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242nd National Meeting and Exposition August 28 - September 1, 2011 Denver, Colorado, USA



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FALL 2011 AGRO MEETING SCHEDULE

Program: page 61; Abstracts: page 80

AGRO SYMPOSIA & MEETINGS THE COLORADO CONVENTION CENTER

AGRO POSTER SESSIONS with the AGRO COFFEE HOURS

Mon: 9:30 AM - 3:30; Tues: 9:30 AM - 4:00 in Hall D

AGRO COFFEE HOURS

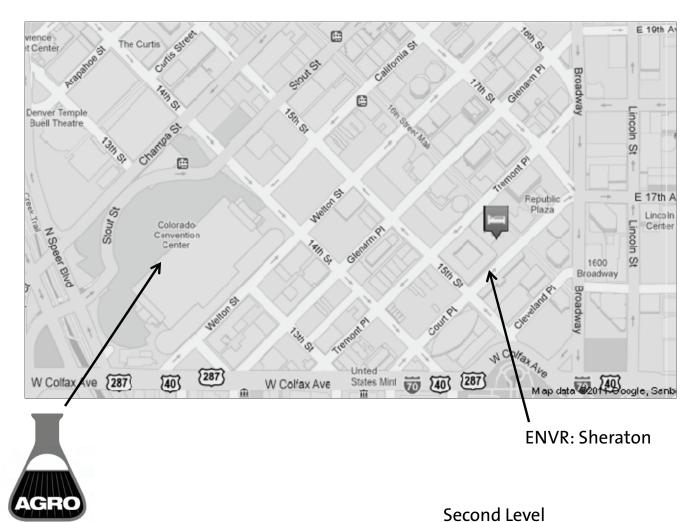
Sunday, Wednesday, Thursday Room 712
Please be quiet during the sessions

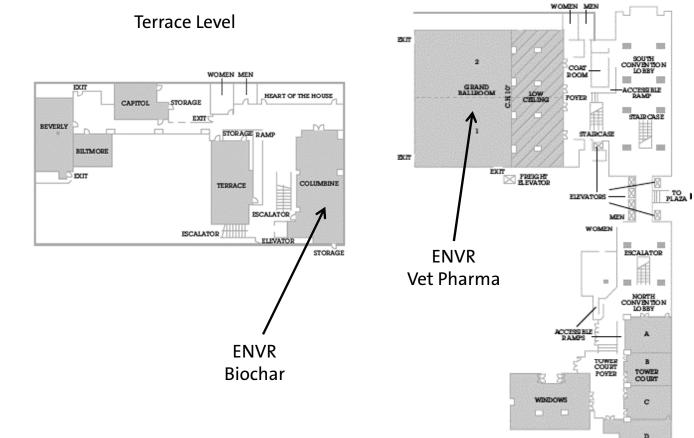
SCI-MIX - Hall D

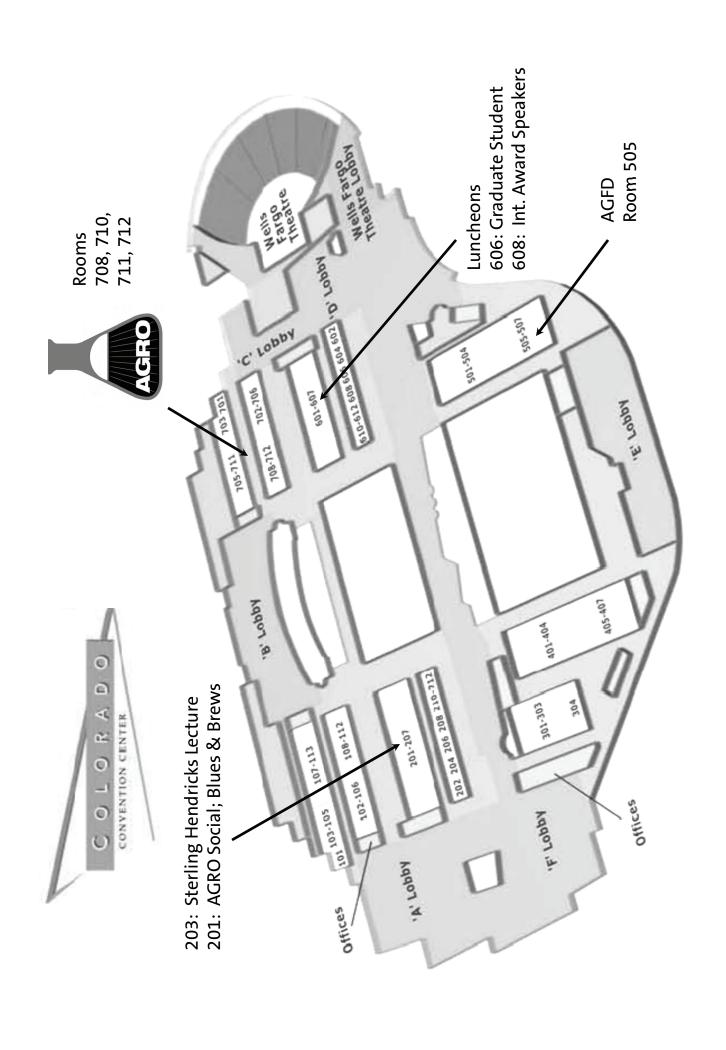
Co-Sponsored ENVR Symposia are at the Sheraton Co-Sponsored AGFD Symposia are at the Colorado Convention Center

SYMPOSIUM OR SESSION/SECTION	Room	Sun	Mon	Tue	Wed	Thu	
Analytical Challenges for Crop Protection Products	712	Р					
Bioavailability and Extractability of Pesticide Residues	710	Р					
Evaluating Agrochemical Aquatic Exposure Modeling in Relation to Risk Evaluator Needs	711	Р	А				
AGRO Education Award Poster Session	Hall D		Α				
Agrochemical Use on Tribal Lands in the United States: Understanding Benefits, Issues, and Cultural Influences	708		А				
Managed Ecosystems, Pesticides, and Biodiversity	712		D				
Symposium in Honor of Dr. George P. Lahm for his Contributions to the Discovery of New Insecticides (International Award Symposium)	710		D	А			
Advances in Characterizing Exposure of Humans and Ecosystems to Pesticides in Surface Waters	711		Р				
New Investigator Symposium	708		Р				
Sci-Mix	Hall D		E				
Sterling B. Hendricks Memorial Lectureship Award				М			
Advances in Protection of Agricultural Productivity, Public Health, and the Environment	711			D			
Endangered Species Act and Pesticide Regulation: Scientific and Process Improvements	710			D	D	D	
Modern Agriculture and Biotechnology: Tools for Sustainability (New Investigator Award - Wednesday AM)	712			D			
Agriculture and Air Quality: Emission Measurements and Models	712				D	D	
Parameters for Pesticide QSAR and PBPK/PD Models	711				D	D	
AGFD							
Future Agricultural Consumer Safety Demands for the Global Market	505				D		
ENVR							
Black Carbon and Biochar for Soil Fertility and Carbon Sequestration	Sheraton: Columbine		D		E		
Veterinary Pharmaceuticals in the Environment	Sheraton: Grand Ballroom 1			D	Α		

Legend: A = AM; MD = mid-day; P = PM; PL = late PM; D = AM/PM; E = evening







From the Communications Chair......

Welcome to Denver!

Many new things are happening in AGRO and much of it in response to the new Strategic Plan.

One task is that all committees have been asked to examine their duties and responsibilities in collaboration with the Committee on Committees. The Communication Committee has been part of this process and it is likely that some of our responsibilities will change so that AGRO is better coordinated.

Communication plays a central role in the success of any organization and AGRO is no exception. The Communication Committee will be part of each of the 3 Goals in the new Strategic Plan. We are looking for new volunteers to help in these efforts.

Are you receiving the monthly AGRO eNewsletter? This tool will allow AGRO to keep members up-to-date on all the latest information on meetings, awards, and new initiatives. Members can even submit job postings by the third Tuesday of every month to updates@agrodiv.org to be included in the next issue.

If you are not receiving the AGRO eNewsletter, visit our website www.agrodiv.org or see inside the back cover for how to sign up! And if you want to place an ad in the eNewsletter, please contact Laura McConnell (laura.mcconnell@ars.usda.gov).

Our new branding efforts are in full swing. The website has been updated and we are working to interface more effectively with other electronic venues. We hope you like our new look and our new products. Let us know what you think!

Finally, have you seen the latest on the ACS website? You can establish or join a network or discussion of like minded chemistry friends. Check it out under Membership and Networks! ACS is looking for feedback on this new tool.

Enjoy the Meeting!

CJ Hapeman, PICOGRAM Editor cathleen.hapeman@ars.usda.gov



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The ACS Symposium Series Online contains the entire collection of high quality, peer-reviewed books developed from the ACS technical divisions' symposia since 1950. Over 1,300 individual book titles comprised of more than 19,000 individual chapters are now integrated into the award-winning ACS Web Editions Platform, enabling you to discover chapters from the eBooks via online searches with book results presented alongside journal articles from ACS. This means that the same features, functionality and related content linking you've come to value in ACS online journal product offerings are now available for the ACS Symposium Series Online.

The ACS Division of Agrochemicals is well represented in the ACS Symposium Series Online, with a total of 83 titles published since 1950. The three latest AGRO division books published over the past 18 months include:



Non-Dietary Human Exposure and Risk Assessment

Editor(s): Michael E. Krolski, Curt Lunchick



Turf Grass: Pesticide Exposure Assessment and Predictive Modeling Tools

Editor(s): Mary T. Nett, James N. Carleton, Joseph H. Massey





Veterinary Pharmaceuticals in the Environment

Editor(s): Keri L. Henderson, Joel R. Coats

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Division of Agricultural and Food Chemistry e-Books to be published as part of the ACS Symposium Series Online in 2011

Understanding Greenhouse Gas Emissions from Agricultural Management – Editors: Lei Guo, Laura McConnell and Amrith Gunasekara

Chiral Pesticides: Stereoselectivity and its Consequences – Editors: A Wayne Garrison, Jay Gan and Weiping Liu

Recent Developments in Invertebrate and Vertebrate Repellents – Editors: Gretchen Paluch and Joel Coats

Invasive Plant Management Issues and Challenges in the United States - Editors: Anne Leslie and Randy Westbrooks

Pesticide Mitigation Strategies for Surface Water Quality - Editors: Kean Goh, Jay Gan, Brian Bret and Thomas Potter



HOSPITALITY COMMITTEE REPORT

Fifteen companies graciously donated a total of \$3000 to support our coffee lounge at our last National ACS meeting in San Francisco. Several firms provided literature to promote their services to meeting attendees. We thank the coffee lounge contributors.

If you wish to join these companies in supporting our coffee lounge, please contact any of our committee members or AGRO officiers. Our coffee lounge offers a brief respite from our technical sessions and provides an alternative forum for exchange of ideas and networking.



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Compliance Services International
EN-CAS Analytical Laboratories
ARCADIS
North Coast Regional Science LLC
Schocken Consulting, LLC
Stone Environmental, Inc



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AGRO Social at San Francisco

The AGRO Division Awards & Social was held at the Moscone Center on Tuesday, March 23, 2010. Shinzo Kagabu was recognized as the recipient of the ACS International Award for Research in Agrochemicals and Chris Somerville as the receipint of the Sterling B. Hendricks Memorial Lectureship Award. Also honored were Daniel Cordova, John Freudenberger, Thomas Selby, and Thomas Stevenson for the

ACS Team Innovation Award; George Lahm for the Kansas City Section Spencer Award; and Kyong Sup Yoon for the AGRO New Investigator Award. We also introduced the winners of the AGRO Education Awards to the revelers in attendance. Our inevitable prize drawing could not be stopped and drew smiles from surprised winners

HOSPITALITY COMMITTEE MEMBERS - James Brady, Julie Eble, Joseph Massey & Patricia Rice SOCIAL CO-CHAIRS - Al Barefoot & Jeff Jenkins

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FROM THE CHAIR'S DESK

KEN RACKE

On behalf of AGRO, I would like to welcome those of you participating in our program activities as part of the Denver ACS meeting and also provide my greetings to colleagues unable to attend. Now that AGRO is programming at one ACS national meeting per year, I trust that members will make every effort to include this centerpiece as one of their annual must-attend events. In addition, or as an alternative if you do have a scheduling conflict, please consider the cooperative program activities we are pursuing to diversify our offerings. AGRO is increasing its participation and sponsorship of national and international conferences and workshops; our goal is to offer one or more program options every year to complement efforts at the national ACS meeting.

Program Chair Al Barefoot and his team of innovative symposium organizers have done a fantastic job of planning our scientific program for the *Denver ACS meeting*. We have a strong and diverse set of symposia sessions planned, including some excellent cooperative efforts with both AGFD and ENVR. It is going to be another meeting where AGRO members have multiple options from which to choose and may not be able to attend every one of the papers of interest.

Other AGRO cooperative program efforts for 2011 have revolved around analytical, residue, and environmental chemistry. AGRO activities at all three events are supported by funds from ACS Innovative Grant Projects.

- On May 8 to 11, the 3rd Latin American Pesticide Residue Workshop (LAPRW) occurred in Montevideo, Uruguay which attracted more than 300 attendees. Steve Lehotay served as our representative and most ably supervised the poster award competition sponsored by AGRO (see page 45).
- Once again, AGRO co-sponsored the 48th Annual Florida Pesticide Residue Workshop (FPRW) held in St. Pete, Florida on July 17 to 20. We appreciate the efforts of Kevin Armbrust and Steve Lehotay in advancing AGRO interests through this event.
- Finally, in cooperation with IUPAC and SETAC, AGRO cosponsored a 2-day symposium on August 1st and 2nd entitled "Advanced Physico-Chemical Techniques to Solve Environmental Science Challenges" as part of the 43rd IUPAC World Chemistry Congress in San Juan, Puerto Rico. This symposium was organized by Laura McConnell and we are most grateful.

New date and location for 5th Pan-Pacific Conference

Please note the new date, September 17 to 21, 2012, and location, Beijing, China, for the 5th Pan-Pacific Conference on Pesticide Chemistry. AGRO is joining forces with the Pesticide Science Society of Japan in supporting merged organization of the conference in conjunction with a previously scheduled event organized by IUPAC, the Beijing Pesticide Society, and China Agricultural University (see announcement on page 47).

Where is AGRO headed in the future?

This will depend in part on *your ideas and contributions*. During the past half dozen years we have attempted to be more intentional and forward-looking as a Division through utilization of a strategic planning process. Following a survey of the membership completed in late 2010, a cross-section of AGRO members met during January to hammer out the latest version of an **AGRO strategic plan for 2011 – 2014**. This exciting new plan was recently approved by the Executive Committee and implementation efforts are now moving forward around three broad initiatives:

- AGRO will enhance the membership experience by providing an interactive and supportive environment for professional growth.
- AGRO will develop the infrastructure for innovative, long range program planning to meet the needs of members and the scientific community.
- AGRO will be a global platform for collaboration and information exchange to advance innovative solutions for a sustainable food supply, the protection of the environment and public health.

A variety of initiatives is contemplated or has already been launched as part of the plan. For example, Laura McConnell, Steve Duke, and Amrith Gunasekara are leading efforts to increase communication with our members (such as the AGRO eNewsletter), revamp our committee structure, and improve AGRO outreach, respectively (Goal 1). Al Barefoot and John Clark are seeking to revitalize the Programming Committee and to include more long-range programming and innovative programming ideas (Goal 2). Jay Gan and I are in the process of forming a new International Activities Committee to guide and to energize our global alliances and co-sponsorships and to increase international participation and membership in the Division (Goal 3).

For a full description of the AGRO strategic plan and the many opportunities for volunteers it provides, you can download a copy from our website (www.agrodiv.org). A summary of the strategic plan can also be found on pages 6-9.

We are in urgent need of fresh volunteers, especially new scientists or longstanding members with a second wind, to lead or to contribute to the strategic plan initiatives.

Feel free to volunteer your services by contacting any of the initiative coordinators directly. Or, you can contact me or the Strategic Planning Committee Chair, Laura McConnell, with your ideas and to find out how you can become engaged. Please get involved and help determine the future for our discipline and for AGRO.



American Chemical Society AGRO Division Report from the Strategic Planning Retreat January 19 – 21, 2011 Ft. Worth, Texas

Overview

The AGRO Division convened a strategic planning workshop January 19 – 21, 2011 to evaluate and revise its current strategic plan. Twelve members were recruited to serve on a Strategic Planning Committee, representing a diversity of affiliations, disciplines, and tenure with AGRO: Ellen Arthur, Aldos Barefoot, Ashli Brown, Keri Carstens, John Clark, Steve Duke, Jay Gan, Amrith Gunasekara, Marja Koivunen, Laura McConnell, Kenneth Racke, Jeanette Van Emon. Also in attendance were Bernard Reynolds, facilitator, and Laura Melohn, ACS staff support.

Benefits of Strategic Planning

Previous efforts at strategic planning has helped the Division look beyond the next one or two national ACS meetings to longer-term needs; has fostered innovative thinking and actions; has served to revitalize the Division and stabilize membership; has provided a structure for the Division to be productive and guide the allocation of resources; has increased the quality and quantity of programming at multiple venues; and has increased the Division's international visibility and reach.

Meeting Objectives

- Develop an updated strategic plan for AGRO that will best serve the current and future membership
- Evaluate impact, successes, and shortcomings of the most recent strategic plan
- 3. Reflect on AGRO needs and member feedback

- 4. Brainstorm on the future possibilities
- Develop critical goals and an action plan to implement supporting activities

The Process

The AGRO planning team participated in an open discussion about various aspects of the Division's operations, programs, services, membership, and finances. The purpose of the review and discussion was to create a shared understanding about the Division's operations and outcomes. To help with these discussions, the facilitator prepared the several reports and summaries which were distributed to the Planning Team prior to the meeting. The information summarized and was used in a variety of exercises throughout the workshop to revise the existing mission statement and vision for the Division.

The Result

Three new goals were crafted and activities related to each goal were developed. The strategic plan will be a living document and will be reviewed annually to see if changes are needed. It is likely new activities will be developed as others are completed. Some activities may be removed. The 2011-2014 AGRO strategic plan was reviewed and accepted by the AGRO executive committee on March 23, 2011. The participants of the workshop will continue to serve on the strategic planning committee for the next three years.

State of the Division Reports

AGRO Member Needs Survey

The needs assessment survey collected the opinions of 371 AGRO members and was used to inform the workshop discussions. The 15 question survey was delivered online and all AGRO members were invited to participate. The invitation to complete the survey was issued on or around November 9, 2010. Reminders were issued on or around November 11 and 17, 2010. The survey closed on November 23, 2010.

AGRO Planning Team Survey

The planning team survey collected the opinions of the AGRO strategic planning team. They were asked to assess the current status of the Division and its strategic plan goals, to identify

three key goals for the future, and to discuss their expectations for the planning workshop.

2008 Strategic Plan Summary

The facilitator prepared a review of the goals and strategies mapped over a three-year period.

AGRO Member Demographics

The report was prepared by ACS and reflects the membership as of December, 2010.

A summary of these reports and some findings by the planning committee are provided below.



American Chemical Society AGRO Division Strategic Plan 2011 – 2014

Mission Statement

AGRO, a Division of the American Chemical Society, brings together a worldwide community of scientists and stakeholders to advance knowledge and promote innovative solutions for the protection of agricultural productivity, public health and the environment.

Rationale: The proposed revision to the AGRO mission statement places more emphasis on who the Division serves (a worldwide community of scientists and regulators, academicians, etc,...), what the Division does (brings these individuals together via our programming and communications), and why we do it (to advance knowledge and promote innovative solutions for the protection of agricultural productivity, public health and the environment).

Vision

AGRO will provide its members an interactive and supportive environment for professional growth, based on innovative programming and services that meet member needs. It will also serve as a community where collaboration and exchange of information will advance innovative solutions for a sustainable supply of food and fiber and protection of the environment and public health.

Rationale: The revised vision statement shifts the focus away from increasing the recognition of the division to a customer focus on serving the membership. Also, the object of our activities was revised from the more vague "challenges facing our world" to a more defined outcome.

Goal 1

AGRO will enhance the membership experience by providing an interactive and supportive environment for professional growth.

Leader: Laura McConnell, laura.mcconnell@ars.usda.gov

Proposed Activities:

- Develop systems to increase member feedback
- Revamp committees to serve division priorities
- Improve networking opportunities and outreach
- Facilitate discussion of news, international developments and scientific breakthroughs among members

Metrics to measure success:

Increased overall membership

Greater proportion of membership in the 5-10 year range Increased member satisfaction from survey responses All new committees populated, goals submitted for EC approval Increased hits to website and on eNewsletter messages and more signups for eNewsletter

Goal 2

AGRO will develop the infrastructure for innovative, long range program planning to meet the needs of members and the scientific community.

Leaders: Aldos Barefoot, aldos.c.barefoot@usa.dupont.com John Clark, jclark@vasci.umass.edu

Proposed Activities:

- Revitalize the programming committee for long range, innovative planning
- Reach out in the US to other ACS divisions, professional societies and non-governmental organizations to develop collaborative programming
- Increase pool of symposium organizers
- Develop innovative, web-based electronic programming

Metrics to measure success:

Program Committee meets on a regular basis and provides an annual report to the membership which includes a 3+year future program plan

Increased number of co-sponsored symposia with other ACS Divisions and outside organizations

More than one-half of symposia include at least one first-time co-organizer

Increased percentage of members actively involved in AGRO programming

Goal 3

AGRO will be a global platform for collaboration and information exchange to advance innovative solutions for a sustainable food supply, the protection of the environment and public health.

Leaders: Ken Racke, kracke@dow.com Jay Gan, jgan@ucr.edu

Proposed Activities:

- Set up an International Activities Committee to direct and energize AGRO initiatives
- Establish strategic alliances and collaborations with key international groups of scientists in agricultural disciplines to increase recognition and participation
- Annually sponsor at least one international programming collaboration
- Increase AGRO membership and participation of international scientists

Metrics to measure success:

Increased international membership

At least one international programming collaboration per year

Survey Results and Planning Committee Findings

Membership

AGRO membership was 1,247 in December 2010. Major member segments (by affiliation) included 34% manufacturer, 18% academic institutions, 14% independent consultant or laboratory, and 10% government agency. The median age of members was 55 with 75% who were 45 and older.

Historically, membership increased during period 1976 to 1993, declined after 1993, and has somewhat stabilized in past several years. A summary of membership from past reports in the PICOGRAM is listed below:

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1976: 1000 members	2000: 1630 members
1993: 2084 members	2002: 1425 members
**high water mark	2005: 1282 members
1998: 1719 members	2010: 1274 members

Information related to membership demographics in terms of years of service was evaluated. The number of members with 6 to 10 "Years of Service in the Division" drops sharply compared to those with 1 to 5 and also compared to those with greater than 10 years of service. This may reflect an issue with retention after five years. Membership stabilized after the implementation of the 2008 plan, so the bulge of those with 1 to 5 years of service in the Division may reflect newer members recruited after implementation of the 2008 strategic plan.

The planning team identified a number of potential membership issues that the new plan may wish to address:

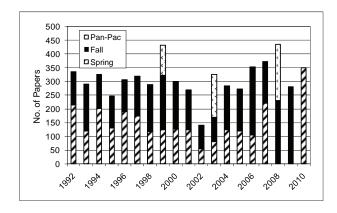
- The need to recruit younger members
- The need to improve retention (beyond 1 − 5 yrs)
- Effective outreach to various AGRO member segments, in particular government (beyond USDA) and industry
- The need to track changes and trends in Agro Science, assessing its impact on members and programs (e.g., pesticides, biotechnology, bioenergy, bioproducts)
- The need to understand and take advantage of ACS meeting venues in attracting member prospects and serving existing members

Scientific Programs

The planning team observed that AGRO technical programs at the ACS national meetings are a strong, core activity. The Division provides innovative topics and excellent symposia. Program metrics are healthy in terms of number of presented papers, symposium attendance, involvement of non-members in symposia on "hot topics", and extent of poster sessions.

The Division is aware that ACS national meeting venue selection may significantly influence attendance at AGRO programming. Members generally do not attend every Division meeting, preferring to attend meetings which include symposia of interest and also those in desirable locations (e.g., San Francisco, Washington DC) and closest to their location. Strength of participation for West Coast and East Coast

meetings may also reflect geographic concentration of Division membership.



In the 2008 strategic planning process, the Division sought to improve the quantity, quality, and diversity of programming as well as attendance by offering technical programming at only one ACS national meeting per year rather than at both meetings as had traditionally been practiced. After a 3-year trial period (2008 – 2010), the Division has now decided to remain with once-a-year programming at the Fall ACS National Meeting, and this was based on an increase in numbers of presented papers at individual meetings during the trial period as well as an overall increase in meeting attendance.

Venue	ACS National Meeting	Total AGRO Symposium Session Attendees	Mean No. Attendees per Symposium Session	Median No. Attendees per Symposium Session
Washington DC	Fall 2005	998	45	43
Atlanta	Spring 2006	490	33	30
San Francisco	Fall 2006	1063	44	39
Chicago	Spring 2007	1056	50	38
Boston	Fall 2007	591	39	38
*** Switch to prog	gramming at or	ne national med	eting ***	
Philadelphia	Fall 2008	1191	42	35
Washington DC	Fall 2009	1786	47	42
San Francisco	Spring 2010	2190	55	39

Results of the membership survey indicate that during the past three years, around one-quarter of the members participated in AGRO programming during any one ACS National meeting (somewhat less at the Pan-Pacific Pesticide Conference). For the 3-year period, slightly over one-half of the membership participated in at least one meeting.

Membership Attending

San Francisco, Spring 2010	27.3%
Washington DC, Fall 2009	27.6%
Philadelphia, Fall 2008	18.5%
Honolulu, Pan-Pacific	
Summer 2008	7.5%
At least one AGRO meeting	
during 2008 – 2010	54.1%
Not attending any AGRO meetings	

45.9%

during 2008 - 2010

Member Satisfaction and Needs

The member survey indicated that members are generally satisfied with the programs of the Division. Approximately two-thirds of the respondents rated the overall service and programs of AGRO as either "Outstanding" or "Good. This is a more positive response than the survey completed prior to development of the 2008 AGRO strategic plan; implementation of the plan has likely had an impact.

The most valuable benefits of AGRO cited by survey respondents were:

- Keeping informed of developments in the field
- Participation in symposia at national meetings
- Professional networking opportunities

A significant proportion of members responding to the survey were "Somewhat interested" or "very interested" in these potential AGRO programs

Members Interested				
Networking	63.5%			
Webinars	58.0%			
Outreach to other				
professional societies	52.4%			

47.7%

Volunteers and Leadership

Job posting

The Division has a number of volunteer committees. The Divisional officer succession process (Vice Chair →Program Chair →Division Chair) appears to be working reasonably well with sufficient number of volunteers and nominations for key Divisional leadership roles. The electronic ballot system instituted by the 2008 Strategic plan is working.

However, the planning team did not think all committees were fully functional. Committee purpose, operations, and deadlines were not always well documented. In addition, not much documentation exists to facilitate orientation and training of new committee chairs or Division officers.

Some 20% of members responding to the survey described themselves as either "highly involved" or "somewhat involved", while two-thirds of members classify themselves as either "not very involved" or "not involved at all." Yet in the same survey a significant number of respondents indicated a strong interest to become involved in Divisional activity opportunities including serving on various committees.

20.8%
16.4%
13.7%
9.1%
5.6%
5.0%
3.8%
1.8%
1.5%

Members with Interests/skills to Volunteer for Division Activities

Working with students	
and new/young scientists	26.9%
Symposium organization	25.7%
Networking with scientists	
in other countries	24.0%
Long-range planning	10.8%

AGRO Publications and Communications

The PICOGRAM has long served as the primary vehicle of AGRO communication with the membership, and it continues to undergo improvements and upgrades. Electronic forms of communication are becoming increasingly important, however. Based on implementation of the 2008 strategic plan, the AGRO website has evolved to become another important means of communication with the membership, and recently an enewsletter has been launched to provide frequent updates and direct members to resources posted to the website (for which a further redesign was launched in early 2011).

Other ACS publications of member interest include *Journal of Agriculture and Food Chemistry* and *Environmental Science and Technology*, although member participation has decreased somewhat in recent years due to an increasingly wide variety of non-ACS journals catering to member interests. The Division has also had strong historical participation in publishing outcomes of scientific symposia via the ACS Symposium Series books. At one time these ACS books were a major source of income for the Division, but difficulties with series management (by Oxford Press) and a decreasing number of AGRO-related volumes had served to decrease income from this source. However, ACS Books has now taken over management of the Symposium Series and provide electronic access to single book chapters or an entire book. Electronic access to these volumes will likely lead to increased royalties for the Division.

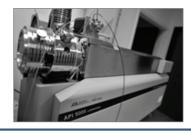
Awards

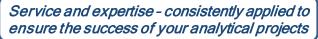
AGRO has traditionally had a very strong International Award program, and for a number of years also sponsored a Young Scientist award targeting pre-doctoral students). Following implementation of the 2008 strategic plan, AGRO developed two new awards programs to replace the Young Scientist Award: the New Investigator Award targeting early career scientists and the Graduate Student Poster Travel Awards Recently, the awards committee has also initiated an Innovation Award (see page 25).



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PAST WINNERS OF THE AGRO DIVISION FELLOW AWARD

1971	Dr. Louis Lykken	1978	Dr. S. Kris Bandal	1993	Dr. Larry Ballantine
	Dr. Tom H. (Bucky) Harris		Dr. Paul Hedin	1994	Dr. James Heitz
	Dr. Herman Beckman	1979	Dr. Rodney D. Moss		Dr. Ralph Mumma
	(Posthumous)	1980	Dr. G. Wayne Ivie		Dr. Willis Wheeler
1972	Mr. Wendell F. (Bud) Phillips		Dr. John B. Siddall	1996	Dr. John Bourke
	Dr. Don G. Crosby		(Posthumous)	1998	Dr. Hank Cutler
	Dr. Elvins Y. Spencer	1981	Dr. Robert M. Hollingsworth		Mr. Paul Giesler
1973	Mr. Roger C. Blinn		Dr. Gino J. Marco	2000	Dr. Barry Cross
	Dr. Philip C. Kearney	1983	Dr. John Harvey, Jr.	2001	Dr. Robert Hoagland
	Dr. Julius J. Menn	1985	Mr. Henry Dishburger	2003	Dr. Judd O. Nelson
1974	Dr. Morton Beroza		Dr. Richard C. Honeycutt	2005	Dr. Rodney Bennett
	Dr. James P. Minyard, Jr.	1986	Dr. Gunter (Jack) Zweig	2006	Dr. Terry D. Spittler
	Dr. Joe C. Street	1987	Dr. Willa Garner	2007	Dr. Ann T. Lemley
1975	Dr. Hank F. Enos	1988	Dr. Jan Chambers		Dr. R. Don Wauchope
	Dr. Maurice B. Green		Dr. James Seiber		Dr. John M. Clark
	Dr. Charles H. Van Middelem	1990	Dr. Joseph Fenyes	2008	Dr. Allan S. Felsot
1976	Dr. Marguerite L. Leng	1991	Dr. Nancy N. Ragsdale		
	Dr. Jack R. Plimmer	1992	Dr. Don Baker		
	Dr. Gerald G. Still		Dr. Joel Coats		
1977	Dr. Gustave K. (Bob) Kohn		Dr. Guy Paulson		

AWARDS COMMITTEE REPORT

The AGRO Division Executive Committee approved addition of a new award: **Award for Innovation in Chemistry of Agriculture**. The new award will be supported by BASF Corporation. This new award is in addition to the long-standing International Award for Research in Agrochemicals, supported by DuPont Crop Protection, which recognizes career-long contributions to the field of Agrochemicals research. Criteria and nomination information for this awards can be found on page 25.

In part prompted by the addition of the new award and in part to add expertise and new viewpoints to the committee, the AGRO Awards Committee has expanded. The expansion was approved by the AGRO Executive Committee. Members of the committee are: Jim Seiber (chair), John Casida, Janice Chambers, John Marshall Clark, Joel Coats, Steve Duke, Bruce Hammock, Ernest Hodgson, Robert Hollingworth, Robert Krieger, Ralph Mumma, Hideo Ohkawa, Sharon Papiernik, Nancy Ragsdale, Will Ridley, David Soderlund, Don Wauchope, Willis Wheeler, and Izuru Yamamoto.

Dr. George P. Lahm of DuPont Crop Protection will receive the International Award for Research in Agrochemicals at the Fall 2011 ACS National Meeting in Denver, Colorado for his contributions in discovery of the anthranilic diamide insecticides. DuPont Crop Protection and BASF Corporation will co-sponsor the award. A committee led by Dr. Thomas M. Stevenson has organized an award symposium to be held on Monday, August 29. Per vote of the AGRO Awards Committee,

Dr. Thomas C. Sparks will receive the International Award at the Philadelphia meeting in 2012 to be sponsored by DuPont Crop Protection. He receives the award for his research and exceptional accomplishments in applying new technology from a number of disciplines to the discovery of new pest control agents. Nominations for the 2013 International Award for Research in Agrochemicals are currently being accepted; the

nomination form and criteria for the 2013 award can be found on page 23 and are due December 31, 2011.

Dr. Laura L. McConnell of USDA-Agricultural Research Service will receive the Division Fellow Award. The Awards Committee is accepting new award nominations for the Division Fellow Award. Criteria for the award and what to submit are shown below; nominations must be submitted by May 31, 2012.

Dr. Deborah P. Delmer, Professor Emeritus at University of California, Davis, will receive the 2011 Sterling Hendricks Lectureship Award, which is sponsored by USDA-Agricultural Research Service, hosted by AGRO, and cosponsored by AGFD. Dr. Delmer will present her lecture on Tuesday, August 30, at 11:30 am, which will be followed by a reception. Nominations for the 2012 award are being solicited by ARS; the nomination form can be found on page 27.

Dr. Cody J. Howard of USDA-Agricultural Research Service will receive the New Investigator Award (NIA). He will present his paper on Wednesday morning, August 31, along with two other nominees. Several additional NIA nominees will present their papers on Monday afternoon, August 29. In addition, twenty students were selected to receive the AGRO Education Travel Grants (see page 33) and will present their posters on Monday, August 29. Application information for these awards can be found on pages 31 and 35. Please attend the NIA symposium and presentations and visit the student posters. We welcome all these new scientists to the AGRO Division.

Finally, consider nominating a deserving colleague for the AGRO Division awards.

Respectfully submitted, James N. Seiber, Chair Awards Committee



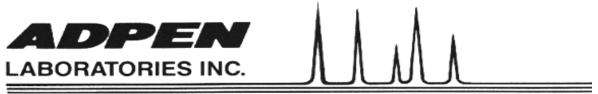
CALL FOR NOMINATIONS AGRO DIVISION FELLOW AWARD

The AGRO Division has established the *Division Fellow Award* to recognize its members whose dedicated and enthusiastic service has kept the Division moving forward.

Criteria shall be -

Continued and substantial contributions of time, talents, and service to the Division of Agrochemicals, ACS, and agrochemical science over a period of at least six years. Nominations include a letter, noting the contributions to the Division, and a current *curriculum vitae*. Deadline for submitting nominations is May 31 of each year. Contact the Awards Committee for further information. Submit nomination electronically to:

Dr. James N. Seiber AGRO Awards Committee Chair 530-754-7005 jnseiber@ucdavis.edu



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ACS International Award for Research in Agrochemicals George Lahm



AGRO Fellow Award

Laura McConnell

AGRO New Investigator Award Cody Howard

AGRO Education Award Winners

Fun, Food, Good Company, Door Prizes, and a Cash Bar 6:00 - 8:00 pm Tuesday, August 30 The Colorado Convention Center - Room 201



ALL AGRO DIVISION MEMBERS, SPEAKERS, AND THEIR GUESTS/SPOUSES/SOS, ARE INVITED TO JOIN US



DuPont Crop Protection is proud to support the ACS International Award for Research in Agrochemicals. We believe that through science-driven innovations we can all improve the productivity and the profitability of the agricultural industry. We are committed to finding sustainable solutions that can create a better, safer and healthier life for people everywhere... and to advancing that future... together.

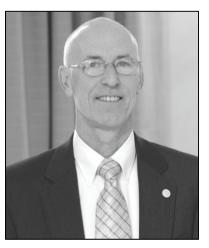




ACS International Award for Research in Agrochemicals

Presented by the AGRO Division of ACS

Co-Sponsored by BASF Corporation & DuPont Crop Protection



DR. GEORGE P.
LAHM is the recipient of the 2011 ACS
International Award for Research in
Agrochemicals. Dr.
Lahm was born in New York City, and grew up on Long Island as the oldest of nine children. He obtained his B.S degree in chemistry from the State
University of New York, Oswego in 1976 and a

Ph.D. in organic chemistry from Indiana University, under Prof. Richard M. Jacobson. He also credits his undergraduate professor Dr. Augustine Silveira Jr. for his commitment and dedication to his students and the outstanding education he bestowed. In 1980, he joined the DuPont Biochemicals Department and initiated his career in the Insecticide Discovery group. In 2010, Dr. Lahm was appointed Dupont Distinguished Scientist, the company's highest technical rank.

Dr. Lahm's pioneering research in the area of sodium channel blocking insecticides set the stage for the discovery of the novel sodium channel blocker, indoxacarb, the first agricultural product to work by this mechanism. In 1999, he discovered the anthranilic diamides, a new insecticide class, and led DuPont research teams in the discovery of Rynaxypyr® and CyazypyrTM. The team drove a remarkable advance from lead discovery to two of the most active insecticides ever developed.

Both Rynaxypyr® and CyazypyrTM represent landmarks for insect control. They set new standards for efficacy, use rate and plant protection. Both products also exhibit low toxicity to the environment, farmers, and consumers due to their unique mode of action, ryanodine receptor activation, with high insect specificity. First introduced in 2008, Rynaxypyr® has achieved remarkable success with 2010 sales of approximately \$400 million and anticipated sales in excess of \$500 million in 2011. CyazypyrTM possesses a complementary spectrum of activity and is anticipated to be a game changing product when introduced next year.

Dr. Lahm was the co-recipient of the 2003 ACS Team Innovation Award for the discovery of indoxacarb and the recipient of the 2009 Spencer Award for outstanding achievement in the field of agricultural and food chemistry. He has been the recipient of several DuPont honors including the 2004 Pedersen Medal for scientific achievement, the 2003 and 2008 Bolton-Carothers corporate team awards for the respective discoveries of indoxacarb and Rynaxypyr®, and a 2004 Crop Protection R&D award for the discovery of CyazypyrTM. In 2010, Dr. Lahm was awarded the Lavoisier medal, DuPont's highest technical award for lifetime contributions.

George and his wife Louise have two children, Sarah and Michael and a very recent grandchild, Grace. He enjoys the outdoors and is an avid runner having competed in numerous marathons including New York and Boston. Dr. Lahm currently holds over 50 US and World patents and has published extensively at scientific meetings and in peer reviewed journals.

Please join us in a two part symposium entitled

Symposium in Honor of Dr. George P. Lahm for his Contributions to the Discovery of New Insecticides

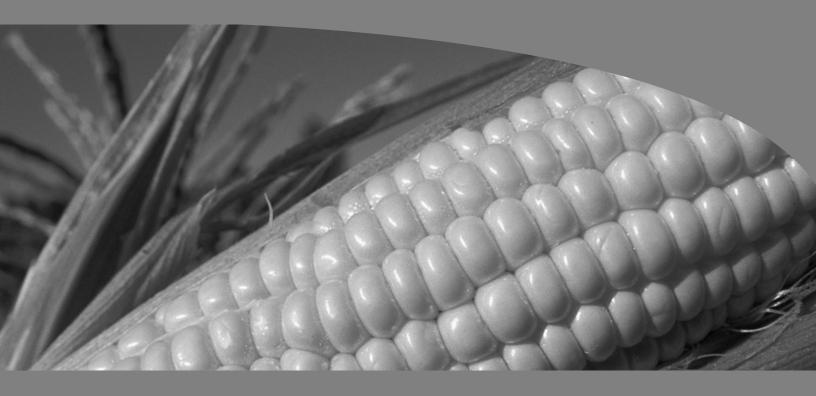
on Monday, August 29, at 8:30 AM in The Colorado Convention Center - Room 710

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DR. DEBORAH P. **DELMER** received her B.A. degree with honors in Bacteriology in 1963 from Indiana University and her Ph.D. in Cell Biology in 1968 from the University of California San Diego. Her first faculty position was at the MSU Plant Research Laboratory, where she held positions of Assistant and then Associate Professor and began her many studies on the biosynthesis of

the plant cell wall. She subsequently held positions as a Principal Scientist at the ARCO Plant Cell Research Institute in Dublin CA, as Professor at The Hebrew University of Jerusalem and, more recently, as Professor and Chair of the Section of Plant Biology at the University of California Davis.

Together with colleagues at Calgene, Inc., Dr. Delmer's group was the first to identify plant homologs of bacterial genes that encode the catalytic subunit of the cellulose synthase, and much of her later research focused on the role of this gene family in cellulose synthesis in plants. In 2004, she received from the American Chemical Society the Anselme Payen Award in recognition of excellence in the science and chemical

technology of cellulose. Dr. Delmer also served as President of the American Society of Plant Biologists in 2000. In 2004, she was elected to membership in the US National Academy of Sciences.

In 2002, at the age of 60, Dr. Delmer surprised all of her colleagues with an interesting change in career goals. She relocated to New York City to serve as Associate Director for Food Security for the Rockefeller Foundation where she was charged with grant making and policy relating to the role biotechnology can play in advancing the improvement of crops for the developing world. In particular, she helped discover talented young scientists in Africa and played a role in partnering these with advanced scientists around the world to help address issues that constrain agricultural production.

Dr. Delmer retired from the Foundation in early 2007 and now serves on a number of advisory boards and works independently as a consultant to foundations, industry, and governments on developing world agriculture and on issues surrounding biomass production. In 2009/10, she also served as Program Director to help roll out a new program called BREAD that supports innovative research that addresses issues of importance to small-holder farmers in the developing world and is jointly funded by the US National Science Foundation and the Bill & Melinda Gates Foundation. In 2010, she became a member of the Board of Governors of The International Center for Research on the Semi-Arid Tropics (ICRISAT), one of the 15 centers of CGIAR devoted to research that promotes agriculture in the developing world.

Dr. Delmer will deliver her lecture immediately following presentation of the Sterling Hendricks Award on

> August 30 at 11:30 am in the The Colorado Convention Center - Room 203

A reception will follow at 12:45 pm

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AGRO DIVISION FELLOW AWARD

For continued and substantial contributions of time, talents, and service to the AGRO Division and agrochemical science



DR. LAURA L. MCCONNELL is a Research Chemist at the US Department of Agriculture, Agricultural Research Service in Beltsville, Maryland. Dr. McConnell specializes in the investigation of processes controlling the movement of pesticides, volatile organic compounds, and other pollutants from agricultural operations into the atmosphere or surface waters with the ultimate goal of designing more

sustainable farming systems that will minimize negative impacts on surrounding ecosystems. She is Lead Scientist on an ARS project entitled, "Discerning the Fate of Atmospheric Agricultural Emissions in the Chesapeake Bay Region", and she has authored more than 75 peer-reviewed publications.

She was honored by ACS early in her career when she received the lota Sigma Pi, Anna Louise Hoffman Award for Outstanding Achievement in Graduate Research (sponsored by the Women Chemists Committee) and the American Chemical Society, Division of Environmental Chemistry, Graduate Student Paper Award. After coming to the Beltsville Agricultural Research Center, she received the ARS Herbert L. Rothbart Outstanding Early Career Scientist of the Year for her work on the Chesapeake Bay, and she later received the Rhône Poulenc Environmental Poster Prize presented at the 9th International Congress on Pesticide Chemistry in London, UK.

Dr. McConnell has provided leadership on a large number of initiatives within the AGRO division. As an active member she

was elected to the Executive Committee in 2000 and became editor of the *PICOGRAM*. In 2005, she assumed a more qctivie leadership role when she was elected Vice Chair and subsequently served as Program Chair in 2006 and Chair in 2007. She has co-organized a number of symposia on topics such as "Agrochemical and Nutrient Impacts on Estuaries"; "Managing gas and particle emissions from Agriculture"; and "Modern Pesticides in Urban Environments Risk Assessment and Management", the first symposium sponsored by an ACS division at a Society of Environmental Toxicology and Chemistry (SETAC) Annual meeting.

In 2008, she led the development of a strategic planning workshop for the division. The resulting strategic plan has governed the activities of the division and has led to an improvement in member services and has expanded the quality and impact of AGRO programming. She has continued as Strategic Planning Chair, organizing a new workshop and the development of a newly updated strategic plan in 2011.

She has obtained funding for three different innovative grant proposals for the division. The first proposal supported intersociety cooperation at the 3rd International Workshop on Crop Protection Chemistry in Latin America in Rio de Janeiro, Brazil. Another led to the redevelopment of the AGRO logo and website and the initiation of an e-newsletter. The third facilitated development of publicity materials and a new website for the 13th IUPAC International Congress of Pesticide Chemistry to be hosted by AGRO at the ACS National Meeting in San Francisco in 2014.

Most recently Dr. McConnell served as a Special Symposium Organizer at the 43rd IUPAC World Chemistry Congress in San Juan, Puerto Rico entitled, "Advanced physico-chemical techniques to solve environmental science challenges." This symposium was selected as one of three to receive \$25K in funding from the ACS as part of International Year of Chemistry celebration with additional funding from two ACS divisions and SETAC.

Congratulations Laura!

Thank you for all you do for the Division and contribute to science!



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AGRO NEW INVESTIGATOR AWARD

Sponsored by Dow Agrosciences

DR. CODY J. HOWARD is the 2011 winner of the New Investigator Award sponsored by the ACS AGRO Division and DOW Agrochemicals. He received his Ph.D. in environmental engineering in 2009 from the University of California at Davis under the direction of Dr. Michael Kleeman. While at UC Davis, he developed a field method for determining ozone formation potential of livestock, silage, and pesticide inert emissions using a transportable smog chamber. The field data was coupled with simulated chemistry mechanisms to predict the effect of agricultural emissions on ozone concentrations in California's San Joaquin Valley.

Dr. Howard's discovered that corn silage is a major contributor to ozone pollution in the region, which has increased research efforts by others in California and within the USDA. His data are being utilized in regional transport models to evaluate the confluence of rural and urban emissions on ozone concentrations and are being used by the California Air Resources Board to develop new regulations concerning pesticide and animal emissions.

Dr. Howard is currently a post doctoral researcher with the Agricultural Research Service division of the United States Department of Agriculture in Beltsville, Maryland working with Drs. Cathleen Hapeman and Laura McConnell. His current work focuses on utilizing computer models and field data to predict the fate and transport of pesticides, particulate matter, ammonia, and VOCs from agricultural operations and to discern their effects on air quality and ecosystem health in the



Chesapeake
Bay region.
He will be
presenting his
recent work
entitled
"Pesticide
Emissions
Model:
Evaluation of
performance
in predicting
pesticide

emissions from the Chesapeake Bay region" during the AGRO symposium, Agriculture and Air Quality: Emissions Measurements and Models. The research concerns validation of the Pesticide Emissions Model (PEM) against a multi-year, high-resolution dataset of pesticide emissions carried out at USDA-ARS, Beltsville by Drs. John Prueger and Timothy Gish. After validation, PEM was used in conjunction with land use data to estimate emissions from pesticide use in the Chesapeake Bay Region.

Dr. Howard recently represented the USDA at a NIST workshop on Aerosol Metrology and Climate and serves as the liaison between ARS and US EPA Atmospheric Modeling and Analysis Division for the PEM. A member of ACS since 2009, he will be co-chairing the aforementioned symposium.

Dr. Howard will present his paper on Wednesday, August 31 at 9 am Colorado Convention Center - Room 712

AGRO New Investigators

The AGRO **New Investigator Symposium** will be held on **Monday afternoon, August 29** in the Colorado Convention Center – Room 708 where five New Investigators will present their research: Drs. Christian Dimpka, Sheng-Peng Sun, Jun Wang, Paul White, and Xin Zhang.

On **Wednesday morning, August 31** in the Colorado Convention Center – Room 712, two New Investigators, Drs. Sasha Hafner and Lifang Luo, will present their research with Dr. Howard in the Agriculture and Air Quality: Emissions Measurements and Models Symposium.

We welcome all these new researchers to AGRO

The AGRO Division is grateful for the sustained support of the New Investigator Award sponsor



PAST AWARDEES OF THE BURDICK AND JACKSON INTERNATIONAL AWARD

1969	Dr. John E. Casida, University of California, Berkley	1981	Dr. Philip C. Kearney, USDA-ARS, Beltsville,
	1970 Dr. Richard D. O'Brien, Cornell University		Maryland
1971	Dr. Robert L. Metcalf, University of Illinois	1982	Dr. Jack R. Plimmer, USDA-ARS, Beltsville,
1972	Dr. Ralph L. Wain, Wye College, University of		Maryland
	London, England	1983	Dr. Karl Heinz Buechel, Bayer AG, Germany
1973	Dr. Hubert Martin, British Crop Protection Council,	1984	Dr. Jacques Jean Martel, Roussel Uclaf, Paris
	England	1985	Dr. Junshi Miyamoto, Sumitomo Chemical Co.,
1974	Dr. T. Roy Fukuto, University of California, Riverside		Japan
1975	Dr. Michael Elliot, Rothamsted Experiment Station,	1986	Dr. James Tumlinson, USDA-ARS, Gainesville,
	England		Florida
1976	Dr. Morton Beroza, USDA-ARS (retired)	1987	Dr. Fumio Matsumura, Michigan State University
1977	Dr. Francis A. Gunther, University of California,	1988	Dr. Ernest Hodgson, North Carolina State University
	Riverside	1989	Dr. Toshio Narahashi, Northwestern University
1978	Dr. Julius J. Menn, Stauffer Chemical	1990	Dr. David Schooley, University of Nevada, Reno
1979	Mr. Milton S. Schecter, USDA (retired)	1991	Dr. Stuart Frear, USDA-ARS, Fargo, North Dakota
1980	Dr. Minuro Nakajima, Kyoto University, Kyoto, Japan		

PAST WINNERS OF THE ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

Co-Sponsored by BASF Corporation & DuPont Crop Protection

1992	Dr. Bruce Hammock, University of California, Davis		
1993	Dr.Morifuso Eto, Kyushu University, Fukoka, Japan	2002	Dr. Keith Solomon, University of Guelph, Ontario,
1994	Dr. Toshio Fujita, Kyoto University, Kyoto, Japan		Canada
1995	Dr. Mohyee Eldefrawi, University of Maryland,		Dr. Marinus Los, American Cyanamid
	Baltimore	2003	Dr. Bob Hollingworth, Michigan State University
	Dr. Koji Nakanishi, Columbia University, New York		Dr. Hideo Ohkawa, Kobe University, Japan
1996	Dr. Günther Voss, Ciba, Basel, Switzerland	2004	Dr. Stephen Duke, USDA-ARS, Oxford, Mississippi
	Dr. Klaus Naumann, Bayer, Leverkusen, Germany		Dr. John Marshall Clark, University of Massachusetts
1997	Dr. Fritz Führ, Jülich, Germany	2005	Dr. Robert Krieger, University of California, Riverside
	Dr. Izuru Yamamoto, University of Tokyo, Japan		Dr. Janice E. Chambers, Mississippi State University
1998	Dr. George Levitt, DuPont, Wilmington, Delaware	2006	Dr. Joel Coats, Iowa State University
	Dr. Leslie Crombie, University of Nottingham,		Dr. Isamu Yamaguchi, Agricultural Chemicals
	England		Inspection Station, Tokyo Japan
1999	Dr. Don Baker, Zeneca, Richmond, CA	2007	Dr. Gerald T. Brooks, West Sussex, UK
	Dr. James Seiber, University of Nevada, Reno		Dr. Fredrick J. Perlak, Monsanto
2000	Dr. George P. Georghiou, University of California,	2008	Dr. David M. Soderlund, Cornell University
	Riverside	2009	Dr. R. Donald Wauchope, USDA-ARS (retired),
	Dr. Herbert B. Scher, Zeneca		Tifton, Georgia
2001	Dr. Donald Crosby, University of California, Davis	2010	Dr. Shinzo Kagabu, Gifu University, Gifu, Japan
	Dr. Ralph Mumma, Pennsylvania State University		



CALL FOR NOMINATIONS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS Sponsored by DuPont Crop Protection

2013 Fall ACS National Meeting in Indianapolis, Indiana

The ACS Award for Innovation in Chemistry of Agriculture is given to an active researcher working in North America for a chemical innovation that significantly enhances agricultural or veterinary pest management and productivity. The awardee will be asked to give an award address at the National ACS meeting.

- The nomination letter will include the following statement: "I hereby nominate [insert first, middle, last name] as a candidate for the ACS International Award for Research in Agrochemicals." It will also include the nominee's birthplace, date of birth, citizenship, business address and a description (200 – 1000 words) of the reasons why the nominee should receive this award, stressing the individual's major accomplishments.
- Include a current curriculum vitae of the candidate that includes: places and nature of employment, professional affiliations, honors and awards received, and a list of publications and patents.
- Nominations often include **one or two letters of support**, although this is optional.

Deadline: Nominations should be received by the committee chair by *December 31* of each year. Balloting will be conducted in January/February and results will be announced in the spring of the following year.

The nominating official(s) should be prepared to assist in organizing a symposium at the National ACS meeting in honor of the awardee.

Please email this information to:

Dr. James N. Seiber AGRO Awards Committee Chair jnseiber@ucdavis.edu 530-754-7005

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2012 Fall ACS National Meeting in Philadelphia, Pennsylvania

The ACS Award for Innovation in Chemistry of Agriculture is given to an active researcher working in North America for a chemical innovation that significantly enhances agricultural or veterinary pest management and productivity. The awardee will be asked to give an award address at the National ACS meeting.

The Nomination email will include the following as attachments:

- 1. A formal letter of nomination that includes
 - Name, business address, phone and email address of the nominator
 - Name, birth date, business address, phone and email address of the nominee
 - A nomination statement (200-1000 words) giving reasons why the nominee should receive this award, stressing the chemical innovation and how it has enhanced agricultural or veterinary pest management and productivity.
- 2. The nominee's current curriculum vitae

- 3. One or two letters of support
- Reference or e-mail link to 1 or 2 published manuscripts that report on the work which supports the award nomination

A single Nomination email, with all attachments listed above should be emailed to:

Dr. James N. Seiber AGRO Awards Committee Chair jnseiber@ucdavis.edu 530-754-7005

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CALL FOR NOMINATIONS 2012 STERLING B. HENDRICKS MEMORIAL LECTURESHIP

Sponsored by USDA-Agricultural Research Service Co-Sponsored by AGRO & AGFD Divisions

The USDA-Agricultural Research Service (ARS) is seeking nominations for the 2012 Sterling B. Hendricks Memorial Lectureship Award. This Lectureship was established in 1981 by ARS to honor the memory of Sterling B. Hendricks and to recognize scientists who have made outstanding contributions to the chemical science of agriculture. Dr. Hendricks contributed to many diverse scientific disciplines, including soil science, mineralogy, agronomy, plant physiology, geology, and chemistry. He is most frequently remembered for discovering phytochrome, the light-activated molecule that regulates many plant processes. The lecture should address a scientific topic, trend, or policy issue related to agriculture. Deadline is **November 3, 2011.**

The AGRO Division and the Agricultural & Food Chemistry Division (AGFD) co-sponsor the Lecture which will be held in a joint session of these divisions. The lectureship is presented at an AGFD symposium in even-numbered years and in an AGRO symposium in odd-numbered years. The award includes an honorarium of \$2000, a bronze medallion, and expenses to attend the meeting.

Nominees will be outstanding senior scientists in industry, universities, consulting, or government positions. *Current ARS employees are not eligible*. The Award will be presented during an American Chemical Society National Meeting held in 2012 in Denver prior to the Lecture. Giving the presentation is a requirement of the honor.

The **Nomination Package** includes:

- A letter explaining the nominee's contributions to chemistry and agriculture,
- A current *curriculum vitae* (hard copy only)

Nomination letters may be sent electronically to: Kim Kaplan, Lecture Coordinator kim.kaplan@ars.usda.gov

Hard copy nominations and *curriculum vitae* are to be submitted via courier to:

Kim Kaplan, Lecture Coordinator ARS Information Office Room 1-2253, Mail Stop #5128 5601 Sunnyside Ave Beltsville, MD 20705 301-504-1637 – phone

PAST STERLING B. HENDRICKS MEMORIAL LECTURESHIP AWARD WINNERS

Norman E. Borlaug, Nobel Laureate, International	1995	Winslow R. Briggs, Carnegie Institution of
Maize and Wheat Improvement Center, Mexico City		Washington
Warren L. Butler, University of California, San Diego	1996	Hugh D. Sisler, University of Maryland
Melvin Calvin, Nobel Laureate, University of	1997	Ernest Hodgson, North Carolina State University
California, Berkeley	1998	Morton Beroza, USDA-ARS, Maryland (retired)
Frederick Ausubel, Harvard Medical School and	1999	Bruce D. Hammock, University of California, Davis
Massachusetts General Hospital, Boston, MA	2000	William S. Bowers, University of Arizona
Alan Putnam, Michigan State University	2001	Malcolm Thompson, USDA-ARS, Maryland (retired)
Ralph Hardy, Cornell University and BioTechnica	2002	Ervin E. Leiner, University of Minnesota
International	2003	Kriton Kleanthis Hatzios, Virginia Polytechnic
Mary-Dell Chilton, Ciba-Geigy Corporation,		Institute and State University
Research Triangle Park, NC	2004	Robert L. Buchanan, Food & Drug Administration
Bruce N. Ames, University of California at Berkeley	2005	Donald L. Sparks, University of Delaware
Sanford A. Miller, University of Texas Health Science	2006	Stanley B. Prusiner, Nobel Laureate, University of
Center at San Antonio		California, San Francisco
Roy L. Whistle, Purdue University	2007	Bruce E. Dale, Michigan State University
Peter S. Eagleson, Massachusetts Institute of	2008	Fergus M. Clydesdale, University of Massachusetts,
Technology		Amherst
John E. Casida, University of California, Berkeley	2009	Charles J. Arntzen, Arizona State University, Tempe
Philip H. Abelson, Deputy Editor, Science, and	2010	Chris Somerville, Director of the Energy Biosciences
Scientific Advisor to AAAS		Institute, Berkeley
Wendell L. Roelofs, Cornell University	2011	Deborah P. Delmer, University of California, Davis
	Maize and Wheat Improvement Center, Mexico City Warren L. Butler, University of California, San Diego Melvin Calvin, Nobel Laureate, University of California, Berkeley Frederick Ausubel, Harvard Medical School and Massachusetts General Hospital, Boston, MA Alan Putnam, Michigan State University Ralph Hardy, Cornell University and BioTechnica International Mary-Dell Chilton, Ciba-Geigy Corporation, Research Triangle Park, NC Bruce N. Ames, University of California at Berkeley Sanford A. Miller, University of Texas Health Science Center at San Antonio Roy L. Whistle, Purdue University Peter S. Eagleson, Massachusetts Institute of Technology John E. Casida, University of California, Berkeley Philip H. Abelson, Deputy Editor, Science, and Scientific Advisor to AAAS	Maize and Wheat Improvement Center, Mexico City Warren L. Butler, University of California, San Diego Melvin Calvin, Nobel Laureate, University of California, Berkeley 1998 Frederick Ausubel, Harvard Medical School and 1999 Massachusetts General Hospital, Boston, MA 2000 Alan Putnam, Michigan State University 2001 Ralph Hardy, Cornell University and BioTechnica 2002 International 2003 Mary-Dell Chilton, Ciba-Geigy Corporation, Research Triangle Park, NC 2004 Bruce N. Ames, University of California at Berkeley Sanford A. Miller, University of Texas Health Science Center at San Antonio Roy L. Whistle, Purdue University Peter S. Eagleson, Massachusetts Institute of Technology John E. Casida, University of California, Berkeley Philip H. Abelson, Deputy Editor, Science, and Scientific Advisor to AAAS



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- Regulatory Approaches
- · Bioaccumulation

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- Risk Mitigation
- Vulnerability Analysis
- Spatial and Temporal Exposure Characterization
- · Risk Mapping

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- Bioaccumulation Studies
- Runoff, Surface Water, and Groundwater Monitoring
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Advisory Committee on Crop Protection Chemistry

Call for Nominations

IUPAC 2012 International Award for Advances in Harmonized Approaches to Crop Protection Chemistry

This award recognizes individuals in government, intergovernmental organizations, industry, and academia who have exercised personal leadership for **outstanding contributions to international harmonization for the regulation of crop protection chemistry**.

The award is administered by the IUPAC Advisory Committee on Crop Protection Chemistry, and is

presented on a biennial basis during even-numbered years in conjunction with an IUPAC-sponsored conference or special symposium.

Awardees receive a \$3,000 honorarium plus travel and per diem reimbursement to attend the award presentation ceremony. Corporate sponsorship for the award has been arranged with Dow AgroSciences.

Nominations will consist of:

- A nomination letter including the nominee's birthplace, date of birth, citizenship, business address, and a description (200-1000 words) of the reasons why the nominee should receive this award, stressing the individual's major accomplishments toward international harmonization for the regulation of crop protection chemistry.
- A curriculum vitae of the candidate that includes places and names of employment, professional affiliations, committee and working group assignments, and listing of relevant regulatory guidance documents, reports, and/or publications.
- One or more letters of support.

Nominations for the 2012 award are due **December 1, 2011**, and should be sent to:

Dr. John Unsworth, Chairman
IUPAC Advisory Committee on Crop Protection
Chemistry
25 Vellacotts
Chelmsford, Essex CM1 7EA
UNITED KINGDOM
Phone: +44 1245 440 056
unsworjo@aol.com

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2012 Fall ACS National Meeting in Philadelphia

The AGRO Division seeks nominations for the New Investigator Award to be awarded at the ACS meeting in Philadelphia in August 2012. The purpose of the New Investigator Award is to recognize scientists who have obtained a doctoral degree and are actively conducting academic, industrial, consulting, or regulatory studies.

The Division is interested in work on all aspects of agrochemicals which are broadly defined to mean pesticides of all kinds (e.g., chemical pesticides, biopesticides, pheromones, chemical attractants, fumigants, plant incorporated protectants, disinfectants) as well as biotechnology-derived crops (e.g., Bt crops, Roundup Ready crops, etc.). The categorical areas of study related to agrochemicals are very broad and encompass environmental chemistry, toxicology, exposure assessment, risk characterization, risk management, and science policy.

Studies of veterinary pharmaceuticals and antibiotics are included in the Division's mission. The Division especially encourages submissions related to public health protection as well as crop, livestock, aquaculture, and wildlife protection.

AGRO is also interested in the environmental chemistry and effects resulting from agricultural production (e.g., soil processes, water and air quality) and in chemical products made from agricultural commodities and byproducts. This includes biofuels and bioproducts and the issues surrounding their production and use.

- To be eligible for the award, the scientist must have obtained his or her doctorate no more than five years before the time of the Fall ACS National Meeting.
 Thus, for 2012, applications will be considered from scientists who have obtained their doctorates no earlier than the year 2007.
- The award winner will be expected to deliver an oral presentation in their area of interest in one of the AGRO Program sessions.
- The award winner will receive a \$1000 honorarium, a commemorative plaque, one-year complementary membership in the AGRO Division, a meeting registration fee waiver, and reimbursement for travel expenses in association with the Denver meeting.

Applications for the New Investigator Award will consist of the following elements:

- 1. A three to five-page paper by the applicant describing their current research and/or other work relevant to the broad mission of the AGRO Division. The paper may be structured as a research paper (i.e., contains the main elements of a typical journal article) or as a critical review of one's particular contributions to the scientific fields covered by the AGRO Division. The impact, or potential impact, of this work should be included in the discussion.
- Submission of a 150-word abstract for the submitted paper to the ACS PACS abstract submission website. http://abstracts.acs.org/

- 3. A current curriculum vitae
- 4. At least **one letter of recommendation** from a current supervisory scientist (e.g., a business manager, a departmental chair, post-doctoral mentor).

For consideration of an award at the Fall ACS National Meeting in Philadelphia, a full application must be **submitted via email no later than March 19, 2012 to**

Cathleen Hapeman, Organizer phone: 301-504-6451 cathleen.hapeman@ars.usda.gov

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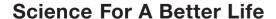


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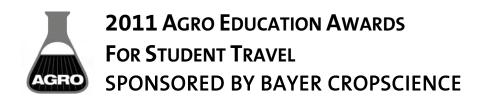
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Congratulations to all our travel grant winners

First and second place winners will be announced at the AGRO Awards & Social on Tuesday evening.

Anna-Marie Alves. Deltamethrin increases peak current and slows deactivation kinetics of the voltage-gated calcium channel ($Ca_v2.2$) from rat brain following PKC dependent phosphorylation. *John Clark U Massachusetts, Amherst* **AGRO 69**.

Edinalvo Camargo. Degradation of saflufenacil as affected by moisture content and soil characteristics. *Scott Senseman, Texas A&M* **AGRO 53**.

Zhenshan Chen. DDA, a new water-soluble degradation product and biomarker of DDT in the Los Angeles Bight. *Robert Krieger*, *U California, Riverside* **AGRO 54**.

Jonathan Childress. Evaluating the mode of action of terpenoids as insecticides: Evidence for membrane interaction. *Joel Coats, Iowa State U* **AGRO 70**.

Yuping Ding. Assessing bioavailability and toxicity of permethrin and p,p'-DDT in sediment using matrix solid phase microextraction. *Michael Lydy, Southern Illinois U* **AGRO 58**.

Lorena Fernandez, Biological stability and delivery studies to elucidate the role of thickener solid particles on water-in-oil emulsion containing microalgae. *Jean VanderGheynst, U California, Davis* **AGRO 76.**

Amanda Harwood. Predicting the toxicity of permethrin to *Daphnia magna* in water using SPME fibers. *Michael Lydy, Southern Illinois U* **AGRO 61**.

Qiang Huang. Raman microscopic analysis of PM₁₀ for assessing source distributions from agricultural operations. *Alba Torrents, U Maryland* **AGRO 77**.

Yu Huang. Optical fiber ammonia gas sensor using a dual layer poly(methyl methacrylate)/ chlorophenol red coating. *Shiquan Tao, Texas A&M* **AGRO 78.**

Lacey Jenson. Mosquito cell lines as an economical platform for discovery of new insecticides to control malaria. *Jeffrey Bloomquist, U Florida* **AGRO 75**.

Weiying Jiang. Insecticide runoff from urban hard surfaces during simulated and natural rainfalls. *Jay Gan, U California, Riverside* **AGRO 52**.

Yu Liu. Cotton socks monitor the indoor distribution, fate, and persistence of fipronil following Frontline[@] application to companion animals. **AGRO 62**.

Terry Lopez. Surrogate system using rubber latex gloves to assess contact transfer and accumulation of surface pesticide residues. *Robert Krieger, University of California, Riverside* **AGRO 63.**

Zhijiang Lu. Oxidation of bisphenol F (BPF) by manganese dioxide. *Jay Gan, U California, Riverside* **AGRO 57.**

James Mutunga. Differential potency and substrate kinetics of acetylcholinesterase peripheral site ligands: The molecular basis of selectivity for *Anopheles gambiae* mosquitoes. *Jeffrey Bloomquist, U Florida* AGRO 68.

Domenic Previte. Extensive permethrin resistance in North American head louse populations detected by quantitative sequencing and serial invasive signal amplification reactions. *John Clark U Massachusetts, Amherst* **AGRO 66**.

Miriam Revellame. Lignocellulosic biomass as a carbon source for biofuels production from oleaginous yeast. *Darrell Sparks, Mississippi State* **AGRO 73**.

Daniel Swale. Enzyme kinetic analysis of allosteric solvent effects when screening mosquito-selective carbamates against *Anopheles gambiae*. *Jeffrey Bloomquist*, *U Florida* **AGRO 65**.

Candace Williams. Isolation of cellulolytic organisms in the gastrointestinal tract of the giant panda and their potential use in the generation of lignocellulosic-based biofuels. *Ashley Brown, Mississippi State* **AGRO 74.**

Xiao Xiao. Decomposition of pharmaceuticals by manganese oxide molecular octahedral sieves. *Ann Lemley, Cornell* **AGRO 55**.

All Graduate Students and Post-Docs

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Support for Poster Presentations
At the 2012 Fall ACS National Meeting in Philadelphia

The AGRO Division has established an endowment fund in collaboration with Bayer CropScience that will be used to promote an understanding of the role of chemistry in agriculture. To address this goal, awards will be made through the Division's Education Committee.

Proposals are sought for the 2012 awards. Undergraduate and graduate students will be awarded up to \$600 each to help defray costs of attendance to give poster presentations at the ACS 244th Fall Meeting, which will be held August 19-23, 2012 in Philadelphia, Pennsylvania. Posters will be displayed in a special poster session of the AGRO Division. First, Second and Third place winners will receive an additional cash award.

The subject of the presentation should pertain to the chemistry of the AGRO Division. Topics should relate to pest management chemistry including synthesis, metabolism, regulatory, biotechnology, delivery, risk assessment, resistance, residues, mode of action, fate/behavior/transport, and agronomic practices. The AGRO Division is also interested in chemical products made from agricultural commodities and byproducts, including biofuels and the issues surrounding their production.

To apply, a graduate student should submit the following to be received no later than March 19, 2012:

- 1. An abstract formatted according to the directions given on the ACS website. Be sure to include name (of applicant), address, and e-mail address.
- A two page extended abstract giving more detail of the research/presentation.
- 3. A short letter of nomination from the faculty advisor.

Submit item 1 to the ACS OASYS abstract submission website.

http://abstracts.acs.org/

Submit item 2 and 3 as a Word or pdf file to Dr. Marja Koivunen at mkoivunen@marronebio.com

For more information, please contact the co-organizers:

Dr. Marja Koivunen Marrone Bio Innovations 2121 Second Street, Suite B-107 Davis, CA 95618 phone: 530-750-2800 mkoivunen@marronebio.com Dr. Diana Aga Chemistry Department, NSC 611 University of Buffalo Buffalo, NY 14260 phone: 716-645-4220 dianaaga@buffalo.edu

Abstracts will be reviewed by the Education Committee.

Submitters will be notified of their selection status in May 2012

Special thanks to our sponsor for their generous contribution!

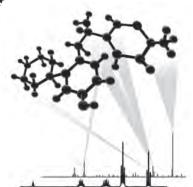


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Notes from the Program Chair

Aldos C. Barefoot

AGRO's goal is to bring together scientists that are seeking solutions to the challenges that our world faces to improve agricultural productivity, public health and environmental protection. As AGRO has developed, updated, and put its strategic plan into action, we have been guided by the recognition that increasing population, changing demands for protein production, conversion of arable land to non-agricultural uses, and the development of sustainability concepts and goals are affecting agriculture and our ability to provide resources necessary for functioning human societies. The changes in the world around us and in expectations for agriculture affect AGRO, and we have responded by renewing our commitment to the world-wide community of scientists involved in research.

The core service that AGRO offers its members and the scientific community is technical programming at the National ACS meetings. Our commitment to high-quality, topical programming will be demonstrated again at the 242nd ACS meeting in Denver. The session *organizers have done an exceptional job* in designing diverse and technically sophisticated symposia on topics of current concern to scientists involved in agriculture, public health, veterinary science, pest management and environmental science of chemicals used to improve agricultural productivity and public health.

The response to our call for Graduate Student Educational Awards and New Investigator Award nominations broke all records. We received 26 requests for Graduate Student Travel Grants and 10 New Investigator Award applications. The Student Poster Session and New Investigator symposium will be Monday. Several additional New Investigators and Cody Howard, the New Investigator Awardee, will present their papers on Wednesday morning. I encourage all of you to attend the sessions and enjoy the opportunity to meet the new scientists who will be the future of research in agriculture and public health.

The International Award for Research in Agrochemicals Symposium will honor George Lahm of DuPont Crop Protection for his contributions to insecticide discovery. Dr. Lahm has been instrumental in the discovery of several insecticides with extraordinary activity on insects and remarkably low toxicity to mammals, fish, birds, and other non-target organisms. Dr. Lahm has received numerous awards, including the Kenneth Spencer Award, and continues to garner recognition for his discoveries.

This year AGRO is the primary sponsor of the *Sterling Hendricks Memorial Lecture Award* which we co-sponsor with AGFD. The award was established by USDA-ARS to recognize scientists who have made outstanding contributions to the chemical science of agriculture. The lecture *Applying Advances in Chemistry to Benefit Developing World Agriculture* will be given by *Deborah Delmer* from UC Davis. The lecture promises to be of interest to many ACS members, and we look forward to a large turnout in the Colorado Convention Center (Rm. 203) on Tuesday at 11:30. A reception sponsored by USDA-ARS, AGRO, and AGFD will follow the lecture. Please join us and help us welcome and congratulate this year's Sterling Hendricks Award recipient.

Symposia at the Denver meeting include several on issues in the news that will drive the work of all *scientists involved in evaluation and regulation of chemicals used or produced by agriculture*: the Endangered Species Act (ESA) and its effect on pesticide regulation, biotechnology and agriculture as tools to create sustainable societies, managing ecosystems to attain biodiversity goals, and assessing air quality in agricultural ecosystems. We are welcome representatives from the Native American Nations who will give presentations on issues concerning *agrochemical use on Tribal Lands*. Developments in toxicology and metabolism, insecticide discovery, analytical methods, environmental fate, water monitoring, and modeling demonstrate a *continuing need for advances in science that affect pesticide discovery, development, and use.*

Adding to the breadth of our program are two symposia resulting from collaboration with ENVR. The interest of both divisions in the fate and effects of *veterinary pharmaceuticals* and in the characterization of *biochars* and effects on nutrients, metals and organics sorption gave us the opportunity to combine the efforts of AGRO and ENVR to create a program with five sessions and two poster sessions. We are also co-sponsoring a symposium with AGFD on *consumer safety in the global market*.

With three concurrent sessions throughout the week (four on Monday) and the co-sponsored symposia with ENVR and AGFD, our program offers many opportunities to sample a wide range of topics or to catch up on developments in specific areas of research, new product commercialization, and regulation.

In addition to our Denver meeting, *AGRO is actively involved* with other groups and societies. AGRO co-sponsored the 2011 Florida Pesticide Residue Workshop and a symposium at the IUPAC World Chemistry Conference in Puerto Rico. Of particular note, the Pesticide Science Society of Japan, with AGRO cosponsorship, has moved the 5th Pan-Pacific Conference on Pesticide Chemistry to Beijing, China to be held on September 17 to 21, 2012 in conjunction with an event organized by IUPAC, China Agricultural University, and the Beijing Pesticide Society. Finally, we are continuing to prepare for our most ambitious effort in two decades, the 13th IUPAC International Congress on Pesticide Chemistry to be held concurrently with the 2014 ACS National Meeting ACS in San Francisco.

Programming activities are already underway for the 244th ACS meeting in Philadelphia in August 2012. John Clark has collected a number of proposals for symposia, and we hope to get a good start on the programs for Philadelphia and Indianapolis (2013) before this fall. We will increase our emphasis on programming for future meetings and work on plans for future program directions at the *Programming Meeting on Sunday morning*. We are also continuing the very successful *Blues and Brews on Wednesday afternoon* where we will welcome ideas and symposium topics from all participants.

It's an exciting time to be involved in agriculture.

Come grow with AGRO.

See you in Denver! – Al



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Comments from the Vice Chair

John M. Clark

Long-Term Planning of the Technical Program for the AGRO Division of ACS

AGRO is beginning to implement its new 3-year strategic plan and has identified long-term programming as a critical need. The Division currently programs technical symposia in approximately 15 standing topics. Recently, an ad hoc steering committee for the standing Programming Committee was formed to direct the revitalization of long-term (2-3) years in advance) programming of technical symposia.

Given the scope of our current symposia, the steering committee felt that no single individual could be an expert on all topics. From this, the committee decided to reach out to our membership and identify individual experts in each topic area to act as 'Champions' of that topic.

We envision that champions will serve as liaisons to the current Vice Chair and Program Chair, providing ideas for

new and timely symposia within their topic area and to assist in identifying possible organizers. The champions will thereby provide the Vice Chair and Program Chair with a long-term institutional memory of the Division's programming efforts as officers rotate into and out of office.

Once champions are in place, the Vice Chair will be responsible in contacting them as necessary and organizing a conference call or two each year.

The identification of champions and how they will function is very much a work in progress. The first step towards getting our programming plans out 2 to 3 years in the future is to identify champions for each area. This is reflected in the Call for Symposia for the 2012 Fall ACS National ACS Meeting on the next pages. I welcome your comments and ideas.

Please come to our Programming Meeting, 9 am Sunday, August 28 in the Colorado Convention Center, Rm. 201

You Are Also Cordially Invited To:

AGRO Brainstorming, Blues & Brews

Нарру Ноиг

August 31, Wednesday 5:00 – 7:00 PM The Colorado Convention Center – Room 201

- Share your ideas about the future AGRO programming

Free refreshments will be served

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244th ACS National Meeting & Exposition ACS Theme: Materials for Health and Medicine

AGRO anticipates an exciting and diverse technical program in Philadelphia, Pennsylvania.

Suggestions and proposals for additional symposia and organizers are most welcome.

Please contact AGRO Program Chair for 2012: John Clark, University of Massachusetts 413-545-1052, jclark@vasci.umass.edu

Symposium proposal template can be found at: www.agrodiv.org

Proposal deadline is November 15, 2011

Award Symposia

AGRO International Award for Research in Agrochemicals Thomas C. Sparks Awardee Sponsored by DuPont

Sterling B. Hendricks Memorial Award Awardee TBA Spring 2012 Sponsored by USDA-ARS Organized in 2012 by AGFD

Innovation in Chemistry of Agriculture Awardee TBA Spring 2012 Sponsored by BASF Scott Jackson, BASF 919-547-2349, scott.jackson@basf.com AGRO New Investigator Award Awardee TBA Spring 2012

Sponsored by Dow AgroSciences
Cathleen Hapeman, USDA-ARS
301-504-6451, cathleen.hapeman@ars.usda.gov

AGRO Education Awards for Undergraduate and Graduate Student Travel Research Poster Presentations Awardees TBA Spring 2012 Sponsored by Bayer CropScience

Sponsored by Bayer CropScience
Diana Aga, University of Buffalo
716-645-4220, dianaaga@buffalo.edu
Marja Koivunen, Marrone Bio Innovations
530-750-2880, mkoivunen@marroneorganics.co

Technical Symposia

Protection of Agricultural Productivity, Public Health and the Environment – General Session

John Clark, Program Chair, jclark@vasci.umass.edu

Advances in Agrochemical Residue, Analytical and Metabolism Chemistry & Metabolomics

Kevin Armbrust, armbrust@msci.msstate.edu Steve Lehotay, steven.lehotay@ars.usda.gov Michael Krolski, mike.krolski@bayercropscience.com Rod Bennet, rodney@bennett@jframerica.com Chad Wujcik, chad.e.wujcik@monsanto.com Teresa Wehner, teresa.wehner@merial.com

Air Quality and Agriculture

Laura McConnell, laura.mcconnell@ars.usda.edu
Jim Seiber, jnseiber@ucdavis.edu
Amrith Gunasekaram, amrith.gunasekara@cdph.ca.gov
Scott Yates, scott.yates@ars.usda.gov

Agrochemical Toxicology and Mode of Action

John Clark, jclark@vasci.umass.edu Tom Sparks, tcsparcks@dow.com Dave Soderlund, dms6@cornell.edu

Bioenergy, Bioproducts, and Biochars: Advances in Production and Use

Cathleen Hapeman, cathleen.hapeman@ars.usda.gov Chris Peterson, cjpeterson@fs.fed.us

Biorationale Pesticides, Natural Products, Pheromones, and Chemical Signaling in Agriculture

Steve Duke, stephen.duke@ars.usda.gov Joel Coats, jcoats@iastate.edu Marja Koivunen, mkoivunen@marroneorganics.com

Development of Value-added Products from Agricultural Crops and Byproducts

Jim Seiber, jnseiber@ucdavis.edu

Developments in Integrated Pest Management and Resistance Management

Jeff Bloomqiust, jbquist@epi.ufl.edu Tory Anderson, anderst@vt.edu Si Hyeock Lee, shlee22@snu.ac.kr

Environmental Fate, Transport, and Modeling of Agriculturally-related Chemicals

Tom Potter, tom.potter@ars.usda.gov Pam Rice, pamela.rice@ars.usda.gov Jay Gan, jgan@ucr.edu

Human and Animal Health Protection: Vector Control, Veterinary Pharmaceutical, Antimicrobial and Worker Protection Products

George Cobb, george.cobb@tiehh.ttu.edu
Laura McConnell, laura.mcconnell@ars.usda.gov
Jay Gan, jgan@ucr.edu
Teresa Wehner, teresa.wehner@merial.com

Human Exposure and Risk Assessment

Bob Krieger, bob.krieger@ucr.edu Kurt Lunchick, kurt.lunchick@bayer.com Dan Stout, stout.dan@epa.gov

Regulatory Harmonization and MRLs

Ken Racke, kracke@dow.com
Philip Brindle, philip.brindle@basf.com
Heidi Irrig, heidi.irrig@syngenta.com

Synthesis of Bioactive Compounds

Thomas Stevenson, thomas.m.stevenson@usa.dupont.com Wenming Zhang, wenming.zhang@usa.dupont.com

Technological Advances and Applications in Agricultural Science (e.g., Nanotechnology, Genetically-modified Organisms and Biocontrol Agents)

John Clark, jclark@vasci.umass.edu
Daniel Goldstein, daniel.a.goldstein@monsanto.com

Urban Agriculture- Turf, Ornamentals, Household Products, and Water-Re-Use

John Clark, jclark@vasci.umass.edu Chris Peterson, cjpeterson@fs.fed.us

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Programming & Outreach Activities 2012 – 2014

Activity/Event	Leaders Champions	Status	Actions Required		
49 th Florida Pesticide Residue Workshop July 2012 St Pete Beach, Florida	Kevin Armbrust Steve Lehotay	Program under development			
5 th Pan-Pacific Conference on Pesticide Science Beijing, China September 17-21, 2012	H. Matsumoto Steve Duke Jim Seiber John Clark	 Meeting location & date changed Meeting under development with Pesticide Science Society of Japan as lead 	Check Pesticide Science Society of Japan website for updates http://wwwsoc.nii.ac.jp/pssj2/en g/index.html		
244 th ACS National Meeting August 19-23, 2012 Philadelphia, Pennsylvania	John Clark	Symposia planning at Blues and Brews on Wednesday August 31, 2011 in Denver	Submit symposia proposals (in Call for Papers format) to John Clark by November 15, 2011 for inclusion in Spring 2012 PICOGRAM		
Activities 2013 – 2014					
246 th ACS National Meeting Indianapolis, Indiana September 8-12, 2013	2012 Vice Chair	Symposia planning at Blues and Brews on Wednesday, August 22, 2012	Submit symposia proposals (in Call for Papers format) to 2012 Vice Chair by November 15, 2012 for inclusion in Spring 2013 PICOGRAM		
248 th ACS National Meeting & 13 th IUPAC Pesticide Congress San Francisco, CA August 24-28, 2014	2013 Vice Chair Laura McConnell Ken Racke	Follow progress on website www.iupac2014.org	Sign up for email updates at website www.iupac2014.org		

Future ACS National Meetings

243rd ACS National Meeting & Exposition March 25-29, 2012, San Diego, California Program Theme: Chemistry of Life

244th ACS National Meeting & Exposition August 19-23, 2012, Philadelphia, Pennsylvania

Program Theme: Materials for Health & Medicine

245th ACS National Meeting & Exposition April 7-11, 2013, New Orleans, Louisiana Program Theme: Chemistry of Energy & Food

246th ACS National Meeting & Exposition September 8-12, 2013, Indianapolis, Indiana Program Theme: Chemistry in Motion **247th ACS National Meeting & Exposition** March 16-20, 2014, Dallas, Texas

248th ACS National Meeting & Exposition August 10-14, 2014, San Francisco, California

249th ACS National Meeting & Exposition March 22-26, 2015, Denver, Colorado

250th ACS National Meeting & Exposition August 16-20, 2015, Boston, Massachusetts

251st ACS National Meeting & Exposition March 13-17, 2016, San Diego, California

252nd ACS National Meeting & Exposition August 21-25, 2016, Philadelphia, Pennsylvania

253rd ACS National Meeting & Exposition April 2-6, 2017, San Francisco, California

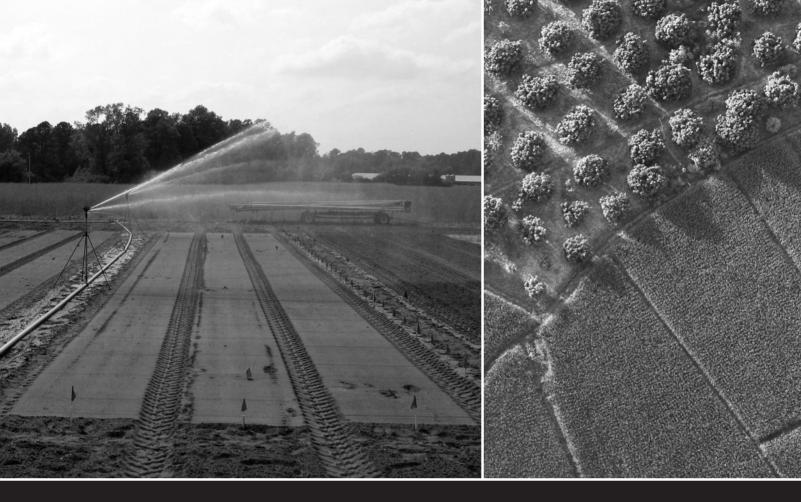
254th ACS National Meeting & Exposition September 10-14, 2017, St. Louis, Missouri

255th ACS National Meeting & Exposition March 18-22, 2018, New Orleans, Louisiana

256th ACS National Meeting & Exposition August 19-23, 2018, Boston, Massachusetts

257th ACS National Meeting & Exposition March 31-April 4, 2019, Orlando, Florida

258th ACS National Meeting & Exposition August 25-29, 2019, San Diego, California



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3rd Latin American Pesticide Residue Workshop May 2011

Meeting Notes by Steve Lehotay

The 3rd Latin American Pesticide Residue Workshop was held in Montevideo, Uruguay from May 8 – 11, 2011. With the help of the Conference Chairman, Prof. Horacio Heinzen, an IUPAC and AGRO table was set up adjacent to the poster session and immediately across from the coffee

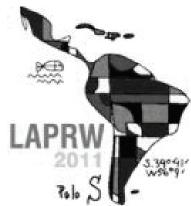


table. The table received maximum foot traffic, and all the IUPAC2014 pens and pins were taken by the participants during the course of the meeting as well as IUPAC magazines and documents.

The meeting was attended by more than 300 participants (the maximum capacity of the conference center) from many countries in North and South America, Europe, and Asia. The program consisted of 43 talks presented in either English or Spanish, and simultaneous translation by on-site interpreters was provided. Additionally, more than 143 posters were presented by the participants, and several vendors showed their latest instruments and products in booths.

AGRO sponsored two \$500 poster awards. The poster judging committee consisted of an AGRO/LAPRW Scientific Committee representative and judges recruited from Latin America, Europe, and the US: myself, Ronald Roy of the US FDA, and Profs. Horacio Beldomenico of Argentina, Eloisa Dutra Caldas of Brazil, Andre de Kok of The Netherlands, and Lutz Alder of Germany.

Posters from industry and non-Latin Americans were excluded and the 108 remaining posters were evaluated for 1) scientific quality, 2) ability of the presenter to discuss their work, 3) quality of the display, and 4) quality of the abstract. It was not an easy task due to the number of high quality poster presentations, but the judges came to unanimous consensus of the two winners.

Dr. Rafael Roehrs and colleagues of Federal Foundation University of Pampa (UNIPAMPA) in Uruguaiana, Rio Grande do Sul, Brazil presented entitled, "Bioremediation of herbicides in water with Enterobacter cloacae combined with Pistia stratiotes." They found in an interesting and well-organized study that there was a synergistic effect between the microorganism and water lettuce to degrade common pesticides (2,4-D, bentazone, quinclorac, propanil, and clomazone) more quickly in water.

Several high quality posters were presented in the analytical category in which the Latin American presenters had visited labs in Europe and the US, where they had used modern MS instruments for their analyses. Despite that instrumentation and expertise advantage, the judging committee was most impressed with the work presented in the poster of a graduate student, *Claudia M. Mamani Moreno of the Laboratorio de Toxicologia Ambiental of IMBECU*, CCT, CONICET-Mendoza, Argentina.

Her poster was entitled, "Determination of Maleic Hydrazide Residues in Garlic Bulbs by HPLC." She collaborated with 5 others including 3 from two different departments at the Universidade Federal de Vicosa in Minas Gerais, Brazil. They used sound scientific principles with simple instrumentation (LC-UV) to successfully meet a real-world need in a very difficult garlic matrix. This method would probably outperform LC-MS/MS due to matrix suppression effects and volatility of the analyte.

At the closing ceremonies, I discussed ACS and AGRO and encouraged scientists to join AGRO and that ACS membership was not required. I thanked and acknowledged the other judges and talked about the qualities of the winning posters. Dr. Roehrs was able to attend the ceremonies and receive the check in the ceremony, but Claudia Mamani Moreno was unable to be there. Her check was sent to her by Prof. Heinzen. Finally, Caroline Harris gave a very nice presentation about IUPAC and the upcoming meeting in San Francisco.



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5th Pan-Pacific Conference on Pesticide Chemistry

4th International Symposium on Pesticides and Environmental Safety

8th IUPAC Workshop on Crop Protection Chemistry and Regulatory Harmonization

Beijing, China September 17-21, 2012











Background

The scientific study, evaluation, and regulation of crop protection chemistry are rapidly developing in countries around the Pacific Rim, particularly with respect to product quality, risk assessment, environmental impacts, and food residues. There is a growing desire on the part of scientists, regulators, and industry leaders throughout the region to consider the applicability of international approaches for management of crop protection chemistry in support of a safe and abundant food supply.

This crop protection chemistry conference will be the 8th in a series of workshops sponsored by IUPAC since 1988, and will be combined in planning with the 4th in a series of environmental symposia sponsored by BPS and CAU.

An exciting new development is that the conference will also now be combined in planning and organization with the 5th Pan-Pacific Conference on Pesticide Chemistry.

Scientific Main Topics

- New pesticide discovery and synthesis
- Pesticide quality, manufacturing & specifications
- Formulation and application techniques
- Pesticide residues in food and international trade standards
- Environmental fate & safety assessment of pesticides
- Global views and harmonized approaches to pesticide regulation

Organizers and Sponsors

- International Union of Pure and Applied Chemistry (IUPAC)
- Beijing Pesticide Society (BPS)
- Pesticide Science Society of Japan (PSSJ)
- China Agricultural University (CAU)
- AGRO Division of the American Chemical Society

For Additional Information

Workshop Secretariat: Zhang Jing (iupac2012@yahoo.cn) Conference Website: www.2012iupac.com

IUPAC website: www.iupac.org/web/act/Beijing 2012-10-08

AGRO Coordinators:

Steve Duke (sduke@olemiss.edu) Jim Seiber (jnseiber@ucdavis.edu)



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MAJOR TOPIC AREAS WILL INCLUDE:

- Discovery, Mode of Action, Resistance Management
- Biotechnology
- Non-Crop Uses
- Environmental Fate and Ecological Effects
- Food Residues and Human Exposure
- Regulation, Stewardship, and Delivery Systems

AUGUST 24-28, 2014

San Francisco, California USA www.iupac2014.org







Councilors' Report

Jeanette Van Emon & Don Wauchope

Jeanette Van Emon and Don Wauchope, who played his horn again for the opening of the Council meeting, attended the Council Meeting held during the Spring 2011 ACS National Meeting in Anaheim. The following is a summary on key actions of the ACS Council and Board of Directors. We welcome your input on any of the items.

In addition to attending the Councilor meeting, Jeanette continued with her appointment on the Divisional Activities Committee and the sub-committee on Innovative Project Grants. The sub-committee met to review and recommend projects for funding. We are pleased to report that AGRO was successful in obtaining funding. Jeanette and Don both attended the Division Caucus prior to the full Council meeting. Jeanette also attended the meeting of the Steering Board for the Western Regional Meeting (WRM); for those of you living in the west, Jeanette is a good point of contact for the WRM.

ACTIONS OF THE COUNCIL

Election Results

The Committee on Nominations and Elections presented to the Council the following nominees for selection as candidates for President-Elect, 2012: Judith L. Benham, Dennis Chamot, Diane Grob Schmidt, and Marinda Li Wu. By electronic ballot, the Council selected Dennis Chamot and Marinda Li Wu as candidates for 2012 President-Elect. These two candidates, along with any candidates selected via petitions, will stand for election in the Fall National Election.

The Committee on Nominations and Elections announced the results of the election to select candidates to represent Districts III and VI on the Board of Directors for the term 2012 – 2014. The Councilors from these districts selected David Lohse & Pat Confalone and Bonnie Charpentier & Carlos Gutierrez as District III and IV candidates, respectively.

• Candidates for Directors-at-Large

The Committee on Nominations and Elections announced the selection of Ken Anderson, William Carroll, Jr., Charles Kolb, and Barbara Sawrey as candidates for Directors-at-Large for the 2012 – 2014 term.

The Society's Finances

In spite of the economic challenges faced in 2010, the Society's operating performance held up remarkably well. Total revenue was \$463.7 million, up +0.8% from 2009, and \$2.4 million (+0.5%) higher than the 2010 budget. The Net from Operations was \$23.8 million, or \$11.9 million favorable to budget. This resulted largely from cost containment initiatives and lower-than-budgeted salaries and fringe benefits.

2012 Member Dues and Division Allotment

The Council voted to set the member dues at \$148 for 2012. This rate is based on an inflation-adjustment formula. Dues

from other organizations were compared with ACS supporting that ACS is still a bargain. Furthermore, the Council voted to continue for three years the current formula for determining allotments to Divisions.

• Local Section Name Change and Grant Deadlines

The Council voted to change the name of the Northeast Oklahoma Section to the Northern Oklahoma Section due to the recent merger of the North Central Oklahoma Section and its territories into the Northeast Oklahoma Section.

Member Statistics

Membership recruitment efforts were exceptionally successful in 2010. It is particularly impressive that due to efficiencies in recruiting efforts, the net cost to recruit the more than 25,000 new members decreased from \$122 per member in 2008 to \$67 in 2010 despite increases in costs for postage and printing. The official membership number for 2011 stands at 163,111.

Attendance Report

The ACS Spring National Meeting attracted approximately 14,047 registrants with a breakout of: Regular attendees, 7,336; Students, 4,682; Exhibitors, 1,097; Exposition only, 599; and Guests, 333.

• Petition to Charter New International Chemical Sciences Chapters

The Council voted to authorize the formation of the following two new international chemical sciences chapters: the Shanghai International Chemical Sciences Chapter and the Thailand International Chemical Sciences Chapter.

ACTIONS OF THE BOARD OF DIRECTORS

During ACS President Joseph Francisco's term, he focused on "Building a Robust Workforce in the US." He appointed two presidential task forces to address the issues chemists face in the U.S. to obtain the skill sets, resources, and external environment to build and sustain a robust workforce in the U.S. The Board received an indepth report from the Presidential Task Force on Innovation in the Chemical Enterprise: New Technologies for the Society, New Jobs for Chemists. Councilors will receive more information on this and other reports which we will pass along to you.

The Society's International Activities

The American Chemical Society and the Federation of Asian Chemical Societies (a federation of 28 chemical societies of countries and territories in the Asia Pacific) agreed to a three-year collaboration alliance characterized by mutual benefits, impact, and commitment to cooperation in service to chemical scientists, engineers and professionals represented by the respective organizations.

2011 AGRO Division Officers



Dr. Kenneth D. Racke Division Chair



Dr. Aldos C. Barefoot Program Chair



Dr. John M. Clark Vice Chair



Dr. John J. Johnston Treasurer



Dr. Liliana Schwartz Secretary

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1970	Elvins Y. Spencer	1984	Robert M. Hollingsworth	1998	Judd O. Nelson
1971	Wendell Phillips	1985	John Harvey, Jr.	1999	Richard Honeycutt
1972	Philip C. Kearney	1986	Henry J. Dishburger	2000	Ann T. Lemley
1973	Roger C. Blinn	1987	James N. Seiber	2001	Jeffery Jenkins
1974	Charles H. Van Middelem	1988	Paul A. Hedin	2002	Terry D. Spittler
1975	Henry F. Enos	1989	Gustave K. Kohn	2003	Jeanette Van Emon
1976	Julius J. Menn	1990	Willa Garner	2004	Rodney Bennett
1977	James P. Minyard	1991	Guy Paulson	2005	Allan Felsot
1978	Gerald G. Still	1992	Joel Coats	2006	R. Donald Wauchope
1979	S.K. Bandal	1993	Larry Ballantine	2007	Laura L. McConnell
1980	Jack R. Plimmer	1994	Nancy N. Ragsdale	2008	John J. Johnston
1981	Marguerite L. Leng	1995	Don Baker	2009	Kevin L. Armbrust
1982	Gino J. Marco	1996	Barry Cross	2010	Ellen L. Arthur

Officers and Committees of the AGRO Division

AGRO DIVISION OFFICERS 2011

Division Chair, Kenneth D. Racke

317-337-4654, kracke@dow.com

Program Chair, Aldos C. Barefoot

302-451-5856, aldos.c.barefoot@usa.dupont.com

Vice Chair, John M. Clark

413-545-1052, jclark@vasci.umass.edu

Secretary, Liliana Schwartz

302-451-5842, liliana.schwartz@usa.dupont.com

Treasurer, John J. Johnston

202-365-7175, john.johnston@fsis.usda.gov

EXECUTIVE COMMITTEE MEMBERS

2009 - 2011

Steve Duke, stephen.duke@ars.usda.gov Cathleen Hapeman, cathleen.hapeman@ars.usda.gov Keri Carstens, keri.carstens@pioneer.com Ann Lemley, atl2@cornell.edu Chris Peterson, cjpeterson@fs.fed.us

2010 - 2012

Todd Anderson, todd.anderson@tiehh.ttu.edu Rodney Bennett, rodney.bennett@jframerica.com Allan Felsot, afelsot@tricity.wsu.edu Laura McConnell, laura.mcconnell@ars.usda.gov Sharon Papiernik, sharon.papiernik@ars.usda.gov

2011 - 2013

Julie Eble, julie.eble@criticalpathservices.com Scott Jackson, Scott.jackson@basf.com Pamela Rice, pamela.rice@ars.usda.gov Jim Seiber, jnseiber@ucdavis.edu Keith Solomon, ksolomon@uoguelph.ca

COUNCILORS 2009 - 2011

Jeanette Van Emon, vanemon.jeanette@epa.gov Don Wauchope, don_wauchope@citcom.net Rodney Bennett, Alternate Barry Cross, Alternate

FERT PROGRAM COMMITTEE

William Hall, Chair 863-428-5099, bill.hall@mosaicco.com

Nominating Committee

Ellen Arthur, Chair 913-433-5328, ellen.arthur@bayercropscience.com Kevin L. Armbrust, armbrust@mscl.msstate.edu John J. Johnston, john.johnston@fsis.usda.gov

AWARDS COMMITTEE

James Seiber, Chair

530-752-1465, jnseiber@ucdavis.edu

John Casida

Janice Chambers

John Marshall Clark

Joel Coats

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Ralph Mumma

Hideo Ohkawa

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Nancy Ragsdale

Will Ridley

David Soderlund

Don Wauchope

Willis Wheeler

Izuru Yamamoto

BYLAWS COMMITTEE

Rodney Bennett, rodney.bennett@jrfamerica.com

COMMITTEE ON COMMITTEES

Steve Duke, Chair

662-915-1036, stephen.duke@ars.usda.gov

Al Barefoot

Rod Bennett

John Clark

John Johnston

Ken Racke

COMMUNICATIONS COMMITTEE

Cathleen Hapeman, Chair

301-504-6451, cathleen.hapeman@ars.usda.gov

Tim Ballard – email newsletter

Laura McConnell - Ads/Website Coordinator

Jay Gan - Abstracts Editor

Sharon Papiernik - Awards Coordinator

Officers and Committees of the AGRO Division

(con't)

EDUCATION COMMITTEE

Diana Aga, Co-Chair

716-645-4220, dianaaga@buffalo.edu

Marja Koivunen, Co-Chair

530-750-2800, mkoivunen@marroneorganics.com

John Bourke, Investment Coordinator

Cathleen Hapeman, New Investigator Award Coordinator

301-504-6451, cathleen.hapeman@ars.usda.gov

David Barnekow

John M. Clark

David Barnekow

John M. Clark

Joel Coats

Barry Cross

Vincent Hebert

Ann Lemley

Glenn Miller

Judd O. Nelson

William Ridley

FINANCE COMMITTEE

Joel Coats, Chair, jcoats@iastate.edu

John J. Johnston, Ex Officio, john.johnston@fsis.usda.gov

Kevin Armbrust

Al Barefoot

Barry Cross

Scott Jackson

Terry Spittler

FUTURE SPECIAL CONFERENCE COMMITTEE

John M. Clark, Chair, jclark@vasci.umass.edu Robert Hollingsworth

HOSPITALITY COMMITTEE

Coffee Hour

Patricia Rice, 919-547-2668

patricia.rice@basf.com

Jim Brady, 336-643-1158, Cell: 336-708-0097

jfbrady@bellsouth.net

Julie Eble, 610-558-3001

Julie_eble@criticalpathservices.com

Joe Massey, 662-325-4725

jmassey@pss.msstate.edu

Social Hour

Aldos Barefoot, 302-451-5856

aldos.c.barefoot@usa.dupont.com

Jeff Jenkins, 541-737-5993

jeffrey.jenkins@orst.edu

International Activities Committee

Ken Racke, Co-chair

317-337-4654, kracke@dow.com

Jay Gan, Co-chair

951-827-2712, jgan@ucr.edu

Michele Arienzo

Paul HendleY

Rai Kookana

Steven Lehotay

Weiping Liu

Laura McConnell

Jim Seiber

Keith Solomon

John Unsworth

MEMBERSHIP COMMITTEE

Dan Stout, Chair

919-541-5767, stout.dan@epa.gov

John J. Johnston, john.johnston@fsis.usda.gov

PATRON RELATIONS COMMITTEE

Scott Jackson, Co-Chair, 919-547-2349

scott.jackson@basf.com

Del Koch, Co-Chair, 573-443-9003

kochd@abclabs.com

Laura McConnell, 301-504-6298

laura.mcconnell@ars.usda.gov

PUBLIC RELATIONS COMMITTEE

Jeff Jenkins, Chair

541-737-5993, jeffrey.jenkins@orst.edu

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STRATEGIC PLANNING COMMITTEE

Laura McConnell, Chair

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Troy Anderson

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Al Barefoot

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Keri Carstens

John Clark

Steve Duke

Jay Gan

Amrith Gunasekara Marja Koivunen

Ken Racke

Jeanette Van Emon

AGRO Division Business Teleconferences

August 5, 2010 1:00 – 4:30 pm CDT Chair – Ellen Arthur

Participants

Kevin Armbrust, Ellen Arthur, John Clark, Joel Coats, Steve Duke, Julie Eble, Cathleen Hapeman, Scott Jackson, John Johnston, Ann Lemley, Laura McConnell, Sharon Papiernik, Chris Peterson, Ken Racke, Pamela Rice, Liliana Schwartz, Jim Seiber, Terry Spittler, Dan Stout, Jeanette VanEmon

Chair's Introduction

Ellen Arthur called the meeting to order

Election Results - Kevin Armbrust

Liliana to send letters to candidates by mid September Kevin will call all candidates.

- 1. Vice-Chair John Clark
- 2. Secretary Liliana Schwartz
- 3. Treasurer John Johnston
- 4. Executive committee: Pam Rice, Jim Seiber, Scott Jackson, Keith Solomon, and Julie Eble

By-Laws Revision

Rod Bennett was not present on call. Ellen will call Rod and follow this through.

Feedback from the 2010 Florida Pesticide Residue Workshop 2010 – *Kevin Armbrust*

 Next year's meeting to be held July 17 to 20, 2011; organizing committee will put together brochure in place for AOAC meeting end of September. PICOGRAM to include brochure – Kevin to get this to Cathleen; she needs after end of September

MOTION for continued co-sponsorship by AGRO passed.

Status of Plans for ACS Meeting in Denver, Fall 2011 – Al Barefoot

 Tentative program distributed via email. Some ideas from Blues and Brews and others.

ACTION: Take a look at program and confirm your organizer commitment. Al will send a note to all potential organizers to get titles, etc. He expects that initial program request will be due to PICOGRAM (and ACS potentially) in December 15. Template for symposium announcement was sent to organizers. These can go into PICOGRAM directly (files need to be a *.doc file and not a pdf)

Hendricks Award -- Denver, Fall 2011 - Steve Duke

- Deadline for nomination November 3. Anyone can nominate
- Steve Duke will ask AGFD to send reminder; Steve will be arranging a conf call in near future to discuss Hendricks nomination;

Awards - Jim Seiber, Al Barefoot, Scott Jackson

 All award nominations – reminder to be sent to membership by Jim Seiber Division

- ACS Fellow award need nominations; Monday is award presentation– Congrats to Jim Seiber!
- Jim will be attending the Korea SABC Aug 24 to 26, 2010. 50th Anniversary and will bring a letter from AGRO Division to congratulate them. Cathleen will send Jim 2014IUPAC promotional items.
- International Award BASF and DuPont to have discussion about splitting Award into two separate Awards. Al Barefoot will plan meeting with Scott Jackson and Jim Seiber.

Pan-Pacific Meeting 2012 - John Clark

- To be hosted by Pesticide Science Society of Japan; at University of Scuba, Japan. John Clark met with Matsomoto, current chair.
- PSSJ wants to know our level of involvement in this
 process; we voted to be part of the process; if we
 decide to cosponsor, then our logo can be used; and
 perhaps we can send a student or two for poster
 competition; travel money for international travel is not
 there.
- AGRO took all financial risk for 4th Pan Pacific and solicited funds to cover all registrations not covered.
- Seiber: we should volunteer to help organize this.
 Suggest Phillip Lee to be involved. Meeting likely July 8-12. 2012.
- Ken Racke would like to see this meeting go forward as well. Offer funding to support speakers \$15K fixed rate to support travel for some of our AGRO memberships – e.g students for poster competition; keep AGRO as coorganizer.
- Steve Duke volunteered as co-program chair/conference co-chair if needed.
- Kevin Armbrust suggested that an innovative grant should be applied for to cover travel support
- Jim Seiber volunteered as co-conference chair. Once this is determined, we could then vote via email on the motion to support the conference and funding from AGRO. We are looking for them to take lead.
- John Clark will draft a letter of agreement prior to communication with Matsomoto.
- Al Barefoot provided historical documents: Meeting budget spreadsheet and Letter of Agreement.

MOTION: Stephen Duke Co-Program Chair; Jim Seiber Co-Conference Chair; \$15K for speakers and travel support for Co-chairs with total of \$25K – Motion Passed

Strategic Planning Meeting 2011 – Laura McConnell

- Attendees: Ken Racke, Ellen Arthur, Aldos Barefoot, 2011 Vice Chair, Steve Duke, Keri Carstens, Jay Gan, Laura McConnell, Troy Anderson, Ashli Brown, Marja Koivunen
- Shifting dates to January 19 to 21, 2011, Fort Worth, TX (Omni Hotel)

ACTION: Laura to check with facilitator to ensure dates will work; Ellen will then check with attendees. Survey will be sent to all members prior to meeting; attendees to receive a survey prior to meeting.

Pacifichem 2010: Dec 2010 - John Johnston

Occurs every 5 years.

- Two AGRO symposia for this meeting, Rodenticides and International Food Safety Issues and Opportunities. List of symposia and accepted talks circulated.
- Cathleen will send John promotional items for IUPAC2014.

IUPAC-ACS Chemistry Congress - Puerto Rico 2011 – Laura McConnell

- Innovative grant was funded.
- IUPAC Congress to be held July 30 to August 7, 2011 in San Juan Puerto Rico (www.iupac2011.org) Planning will begin in September to identify speakers. Anyone who is interested in attending, please let me know.
- Conference call next month to start process to select speakers for the symposium – 2 days with accompanying poster session.
- SETAC Global voted to contribute \$4K for symposium.
 Contact Laura with interest for talk.

IUPAC - San Francisco 2014 - Ken Racke

- Bid was accepted for AGRO to host in San Francisco in 2014. First circular developed; website activated; logo developed; pens, pins.
- At 12th IUPAC in Melbourne, booth where info was distributed. Recruited individuals to help with 2014; good promotion in Australia. Just over 1100 participated in Australia's IUPAC.
- Have requested an official report from Australian IUPAC

 including lessons learned; good coop from office of

 International Affairs
- Innovative Grant submitted for promotional efforts
- ACS Meetings Department to get back to us on plan.
- Expanded list in individuals for program committees or organizing symposia
- Organizing Committee Teleconference to be planned by Ken – and early call for innovative symposia. Check out website: www.IUPAC2014.org

PICOGRAM - Cathleen Hapeman

- PICOGRAM for fall 2010 will only be electronic. It will not have call for papers in it. It will have the table for symposia for Denver. New officers; student winners; announcement for various awards; will be sent out via email
- The next PICOGRAM will be hardcopy and will be sent end of January with call for papers, who will be organizing the International Award for Research and who will organize.

ACTION: September 30 2010 materials to Cathleen for PICOGRAM. Nancy Ragsdale summary for San Francisco. IUPAC Australia summary by Ken to Cathleen. Kevin to provide summary of Florida meeting.

ListServ Update - Laura McConnell

- List from ListServ plus list of emails from membership list all now into new system. This sends out message and allows recipient to opt out of receiving the emails. They can also have email address changed to divert to another email. We will be charged by number of emails that we send.
- We should go to a single email per month with a deadline for the monthly email to go out in a Newsletter format
- · Give Laura feedback on test email.

- Chair will review monthly before going out. Letter will go
 out last Wednesday of every month; Wed before is
 deadline for content. Chair can log in at any time to
 view this.
- Tim Ballard has expressed interest to manage this.

Treasury Report – John Johnston

- Johnston took over Jan 2010; summary of costs for 2010 in report that was circulated.
- Jeannette will follow up on ACS having this report. John recently withdrew \$18K to keep checking account afloat.
- Have we captured all income for San Fran meeting some checks were received before end of 2009.

Finance Committee Report for AGRO - Joel Coats

- Kevin Armbrust will provide historical documents.
- Finance Committee: Joel Coats (Chair), Al Barefoot, Terry Spittler, Kevin Armbrust, Scott Yates, Ann Lemley, John Johnston (Ex Officio).

ACTION: Joel / John will discuss income picture; then he will line up a meeting of the committee to put together next year's budget.

ACTION: Draft by September 30, 2010 of 2011 Budget with a follow-up meeting in October.

Proposal to Move Council to Tuesday during National Meetings – *Ellen Arthur*

- Response needed for ACS. Their concern that if the meeting is moved, then folks will leave meeting earlier.
- A straw vote was sent out among councilors. 50% supported move; 32% opposed; remaining undecided.

ACTION: Jeannette to take lead on responding to ACS on how this will impact AGRO. Due to ACS by Aug 22. Terry Spittler would like meeting to remain on Wed. Should be no imposition for Councilor to stay til Wed noon (JC). In spirit of even programming, makes sense to leave it on Wednesday. Folks will be leaving early if held on Tuesday. Attendance would suffer.

ACTION: Forward comments to Jeanette.

Western Regional Meeting – Jeanette Van Emon

AGRO gave \$500 support for this meeting. They are up for a ChemLuminary Award as a result of the meeting.

Innovative Grants - Laura McConnell

- Expenses associated with IUPAC 2014 launch.
 Innovative Grant proposal submitted.
- Laura submitted a grant for email marketing system to update locate. May offset expenses if funded. Should hear back after fall meeting.
- Innovative grant proposal also submitted by George Cobb of ENVR for joint symposium with AGRO veterinary pharmaceuticals in the environment for Denver Meeting.

Passing of the Chair Position – Ellen Arthur

Mallot is now activated and Ken is now in charge!!! Thanks all. It's been great working with you. Looking forward to more of the same.

Best wishes...Ellen

March 23, 2011 1:00 – 4:30 pm CDT Chair – Ken Racke

Participants

Ken Racke, Al Barefoot, Laura McConnell, Don Wauchope, Ann Lemley, Amrith Gunasekara, Cathleen Hapeman, Ellen Arthur, Allan Felsot, Julie Eble, Rod Bennett, John Clark, Keith Solomon, Pam Rice, Sharon Papiernick, Jim Seiber, Scott Jackson, John Johnston, Steve Duke, and Liliana Schwartz

Chair's Introduction

This is the first Executive Committee meeting in 2011, following the January 19 -21, 2011 Ft. Worth AGRO Strategic Meeting.

Awards Committee Proposal for Revision in Sponsorship of the AGRO International Award and Creation of a New Award – *Jim Seiber*

 The Awards Committee will be proposing an expansion of membership of the committee, in part to accommodate committee activity with two awards per year proposed to the Executive Committee and to stimulate more nominations for the Division fellowship.

MOTION: AGRO adopts two awards: 1) AGRO DuPont International Award (see PICOGRAM) and 2) Award for Innovation in Chemistry and Agriculture sponsored by BASF for ACS or AGRO Active Researchers. Motion passed.

- Jim proposes the expansion of the current AGRO Awards Committee from the current 12 members to 18. The additional 6 members will be selected by the existing committee members from the following 2 lists:
 - Past International Awards Recipients
 - Individuals expressing an interest during the recent member survey

MOTION: AGRO Awards Committee proposes its expansion from the current 12 to 18 members. Motion passed.

Strategic Planning Committee Report and Recommendations – Laura McConnell

 Strategic Planning Meeting held on January 19 – 21, 2011 was more specific than the 2008 meeting. Three goals and their objectives were drafted and they have to be finalized after their review by the Executive Committee (see the attached Executive Summary of the 2011 Strategic Planning Meeting):

Goal 1

AGRO will enhance the membership experience by providing an interactive and supportive environment for professional growth.

- 1.1 Develop and implement a system to obtain member feedback and share with members by December 2011.
- 1.2 Establish committee structure that serves and promotes division priorities by January 2012.
- 1.3 Recruit and retain a better informed membership by December 2014.
- 1.4 Improve networking options and communication to members by December 2012.

Goal 2

AGRO will use all internal and external resources to provide innovative programming and services that meet the needs of members and the global scientific community.

- 2.1 Revitalize the program committee to implement longrange innovative planning by December 2011.
- 2.2 Reach out to other divisions, professional societies and NGOs, and formalize collaborative relationships by August 2012
- 2.3 Create internal working groups with common professional or research interests by December 2012.
- 2.4 Increase pool of symposium organizers by August 2012.
- 2.5 Develop diverse set of virtual tools to foster innovative services by December 2013.

Goal 3

AGRO will be the global platform for collaboration and information exchange to advance innovative solutions for a sustainable food supply and protection of the environment and public health.

- 3.1 Define and communicate clearly the scope and diversity of scientific endeavors included in the AGRO mission by July, 2012.
- 3.2 Establish strategic alliances and collaborations with key groups of world AGRO scientists to increase international recognition and participation by July, 2012.
- 3.3 Facilitate the exchange of news, international developments, and scientific breakthroughs to a global audience by July, 2012.

MOTION: Executive Committee endorses three overall goals as outlined in the plan. Laura will continue to supervise the program implementation for the next four years as Chair of the Strategic Planning Committee. Motion passed.

MOTION: Formation of the AGRO Committee on Committees chaired by Steve Duke charged with carrying Objective 1.2 and advising the Executive Committee. Motion passed.

- The committee metrics should reflect sustainable food supply, more than membership. It was suggested that the committee should come up with a plan that reflects challenging metrics for the next 6 months.
- The Vision and Mission statements were reviewed during the meeting and the Executive Committee decided to vote on the "Mission" statement, while the "Vision" statements has to be further elaborated. Laura M. and Don W. will be revising the "Vision" statement.

Modified AGRO Mission Statement

AGRO, a Division of the American Chemical Society, brings together a worldwide community of scientists and stakeholders to advance knowledge and promote innovative solutions for the protection of agricultural productivity, public health and the environment.

MOTION: AGRO Executive Committee approves new proposed mission statement elaborated during the Strategic Planning Meeting. Motion passed.

MOTION: Formation of an International Affairs Committee to be co-chaired by Jay Gan and Ken Racke. Motion Passed. Jim Seiber is willing to serve.

Program Committee Report on Planning for Denver - Al Barefoot

- The program in Denver contains 14 topics with specific symposiums. The abstracts are ready for review.
- Symposium organizers are still looking for people to submit abstracts, at least 80 papers.
- The biotechnology area needs more papers. The submission deadline is April 4th.
- ACS instructions for symposium organizers have been sent out and they are very helpful this time.
- AGRO is looking to have sessions closed to the Environmental and AGFD sessions.

Treasurer's Report for 2010 - John Johnston

ACS Divisional Allocations are:

* Distribution of Divisional Allocations

	Fraction of		
Allotment Category	Allocations		
Base Allotment	12.50%	\$162,500.00	\$5,121.21
Per Member Allotment	12.50%	\$162,500.00	\$1,823.55
Innovative Projects	10%	\$130,000.00	\$12,500
Allotment			
Total Programming	65%	\$845,000.00	\$10,666.07
Allotment*			
Total		\$1,300,000.00	\$17,610.83

* Distribution of Programming Allotment

	% of Programming		
Category	Allotment		
# attendees at oral	50%	\$422,500.00	\$5,961.72
sessions			
# members at meeting	25%	\$211,250.00	\$2,569.53
# posters presented	25%	\$211,250.00	\$2,134.82

Total San Francisco Meeting expenses were \$36,019 which included the following allocations:

\$6,249 Refreshments

\$3,049 Business Meeting

\$2,979 Blues and Brews

\$9,379 Social

Finance Committee Recommendations for 2011 – *Joel Coats, Kevin Armbrust*

Due to Joel and Kevin's absence from the call, this topic is on hold until the Denver Business Meeting.

Miscellaneous - Ken Racke

- ACS Fellow Program The nomination process deadline is May 2, 2011. Ken asked for suggestions to proceed further with the nominations.
- ACS Web ACS developed an ACS network. It has good capabilities, similar to Facebook's functionality, posting documents, communication, set archives etc. Don W. volunteered to set up an AGRO Executive Committee communication site by using this ACS tool.
- Elections 2011 Ken will be communicating directly with Ellen.

Respectfully submitted, *Liliana Schwartz*, AGRO Secretary

Bylaws of the AGRO Division of the American Chemical Society *

* Effective October 27, 2000. Approved, as amended, by the Committee on Constitution and Bylaws, acting for the Council of the American Chemical Society.

Bylaw I. Name and Objects

Section 1. The name of this organization shall be the Division of Agrochemicals (hereinafter referred to as "the Division") of the AMERICAN CHEMICAL SOCIETY (hereinafter referred to as "the SOCIETY").

Section 2. The objects of the Division shall be to bring together persons particularly interested in agrochemicals, to consider all scientific aspects of chemistry relevant to the control of pests of agricultural or public health significance and to other methods for enhancing or modifying agricultural productivity, to develop and improve the professional stature of chemists with these interests, and to render whatever service it may to the scientific and lay communities on the topic of agrochemicals.

Bylaw II. Members and Affiliates

Section 1. Membership in the Division shall be open to all members of the SOCIETY. Application for membership shall be made in writing to the Secretary of the Division and shall be accompanied by one year's dues.

Section 2. A National Affiliate of the SOCIETY may apply to the Secretary to become a National Affiliate of the Division. Provided that Division dues established for National Affiliates are paid, a National Affiliate shall have all the privileges of membership in the Division except those of voting for or holding an elective position of the Division, voting on articles of incorporation or bylaws of the Division, or serving as a voting member of its Executive Committee.

Section 3. The Division may accept Division Affiliates who are not members or National Affiliates of the SOCIETY but who wish to participate in the activities of the Division. Such affiliates shall be entitled to all the privileges of membership in the Division save those withheld by the Bylaws of the SOCIETY.

Section 4. Members may resign their membership in the Division by submitting their resignation, in writing, to the Secretary during the year for which their dues are paid.

Section 5. The name of any member of the Division who is in arrears in payment of dues by as much as two years shall be stricken from the rolls. A member dropped for nonpayment of dues may be reinstated upon payment of arrearages.

Section 6. Affiliates shall retain affiliate status only so long as payment is made of Division dues. An affiliate's name is to be

stricken from the rolls as soon as the affiliate is in arrears in the payment of dues.

Section 7. The anniversary dates of Division members and National Affiliates of the Division shall coincide with their anniversary dates in the SOCIETY.

Bylaw III. Officers and Councilors

Section 1. The officers of the Division shall be a Chair, a Chair-Elect, a Vice-Chair, a Secretary, and a Treasurer. The Chair-Elect shall automatically succeed to the office of Chair upon expiration of the latter's term of office or if this office becomes vacant. The Vice-Chair shall automatically succeed to the office of Chair-Elect upon expiration of the latter's term of office or if this office becomes vacant. The offices of Secretary and of Treasurer may be held by one individual. Only MEMBERS are eligible to hold elective positions.

Section 2. The duties of the Chair shall be to preside at meetings of the Executive Committee, to carry into effect the decisions and recommendations of the Committee, to preside at stated meetings of the Division, and to appoint all committees except as otherwise provided.

Section 3. The duties of the Chair-Elect shall be to serve in the absence of the Chair of the Division and to act as Chair of the Program Committee.

Section 4. The duties of the Vice-Chair shall be to serve in the absence of the Chair-Elect and to act as Assistant Chair of the Program Committee, with particular emphasis on planning and developing technical programs.

Section 5. The duties of the Secretary shall be to keep minutes of all meetings of the Division and of the Executive Committee; to keep a roll of Division members and affiliates and to submit the same annually to the Executive Director of the SOCIETY for verification as provided in the Bylaws of the SOCIETY; to conduct the business correspondence of the Division as assigned to the Secretary by the Chair or by the Executive Committee; to prepare and submit an annual report of Division activities to the SOCIETY as required in the SOCIETY's Bylaws; to perform such other duties as may, from time to time, be assigned by the Chair or Executive Committee or required by the SOCIETY's Bylaws. The Secretary shall send to each member, at least two weeks before the regular meetings of the Division, abstracts of papers to be presented at said meetings.

Section 6. The Treasurer shall act as custodian of the funds of the Division, collect dues and other revenues, and pay the bills of the Division after the same have been authorized by the Executive Committee. The Treasurer shall maintain accurate records of receipts and disbursements and shall submit a report of the financial condition of the Division at the annual meeting of the Division. The Treasurer shall furnish a surety

bond, the premium for which shall be paid from Division funds.

Section 7. Councilors and Alternate Councilors shall represent the Division on the Council of the SOCIETY as provided in the Constitution and Bylaws of the SOCIETY.

Section 8. The Division shall have an Executive Committee, which shall consist of the officers of the Division; the Immediate Past Chair of the Division; the Councilors and Alternate Councilors; the Chairs, Chairs-Elect, Vice-Chairs, and Immediate Past Chairs of Subdivisions, if any; and fifteen (15) Members-at-Large. The Chair of the Division shall serve as Chair of the Executive Committee.

Section 9. The officers of the Division other than the Chair and the Chair-Elect shall be elected by mail ballot as described elsewhere in these bylaws.

Section 10. At the annual meeting of the Division, the Executive Committee shall appoint a Nominating Committee consisting of at least three members, one of whom shall be the Immediate Past Chair of the Division, who shall serve as Chair of this Committee. This Committee shall nominate two candidates for the office of Vice-Chair and at least ten (10) candidates for the positions as Members-at-Large to be filled on the Executive Committee. This Committee shall nominate candidates for each of the following offices to be filled: Councilor, Alternate Councilor, Secretary, and Treasurer. This Committee shall submit a report in writing to the Chair of the Division for preparation of the ballot to be mailed to the membership. Additional nominations may be made in writing by any group of at least five members and presented to the Chair of the Division not less than three months prior to the fall meeting.

Section 11. Officers and Members-at-Large shall be elected by the members and Division Affiliates of the Division. Only members of the Division may vote for Councilors and Alternate Councilors. The Secretary or other designated officer of the Division shall prepare an election ballot, on which shall appear the names in order chosen by lot of all candidates nominated and found willing to serve. In all Division balloting conducted by mail, the ballot voted shall be sealed, without voter identification, in a special ballot envelope. The special ballot envelope, bearing no voter identification, shall be enclosed in a larger envelope upon which—or within which, on a separate slip—shall be hand-inscribed the name of the member voting; the larger envelope shall then be sealed and forwarded to the Chair of the Tellers Committee. The Tellers shall count the ballots thus received, using the list of members provided by the Secretary to verify the eligibility of all those voting. Any ballot envelope not validated by the voter's accompanying hand-inscribed name shall be rejected. The Secretary shall set and announce in advance of the neither balloting the interval during which ballots must be received to be counted; this interval shall not be less than four nor more than seven weeks following the ballot mailing. The Tellers Committee, appointed by the Chair of the Division, shall be responsible for counting all valid ballots received within the interval and shall certify the results to the Secretary, who shall in turn certify the results to the SOCIETY, the elected officials, and the Division. Elections are to be by plurality, should there be more than two candidates for an office. Resolution of a tie vote shall be made by the Executive Committee.

Section 12. The Chair, the Chair-Elect, the Vice-Chair, the Secretary, and the Treasurer of the Division shall serve for one year or until their successors are elected.

Section 13. The terms of office of the Members-at-Large of the Executive Committee shall be three years. Five Membersat-Large shall be elected each year. Section 14. The terms of Councilors, Alternate Councilors, and all officers excluding the Chair, Chair-Elect, and Vice-Chair shall begin on January 1 following their election. The terms for Chair, Chair-Elect, and Vice-Chair shall begin at the conclusion of the fall meeting of the SOCIETY.

Section 15. Vacancies in offices other than Chair and Chair-Elect shall be filled by the Executive Committee. Incumbents so selected shall serve until the next regular election.

Bylaw IV. Councilors

The Division shall have Councilors and Alternate Councilors whose terms of office shall be three years. Alternate Councilors shall serve only for specific meetings of the Council when a Councilor is not able to attend.

Bylaw V. Committees

Section 1. There shall be a Program Committee, consisting of three or more members, one of whom shall be the Chair-Elect of the Division, who shall serve as Chair of the Committee. A second member of the Committee shall be the Vice-Chair. The Program Committee shall have the entire responsibility for organizing the program of papers for all Division meetings. It shall work cooperatively with other Divisions of the SOCIETY and other bodies in planning joint sessions and symposia of mutual and timely interest.

Section 2. There shall be a Membership Committee of three or more members. This Committee shall aggressively promote membership in the Division by members of the SOCIETY.

Section 3. There shall be a Finance Committee of two or more members. This Committee shall audit the accounts of the Treasurer prior to the business meeting of the Division and report its findings at the annual meeting. This Committee shall advise the Executive Committee on financial resources.

Section 4. There shall be an Awards Committee of at least six members. This Committee shall maintain and develop the Division and International Awards Programs.

Section 5. There shall be a Hospitality Committee of at least two members. This Committee shall direct social events in coordination with other committees and maintain a hospitality table at Division meetings.

Section 6. There shall be a Publication Committee of at least three members. This Committee shall be responsible for publication of the Division newsletter, PICOGRAM, and other Division publications.

Section 7. Special committees may be appointed to consider, conduct, and report upon such special matters as may be delegated to them.

Section 8. Except where otherwise provided, committee appointments shall be made by the Chair, with the advice and approval of the Executive Committee.

Bylaw VI. Dues

Section 1. Members of the Division shall pay annual dues, the exact amount to be decided by the Executive Committee. Dues are payable in advance. Members who have been granted emeritus status by the SOCIETY and who are interested in the work of the Division shall be granted all privileges of Division membership without the payment of annual dues.

Section 2. Affiliates shall pay annual dues of \$2.00 more than members; except that Division Affiliates who are regularly

matriculated students specializing in a chemical science shall pay annual dues of an amount to be decided by the Executive Committee.

Bylaw VII. Subdivisions

Section 1. Composition. The Division may sponsor Subdivisions devoted to specialized fields within the area of Division interest. Membership in the Division shall be a requirement for membership in a Subdivision.

Section 2. Formation. Formation or discontinuance of a Subdivision shall be at the discretion of the Executive Committee of the Division. Steps to initiate a Subdivision may be made by petition of a group of Division members to the Executive Committee or by the action of the Executive Committee. The scope of the activities of any Subdivision shall be defined by the Executive Committee.

Section 3. Officers. Upon approval of the formation of a Subdivision, the Executive Committee of the Division shall appoint a Chair, Chair-Elect, Vice-Chair, and Secretary for the Subdivision. The Chair-Elect shall assume the office of Chair after one year. In succeeding years the Subdivision shall elect at the annual meeting a Chair-Elect and a Secretary. The Chair, a Chair-Elect, and Secretary shall constitute a Steering Committee for the Subdivision. This Steering Committee shall report through the Chair of the Subdivision and be responsible to the Executive Committee of the Division, of which Subdivision Chairs shall be members ex officio.

Section 4. Funds. The necessary expenses for each Subdivision shall be authorized by the Executive Committee of the Division from Division funds and shall be paid by the Treasurer of the Davison upon the usual authentication.

Bylaw VIII. Meetings

Section 1. There shall be a meeting of the Division at each national meeting of the SOCIETY unless the Executive Committee votes otherwise, provided the requirements for a minimum number of meetings as specified in the SOCIETY Bylaws shall be met.

Section 2. The annual meeting of the Division shall be held at the fall meeting of the SOCIETY. Division business requiring vote of the membership shall be conducted only at this meeting, except as provided elsewhere in these bylaws. However, voting by the membership may be conducted by mail or as directed by the Executive Committee.

Section 3. Special meetings of the Division may be called by the Executive Committee, provided notice is given to the membership in writing or by publication in Chemical & Engineering News at least two months in advance. Special meetings may not be held within one month before or after a national meeting.

Section 4. Fifteen (15) members of the Division shall constitute a quorum for the conduct of business.

Section 5. The fee for registration at any special meeting shall be decided by the Executive Committee in accordance with the Bylaws of the SOCIETY.

Section 6. The rules of order in the conduct of Division meetings not specifically provided in these bylaws or in the SOCIETY's documents shall be the most recent edition of Robert's Rules of Order, Newly Revised.

Bylaw IX. Papers

Section 1. The Program Committee may approve or reject papers submitted for presentation before any meeting of the Division.

Section 2. The rules for papers presented before meetings of the SOCIETY as outlined in the Bylaws and Regulations of the SOCIETY shall govern the Division.

Bylaw X. Amendments

Section 1. These bylaws may be amended at any annual meeting of the Division by a two-thirds (2/3) vote of the members present. All amendments shall be submitted in writing to the Secretary at least sixty (60) days prior to the meeting. Upon approval of the Executive Committee, the Secretary shall send the text of the proposed amendment to the members of the Division at least thirty (30) days prior to the annual meeting.

Section 2. Amendments shall become effective upon approval by the Committee on Constitution and Bylaws, acting for the Council, unless a later date is specified.

Bylaw XI. Dissolution

Upon dissolution of the Division, any assets of the Division remaining thereafter shall be conveyed to such organization then existent as is dedicated to objects similar to those of the Division and the AMERICAN CHEMICAL SOCIETY, or to the AMERICAN CHEMICAL SOCIETY, so long as whichever organization is selected by the governing body of the Division at the time of dissolution shall be exempt under Section 501(c)(3) of the Internal Revenue Code of 1954 as amended or under such successor provision of the Code as may be in effect at the time of the Division's dissolution.

American Chemical Society AGRO DIVISION

242nd ACS National Meeting August 28 – September 1, 2011 Denver, Colorado USA

AC Barefoot, Program Chair and KD Racke, Division Chair

PROGRAM

DIVISION BUSINESS

AGRO Long-Range Program Meeting

Sunday 9:00 AM

Colorado Convention Center Hall Room 201

All Members Welcome; see page 39

AGRO Business Meeting

Sunday 5:00 PM

Colorado Convention Center Hall Room 4D

AGRO POSTER SESSIONS & COFFEE

General Topics

AGRO Education Award Poster Session

Monday 9:30 AM – 3:30 PM Colorado Convention Center Hall D

Advances in Protection of Agricultural

Productivity, Public Health, and the Environment

Tuesday 9:30 AM – 4:00 PM Colorado Convention Center Hall D

Sunday, Wednesday, and Thursday coffee only will be served in Colorado Convention Center Hall Room 712. PLEASE BE QUIET IF THE SESSION IS STILL IN ONGOING

SOCIAL EVENTS

International Award Speakers Luncheon

Monday 12:00 – 1:00 PM Colorado Convention Center – Room 608 Invitation Only

Sterling B. Hendricks Award Lecture Reception

Tuesday following the 11:30 AM lecture Colorado Convention Center Hall – Room 203

AGRO Awards Social

Tuesday 6:00 – 8:00 PM *Colorado Convention Center Hall – Room 201* Members/Guests welcomed; see page 13

Graduate Student Luncheon

Wednesday 12:00 – 1:00 PM *Colorado Convention Center Hall – Room 606* Invitation Only; see page 34

Blues & Brews - Program Planning Social

Wednesday 5:00 – 7:00 PM Colorado Convention Center Hall – Room 201 Members/Speakers welcomed; see page 39

SUNDAY AFTERNOON

Bioavailability and Extractability of Pesticide Residues

Implications for Risk Assessment

K. Malekani, P. Francis, D. Tessier, *Organizers* D. Shea, S. Mislankar, *Organizers, Presiding*

Section A

Colorado Convention Center 710

- 1:30 Introductory Remarks
- 1:35 1. Use of 3D force field analysis as a tool for understanding molecular binding mechanisms.S. H. Jackson
- 1:55 2. Effects of aging on retention, transport, and transformation of pesticides in soil. W. C. Koskinen
- 2:15 3. Formation of soil- and sediment-bound residues of sulfonylurea herbicides and their relevance in environmental risk assessments: A case study. R. Allen, R. Fischer, D. Judge
- 2:35 4. ¹⁵N NMR studies on the reaction of aromatic amines with soil organic matter to form bound residues. **K. A. Thorn**
- 2:55 Intermission
- 3:10 5. How do laboratory assessments of S-metolachlor sorption and dissipation agree with field behavior? S. K. Papiernik, A. Cabrera, W. C. Koskinen
- 3:30 6. Use of stable isotopes to predict HOC bioavailability in sediments. L. I. Delgado Moreno, J. Gan
- 3:50 7. Comparing pesticide distribution between formulated and natural sediments. X. Cui, J. M. Giddings, J. Gan
- **4:10 8.** Use of passive sampling devices to estimate the bioavailability of pyrethroids. **K. O'Neal**, D. Shea

Analytical Challenges for Crop Protection Products

Cosponsored by ENVR T. Anderson, Organizer

K. Armbrust, C. Wujcik, Organizers, Presiding

Section B
Colorado Convention Center 712

- 1:30 Introductory Remarks
- 1:35 9. Art of method development: Sensitive analytical methods for the trace residue analysis of crop protection chemicals in plant and environmental matrices using cutting edge technology. M. G. Saha, R. F. Gooding, J. E. Jones
- 1:55 10. Analyzing pesticide formulation adjuvants to assess their impact on pollinator health. C.
 A. Mullin, T. J. Ciarlo, W. Zhu, M. T. Frazier, J. L. Frazier
- 2:15 11. Mass spectrometry based, label-free proteomics: A case study for agricultural applications. L. Riter, P. Jensen, J. Ballam, E. Urbanczyk, S. MacIsaac, H. Valentin
- 2:35 12. Analytical challenges for the analysis of pyrethroids at trace residue levels. **D. A. Koch**, K. L. Clark, D. M. Tessier, C. Lam
- 2:55 Intermission
- **3:10 13.** Improved LC-MS/MS analysis of dicamba and its major metabolites in soy and cotton matrices. **J. E. Foster**, C. E. Wujcik
- 3:30 14. Analytical issues with ion suppression and enhancement in the quantitative analysis of small molecules in various matrices. L. Mallis, C. Cunningham, Jr, J. Eble
- **3:50 15.** LC/MS/MS, GC/MS, and GC/MS/MS methods for the analysis of pesticides and their degradation products in air and water samples. **R. Raina**, L. Sun, M. Etter, N. Fergus, E. Smith, P. Hall
- **4:10 16.** High throughput analysis of glyphosate and aminomethylphosphonic acid in raw agricultural commodities. **N. R. Smith**, J. M. Allan, C. E. Wujcik

Evaluating Agrochemical Aquatic Exposure Modeling in Relation to Risk Evaluator Needs Modeling

M. Barrett, R. Parker, *Organizers* M. Ruhman, *Organizer, Presiding*

Section C Colorado Convention Center 711

- 1:30 Introductory Remarks
- 1:35 17. Aquatic exposure modelling for exposure assessment in support of the regulation of pest control products in the Canada. G. Malis, I. Kennedy, L. Avon, &. Larivière
- 1:55 18. Spatially distributed pesticide exposure assessments in the Central Valley, California. Y. Luo, D. L. Ficklin, E. Luedeling, S. E. Gatzke, M. Zhang
- 2:15 19. Exploring approaches to Pesticide Aquatic Ecological Exposure Assessment: Issues in evaluating risk across the national landscape.

 R. D. Parker, M. R. Barrett, M. Ruhman
- 2:35 20. Evaluation and refinements to Tier 2 US EPA drinking water risk assessments: Methods to improve modeling scenarios. N. Snyder, A. Barefoot
- 2:55 Panel Discussion
- 3:10 Intermission
- **3:25 21.** Meta-modeling of the pesticide fate model PRZM for aquatic risk assessment. **Y. Luo**, F. Spurlock, X. Deng, S. Gill, K. Goh
- 3:45 22. Use of modeling and monitoring in pesticide exposure assessments in a regulatory context. M. R. Barrett, R. D. Parker
- 4:05 23. Prioritizing research and regulatory initiatives to minimize pesticide impacts on threatened and endangered species in California's Central Valley. D. L. Denton, R. S. Breuer, W. M. Williams, G. Hoogeweg, M. Zhang
- **4:25 24.** Aquatic exposure modeling for registration of crop protection products in the European Union. **K. W. Paul**, N. Mackay, R. L. Jones, A. Barefoot
- 4:45 Panel Discussion

International Award for Research in Agrochemicals

Symposium in Honor of Dr. George P. Lahm for his Contributions to the Discovery of New Insecticides

Financially supported by BASF Corporation & DuPont Crop Protection T. Stevenson, Organizer, Presiding

Section A
Colorado Convention Center 710

- 8:30 Introductory Remarks
- 8:40 25. Evolving strategies in insecticide discovery: A career perspective. G. P. Lahm
- 9:30 26. Diamide insecticides: New heterocyclic anthranilic derivatives. A. Jeanguenat, P. Durieux, A. J. Edmunds, R. G. Hall, L. van Innis, O. Loiseleur, M. Mühlebach, A. O'Sullivan, J. Pabba, A. Stoller, S. Trah, J. Wenger, A. C. Dutton
- 10:00 Intermission
- 10:15 27. Design, synthesis, and properties of acyclic spiroindoline insecticides. P. Maienfisch, J. Cassayre, F. Cederbaum, C. Corsi, L. Molleyres, T. Pitterna, E. Hillesheim
- 10:45 28. Benzisothiazoles: A versatile source for new insecticide leads. W. von Deyn, S. Soergel, V. Salgado, B. Wedel

Managed Ecosystems, Pesticides, and Biodiversity

A. Barefoot, B. Wigley, *Organizers* P. Edwards, *Organizer, Presiding*

Section B
Colorado Convention Center 712

- 8:30 Introductory Remarks
- 8:35 29. Managing lands to retain and sustain biodiversity. G. Kittel
- 9:05 30. Strategies for minimizing unintended effects of pesticides on biodiversity. **B. McGaughey**, L. Turner, J. Gagne, J. Giddings
- 9:35 31. Using herbicides to promote native plant communities. G. Beck, S. Nissen, J. R. Sebastian

10:05 - Intermission

- 10:30 32. Indirect effects of forest herbicides on wildlife: A literature review. V. L. Tatum, G. J. Roloff, L. A. Clark, L. L. Irwin
- 11:00 33. Biodiversity and landscape management in and around banana plantations in the humid tropics of Latin America. P. J. Edwards, R. Vargas
- 11:30 34. Use of aquatic herbicides to enhance biological diversity in natural and managed ecosystems. K. Getsinger

Evaluating Agrochemical Aquatic Exposure Modeling in Relation to Risk Evaluator Needs Model Verification and Uncertainties

R. Parker, M. Ruhman, *Organizers* M. Barrett, *Organizer, Presiding*

Section C Colorado Convention Center 711

- 8:30 35. Overview of issues in aquatic exposure modeling in the US EPA Office of Pesticide Programs, Environmental Fate and Effects Division (EFED). R. Parker
- 8:40 36. Integrating regulatory risk assessments, risk management, and best management practices to achieve the water quality objectives of the European Union: A long term initiative of the European Crop Protection Association (ECPA). R. Allen
- 9:00 37. Effects of input uncertainty on VFSMOD modeling of water, sediment, and pesticide trapping by vegetative filter strips. S. M. Folle, M. F. Winchell, T. L. Estes, K. A. Budreski1, J. P. Hanzas, R. L. Breton, P. Whatling
- 9:20 38. Effectiveness of buffers installed at targeted critical drainage areas in Minnesota.

 J. P. Hanzas, Jr, R. G. Struss
- 9:40 39. Quantifying trapping efficiency of vegetative filter strips for pesticide registration. G. J. Sabbagh, G. A. Fox, R. Muñoz-Carpena, D. Desmarteau
- 10:00 Panel Discussion
- 10:20 Intermission
- 10:35 40. Key environmental and physicochemical parameters influencing PRZM-GW predicted groundwater concentrations. T. L. Negley, A. C. Newcombe, D. F. Young
- 10:55 41. Estimation of reliable degradation kinetics parameters for complex metabolite pathways. I. Khanijo, N. Mackay

11:15 – 42. Method for temporal analysis of exposure to residues of concern for a parent compound and degradates. M. Ruhman, M. R. Barrett

11:35 - Panel Discussion

Agrochemical Use on Tribal Lands in the United States: Understanding Benefits, Issues, and Cultural Influences

Financially supported by Waterborne Environmental Inc.

P. Holden, Organizer

R. Gruenig, Organizer, Presiding

Section D Colorado Convention Center 708

- 8:00 Introductory Remarks
- **8:10 43.** Tribal pesticide enforcement in the inland Northwest: Circuit rider approach. **E. Gjevre**
- 8:30 44. Analytical snapshot of agrochemicals associated with marijuana grow operations on the Colville Indian Reservation, Washington.

 D. J. Hurst
- 8:50 45. Pesticide application notification systems.

 M. Aaron
- 9:10 Discussion
- 9:20 Intermission
- 9:30 46. Agricultural pesticide impacts on the health and culture of Maine's Native Americans. F. E. Corey
- 9:50 47. Pesticides and the impact on traditional basketry. D. Caudell
- **10:10 48.** Pesticide impacts on culturally-significant plants. **W. Keenan**
- 10:30 Discussion
- 10:40 Intermission
- 10:50 49. Progress toward control of Eurasian watermilfoil and an invasive hybrid milfoil in Coeur d'Alene Lake Tribal Waters by the Coeur d'Alene Tribe. D. S. Lamb
- 11:10- 50. Pesticide applications near well heads.M. Aaron
- 11:30 51. Integrated pest management on tribal lands. M. Aaron
- 11:50 Discussion

AGRO Division Monday Poster Session & Coffee

General Topics AGRO Education Award Poster Session

Financially supported by Bayer CropScience D. Aga, M. Koivunen, Organizers

9:30 AM - 3:30 PM Authors Present 9:45 - 10:45 AM and 2:30 - 3:30 PM

Section E Colorado Convention Center Hall D

- **52.** Insecticide runoff from urban hard surfaces during simulated and natural rainfalls. **W. Jiang**, D. Haver, A. Soeprono, M. Rust, J. Gan
- **53.** Degradation of saflufenacil as affected by moisture content and soil characteristics. **E. Camargo**, S. Senseman, R. Haney, J. B. Guice, G. McCauley
- **54.** DDA, a new water-soluble degradation product and biomarker of DDT in the Los Angeles Bight. **Z. Chen**, L. Chen, Y. Liu, C. Tang, H. Vega, R. I. Krieger
- **55.** Decomposition of pharmaceuticals by manganese oxide molecular octahedral sieves. **X. Xiao**, A. T. Lemley
- **56.** Environmental fate of the transgenic insecticidal protein Cry1Ab in water within a Bt maize agricultural ecosystem. **S. Mueting**, M. Lydy
- **57.** Oxidation of bisphenol F (BPF) by manganese dioxide. **Z. Lu**, J. Gan
- **58.** Assessing bioavailability and toxicity of permethrin and *p,p'*-DDT in sediment using matrix solid phase microextraction. **Y. Ding**, P. F. Landrum, J. You, M. J. Lydy
- Development of an in vitro method to determine the bioavailability of xenoestrogens in soil. K. N. Engler, A. T. Lemley
- **60.** Effect of exposure method on SPME-based bioavailability estimates for hydrophobic compounds. **A. D. Harwood**, M. J. Lydy
- 61. Predicting the toxicity of permethrin to *Daphnia magna* in water using SPME fibers. A. D. Harwood, A. R. Bunch, J. You, M. J. Lydy
- **62.** Cotton socks monitor the indoor distribution, fate, and persistence of fipronil following Frontline[®] application to companion animals. **Y. Liu**, L.

- Chen, Z. Chen, M. Bigelow Dyk, H. Vega, R. Krieger
- **63.** Surrogate system using rubber latex gloves to assess contact transfer and accumulation of surface pesticide residues. **T. E. Lopez**, L. Chen, Z. Chen, L. Cui, Y. Liu, P. J. Nguyen, G. Sankaran, L. T. Tang, H. Vega, R. I. Krieger
- **64.** Rubber latex gloves as a potential direct dosimeter to estimate pesticide exposure in strawberry harvesters. **G. Sankaran**, L. Chen, Z. Chen, Y. Liu, T. Lopez, H. Vega, R. I. Krieger
- 65. Enzyme kinetic analysis of allosteric solvent effects when screening mosquito-selective carbamates against *Anopheles gambiae*. D. Swale, P. Carier, M. Ma, J. Hartsel, M. Totrov, J. Bloomquist
- 66. Extensive permethrin resistance in North American head louse populations detected by quantitative sequencing and serial invasive signal amplification reactions. D. J. Previte, B. C. Poole, K. Yoon, G. E. Abo El-Ghar, D. Kwon, S. Lee, J. Clark
- **67.** High-throughput screening of terpenoid compounds at the American cockroach octopamine receptor to determine structure-activity relationships. **A. D. Gross**, M. J. Kimber, P. Ribeiro, J. R. Coats
- **68.** Differential potency and substrate kinetics of acetylcholinesterase peripheral site ligands: The molecular basis of selectivity for *Anopheles gambiae* mosquitoes. **J. M. Mutunga**, D. M. Wong, M. Ma, P. C. Lam, M. Totrov, L. Jianhong, P. R. Carlier, J. R. Bloomquist
- **69.** Deltamethrin increases peak current and slows deactivation kinetics of the voltage-gated calcium channel ($Ca_V2.2$) from rat brain following PKC dependent phosphorylation. **A. Alves**, S. Symington, J. Clark
- **70.** Evaluating the mode of action of terpenoids as insecticides: Evidence for membrane interaction. **J. W. Childress**, J. R. Coats
- **71.** Preformed biomarkers in produce may confound biomonitoring in pesticide exposure and risk assessment. **L. Chen**, Z. Chen, Y. Liu, T. Lopez, G. Sankaran, H. Vega, R. Krieger
- **72.** Adduct identification from reactions of phenoxy/propanoic herbicides with DNA in plants. **D. R. Hall**, D. Boerth
- **73.** Lignocellulosic biomass as a carbon source for biofuels production from oleaginous yeast. **M.**

- **L. Revellame**, R. Shivaji, R. Hernandez, D. Sparks, A. Brown
- 74. Isolation of cellulolytic organisms in the gastrointestinal tract of the giant panda and their potential use in the generation of lignocellulosic-based biofuels. C. Williams, W. Holmes, J. Falcone, D. Sparks, C. L. Williams, A. Kouba, S. Willard, A. Brown
- **75.** Mosquito cell lines as an economical platform for discovery of new insecticides to control malaria. **L. J. Jenson**, D. Diykov, J. R. Bloomquist
- 76. Biological stability and delivery studies to elucidate the role of thickener solid particles on water-in-oil emulsion containing microalgae. L. E. Fernandez, H. Guo, H. Scher, J. S. VanderGheynst
- **77.** Raman microscopic analysis of PM₁₀ for assessing source distributions from agricultural operations. **Q. Huang**, W. F. Schmidt, E. Razote, L. L. McConnell, C. J. Hapeman, A. Torrents, R. Maghirang, S. L. Trabue
- **78.** Optical fiber ammonia gas sensor using a dual layer poly(methyl methacrylate)/chlorophenol red coating. **Y. Huang**, S. Tao

DIVISION OF ENVIRONMENTAL CHEMISTRY

Black Carbon and Biochar for Soil Fertility and Carbon Sequestration Production and Characterization

Cosponsored by AGRO

D. Rutherford, C. Hapeman, P. White, T. Potter, *Organizers*

C. Rostad, Organizer, Presiding

ENVR Section B Sheraton Denver – Columbine

- 8:00 Introductory Remarks
- 8:05 ENVR 88. Quality variations of poultry litter biochar generated at different pyrolysis temperatures. M. Guo, Y. Shen
- 8:25 ENVR 89. Ammonia adsorption capacity of biomass and animal-manure derived biochars. K. S. Ro, G. Reddy, I. Lima, D. Mahajan, J. Cyrus
- 8:45 ENVR 90. Characterization of solid pyrogenic black carbon (biochar) by desorption atmospheric pressure photoionization (DAPPI) coupled to Fourier-transform ion cyclotron resonance mass spectrometry. W. T. Cooper, D. C. Podgorski, R. Hamdan, A. R. Zimmerman

- 9:05 ENVR 91. Adsorption properties of biocharbased activated carbon. Z. Gu, K. Muthukumarappan, J. Julson
- 9:25 ENVR 92. Investigation of dissolved organic carbon from water extracts of biochars by electrospray ionization/mass spectrometry. C. E. Rostad, D. W. Rutherford, R. L. Wershaw
- 9:45 ENVR 93. Effect of pH conditions on nutrients leachability and surface characteristics of biochars. P. Kim, N. Labbe, C. W. Edmonds, T. G. Rials, A. Johnson
- 10:05 Intermission
- 10:20 ENVR 94. Predicting biochar impact on soil carbon dynamics and soil quality in EPIC model. T. Lychuk, R. C. Izaurralde
- 10:40 ENVR 95. Do soil biochar additions prime or sequester soil organic carbon? M. Cotrufo, C. Stewart, J. Zheng
- 11:00 ENVR 96. Biochar as a carbon sequestration technology for Central Great Plains soils. F. J. Calderon
- 11:20 ENVR 97. Biochar as a soil amendment on two types of Saskatchewan Chernozemic soils. J. J. Stefankiw, J. J. Schoenau, R. E. Farrell
- 11:40 ENVR 98. Impact of biochar addition rate and soil type on greenhouse gas emissions: The importance of long-term data. C. Stewart, J. Zheng, M. Cotrufo

MONDAY AFTERNOON

AGRO Division Monday Poster Session & Coffee Section E

Colorado Convention Center Hall D

9:30 AM - 3:30 PM

Papers 52 – 78. See Previous Listings Authors Present 2:30 – 3:30 PM

Symposium in Honor of Dr. George P. Lahm for his Contributions to the Discovery of New Insecticides

Financially supported by BASF and DuPont Crop Protection

T. Stevenson, Organizer, Presiding

Section A

Colorado Convention Center 710

1:00 – 79. Piperidine thiazole fungicides. M. Hanagan, R. J. Pasteris, R. Shapiro, Y. Henry, B. Klyashchitsky

- 1:30 80. Sedaxane: A new broad-spectrum seed treatment fungicide. H. Walter, C. Corsi, M. Oostendorp, G. Scalliet, R. Zeun
- 2:10 81. From pyridines to pyrazoles: The discovery of Xemium[®]. J. Dietz, T. Grote, S. Strathmann
- 2:40 82. Fused pyrazole kinase inhibitors as broadspectrum fungicides. T. M. Stevenson, A. E. Taggi, A. D. Crews, M. H. Howard, P. L. Sharpe, J. Andreassi, J. J. Bisaha, C. J. Megatulski, T. M. Cenizal, P. R. Kovacs
- 3:10 Intermission
- 3:25 83. Pyrimidinone methylsulfonylisoxazolines: Novel herbicidal inhibitors of very long chain fatty acid biosynthesis. T. P. Selby, B. T. Smith, A. Travis, D. A. Clark, S. Bolgunas, R. Crosswicks, M. Ruggiero, M. McComrick, C. T. Pedersen, S. Gutteridge
- **3:55 84.** Indaziflam: A new low-dose, non-selective solution for broad-spectrum weed control. **H. Ahrens**, H. Dietrich, K. Minn, T. Auler, H. Bieringer, M. Ford, E. Hacker, M. Hills, H. Kehne, H. Menne, E. Rose
- **4:25 85.** Innovation in agrochemical research: The role of paradigms. **A. Kleemann**

Managed Ecosystems, Pesticides, and Biodiversity

P. Edwards, *Organizer*

B. Wigley, Organizer, Presiding

Section B
Colorado Convention Center 712

- 1:30 Introductory Remarks
- 1:35 86. Forest herbicides: Effective tools for intensive management and sustainable forestry. R. B. Iglay, V. R. Lane, P. D. Jones, D. A. Miller, S. Demarais, S. B. Castleberry, K. V. Miller, T. B. Wigley
- 2:05 87. Operation pollinator: Positive action for pollinators. J. Peters, N. Williams, R. Isaacs, J. Ellis, D. Waage, J. Tuell, A. Pence, K. Ward, D. Wilson, J. Daniels
- 2:35 88. Acute toxicity of forestry herbicide mixtures to aquatic organisms. V. L. Tatum, D. L. Borton, W. R. Streblow, J. Louch, J. P. Shepard
- 3:05 Intermission
- **3:30 89.** Vertebrate pest management: Case studies in pesticides and the management of biodiversity. **M. J. Bodenchuk**

- 4:00 90. Impact of farming practices, pesticides, and landscape management on farmland birds in Europe and the role of Cross Compliance and Agri-Environmental Schemes . P. J. Edwards, G. Siriwardena
- **4:30 91.** Contribution of zero tillage to sustainability in Brazil's tropics. **J. N. Landers**

Advances in Characterizing Exposure of Humans and Ecosystems to Pesticides in Surface Waters: Regional Scale Assessment and Monitoring Approaches

N. Poletika, C. Crawford, *Organizers* R. Gilliom, *Organizer, Presiding*

Section C Colorado Convention Center 711

- 1:15 Introductory Remarks
- 1:20 92. Watershed regressions for pesticides (WARP) for predicting atrazine concentrations in corn belt streams. W. Stone, R. Gilliom
- 1:40 93. Analysis of monitoring data from multiple small watersheds to identify drivers of agrochemical runoff from corn and sorghum agriculture. P. Miller, M. Andrus, C. Harbourt, D. Mao, J. Prenger, P. Hendley, R. Joseph
- 2:00 94. Comparison of SWAT pesticide simulation approaches for ecological exposure assessments. N. Peranginangin, M. F. Winchell, R. Srinivasan
- 2:20 95. Large-scale modeling of historical pesticide applications. G. Hoogeweg, M. Cheplick, W. M. Williams, D. Denton, R. Breuer
- 2:40 Panel Discussion
- 2:55 Intermission
- 3:10 96. Importance of sediment analysis in monitoring current-use pesticides in streams. M. L. Hladik, K. L. Smalling, K. M. Kuivila
- 3:30 97. Sampling plans for water quality assessment. J. W. Green
- 3:50 98. Continuous monitoring for pesticides in freshwater off-channel habitats using a lipid-free tubing passive-sampling device. P. Janney, J. J. Jenkins, K. Anderson
- 4:10 99. Exposure assessment for pronamide drinking water residues in California central coast lettuce production areas. N. Poletika, B. Bret, M. Winchell

4:30 – 100. Pesticides and pesticide degradates in source and finished water of community water systems supplied by rivers. **G. Delzer**, J. Valder

4:50 - Panel Discussion

New Investigator Symposium

Financially supported by Dow AgroSciences
C. Hapeman, Organizer, Presiding

Section D Colorado Convention Center 708

- 1:30 Introductory Remarks
- **1:40 101.** Application of biological mass spectrometry and protein barcodes in agricultural and food chemistry. **J. Wang**
- 2:00 102. WITHDRAWN
- 2:20 Intermission
- 2:35 103. Metolachlor fate in regionally adopted cropping systems of the SE United States. P. M. White, Jr., T. L. Potter
- 2:55 104. Degradation of *p*-nitrophenol by heterogeneous Fenton-like reactions on nanomagnetite: Process optimization using response surface methodology. S. Sun, A. T. Lemley
- 3:15 105. CuO and ZnO nanoparticles affect production by a beneficial pseudomonad of metabolites important in plant performance.
 C. Dimkpa
- 3:35 Concluding Remarks

DIVISION OF ENVIRONMENTAL CHEMISTRY

Black Carbon and Biochar for Soil Fertility and Carbon Sequestration Applications in the Environment

Cosponsored by AGRO

D. Rutherford, C. Rostad, P. White, C. Hapeman, Organizers

T. Potter, Organizer, Presiding

ENVR Section B Sheraton Denver – Columbine

- 1:30 Introductory Remarks
- 1:35 ENVR 125. Herbicide sorption in a biocharamended coastal plain soil under conventional and conservation tillage management. T. Potter, P. M. White, I. M. Lima

- 1:55 ENVR 126. Biochars from sugarcane trash and sugarcane bagasse as soil amendments.

 I. M. Lima, P. M. White, K. T. Klasson, M. Uchimiya
- 2:15 ENVR 127. Biochar-mediated reductive transformation of nitro herbicides. S. Oh, J. Son, P. C. Chiu
- 2:35 ENVR 128. Biochar production for use as low-cost adsorbents: Applications in drinking water treatment serving developing communities. J. P. Kearns, K. Shimabuku, L. S. Wellborn, D. R. Knappe, R. S. Summers
- 2:55 ENVR 129. Biochar field trials in Zambia, Africa: Doubling growth and understanding why. G. Cornelissen, V. Shitumbanuma, G. D. Breedveld, V. Martinsen, J. Mulder, M. Van Leur, V. Alling, S. E. Hale, P. Aagaard, E. Phiri, O. E. Arnesen, J. Studsroed
- 3:15 Intermission
- 3:30 ENVR 130. Nutrient, metals, and organic matter retention in Indonesian and Zambian soils amended with biochar: Batch and column leaching tests. V. Alling, V. Martinsen, G. Breedveld, J. Mulder, S. Hale, V. Shitumbanuma, P. Aagaard, A. Heikens, N. Nurida, P. Setyant, G. Cornelissen
- 3:50 ENVR 131. Biochar characteristics and function as a heavy metal sorbent in soil: Role of surface ligands. M. Uchimiya
- **4:10 ENVR 132.** Biochar for soil remediation on abandoned mine lands: San Juan Mountains, CO. **C. D. PetIz**
- **4:30 ENVR 133.** Heavy metal adsorption capacity of biomass and animal-manure derived biochars. **I. M. Lima**, K. S. Ro, G. Reddy, D. Mahajan, K. T. Klasson, M. Uchimiya
- 4:50 ENVR 134. Sugarcane bagasse and pine wood biochar effects on aerobic soil dissipation of metribuzin and pendimethalin.

 P. M. White, Jr., T. L. Potter, I. M. Lima
- 5:10 Concluding Remarks

MONDAY EVENING

Sci-Mix

A. Barefoot, *Organizer*8:00 - 10:0052 - 59, 61 - 78. See previous listings.

Section A Colorado Convention Center – Hall D

TUESDAY MORNING

Endangered Species Act and Pesticide Regulation: Scientific and Process Improvements Policy and Process

Financially supported by Intrinsik Environmental Sciences, CropLife America, and Dow AgroSciences J. Johnston, S. Jackson, J. Cowles, T. Hall, B. McGaughey, Organizers K. Racke, J. Jenkins, Organizers, Presiding

Section A
Colorado Convention Center 710

- 8:30 Introductory Remarks
- **8:40 –** Federal Panel Perspectives on ESA and Pesticide Regulation.
- 9:15 106. Endangered Species Act: Interfacing with agricultural and natural ecosystems. B. McGaughey, L. W. Anderson, M. J. Bodenchuck
- 9:40 107. Insights from USDA on improving the ESA-pesticide assessment process. S. H. Kunickis, H. D. Coble
- 10:05 Intermission
- 10:25 108. Growers, pesticides, and endangered species: Results of MCFA ESA workshop. D. A. Botts
- 10:50 109. Using litigation to push for programmatic reform of EPA's Endangered Species Protection Program. C. L. Adkins Giese
- **11:15 110.** Integrating FIFRA, ESA, and other legal requirements. **D. B. Weinberg**
- **11:40 111.** Unintended consequences: A historical perspective on pesticides and endangered species with suggestions. **L. Turner**

Modern Agriculture and Biotechnology: Tools for Sustainability

Sustainability Standards

E. L. Arthur, P. Rice, Organizers

P. Rice, J. Van Emon, Organizers, Presiding

Section B
Colorado Convention Center 712

- 8:30 Introductory Remarks
- **8:40 112.** Linking agricultural sustainability with healthy foods. **J. N. Seiber**
- 9:10 113. Studying sustainability from field to market. T. Stone, J. Shaw, B. Lackey, R. Murdock
- 9:40 114. Importance of herbicides for sustainable farming in the United States. L. Gianessi
- 10:10 Intermission
- 10:30 115. Plant biotechnology for sustainable agriculture: Research and development and an enabling policy framework. D. Dewar
- 11:00 116. Metabolism of [¹⁴C]dicamba in dicamba-tolerant cotton. T. L. Whitehead, M. J. Mierkowski, R. C. Chott, M. J. Miller
- 11:30 117. Sustainability standards: Biotech and organic coexistence. T. P. Redick

Advances in Characterizing Exposure of Humans and Ecosystems to Pesticides in Surface Waters Time Intensive Studies and Vulnerability Assessment

R. Gilliom, C. Crawford, *Organizers* N. Poletika, *Organizer, Presiding*

Section C Colorado Convention Center 711

- 8:15 Introductory Remarks
- 8:20 118. Improved characterization of the temporal and spatial variability of potential surface water drinking water exposure by using environmental and historic monitoring databases. P. Hendley, W. Chen, R. Joseph, R. Williams, C. Harbourt
- **8:40 119.** Time series model for estimating pesticide exceedance probabilities for streams. **A. Vecchia**, K. Ryberg
- 9:00 120. Investigating sampling designs for pesticide surface water monitoring using available daily or near-daily measurements.
 W. Chen, P. Mosquin, P. Hendley, R. L. Sielken, R. Joseph, S. Chen, R. Williams, A. Merritt

- 9:20 121. Estimation of upper percentiles of chlorpyrifos surface water concentration from yearly monitoring program data. G. G. Brown, P. L. Mosquin, R. W. Whitmore, N. Poletika
- 9:40 Panel Discussion
- 10:00 Intermission
- 10:15 122. Combining long-term herbicide monitoring with identification of vulnerable areas in restricitve layer watersheds. R. N. Lerch, C. Baffaut, E. J. Sadler, N. R. Kitchen, K. A. Sudduth
- 10:35 123. Application of high resolution elevation data (LiDAR) to assess natural and anthropogenic agricultural features affecting the transport of pesticides at multiple spatial scales. J. J. Amos, C. Holmes, J. Bang, P. Hendley, L. Fish
- 10:55 124. Updates to percent crop area methods: Extending drinking water assessments to tropical climates and refinements to the regional values . N. Snyder, A. Barefoot
- 11:15 125. Development of a modeling system to estimate pesticide runoff from urban areas in California. W. M. Williams, K. Moran, Y. Luo, D. L. Denton, R. S. Breuer, J. M. Cheplick, G. Hoogeweg
- 11:35 Panel Discussion

Sterling B. Hendricks Memorial Lectureship

Sponsored by USDA-Agricultural Research Service Cosponsored by AGFD

K. Kaplan, *Organizers*S. O. Duke, M. H. Tunick, *Organizers, Presiding*

Section D
Colorado Convention Center 203

- 11:30 Award Presentation
- 11:40 AGRO 126. Applying advances in chemistry to benefit developing world agriculture. D. Delmer
- **12:30** Reception

AGRO Division Tuesday Poster Session & Coffee

Advances in Protection of Agricultural Productivity, Public Health, and the Environment A. Barefoot, *Organizer*

> 9:30 AM - 4:00 PM Authors Present 9:45 - 10:45 AM and 2:45 - 3:45 PM

Section E Colorado Convention Center Hall D

- 127. Method for the analysis of atrazine, simazine, metolachlor, and atrazine metabolites in water samples collected by polar organic chemical integrative sampler. T. Mayer, M. F. Pennell, K. M. L'Empeurer, G. S. Moorthy, S. Drummond, S. J. Hill, J. Eble
- 128. LC-MS/MS analytical method for the determination of PREVICUR residues in poultry matrices and eggs. T. Nguyen, S. Moore
- 129. Application of capillary electrophoresis to identification of pesticide photolysis products.R. Weintraub, D. Safapour
- 130. Analysis of bee relevant matrices for imidacloprid, imidacloprid olefin, and 5hydroxy imidacloprid by modified QuEChERS extraction and analysis by LC/MS/MS with stable, isotopically-labeled internal standard. J. Brungardt, B. Leimkuehler
- 131. Quantitative determination of thiamine in corn (Zea mays) grain by high performance liquid chromatography-tandem mass spectrometry. F. A. Claussen
- **132.** Extraction of microbial secondary metabolites from fermentation broths using polymeric resins. **G. Yuen**, R. N. Asolkar, V. Bui, H. Huang, M. E. Koivunen, P. G. Marrone
- 133. New pesticidal compounds from Burkholderia sp. R. N. Asolkar, M. E. Koivunen, A. Cordova-Kreylos, H. Huang, L. Chanbusarakum, P. G. Marrone
- **134.** Using microbes for synthesizing agrochemical metabolites. **M. J. Schocken**
- 135. Discovery of spiroindolines: A new class of insecticides with a novel mode of action. J. Cassayre, P. Maienfisch, R. S. Roberts, P. A. Worthington, D. J. Hughes, L. Molleyres, F. Cederbaum, E. Hillesheim, A. Sluder, F. Earley, S. Shah

- **136.** Effect of halogen and trifluoromethyl substituents on the biological activity of spiroindolines. **P. Maienfisch**, J. Cassayre, L. Molleyres, R. S. Roberts, D. J. Hughes, E. Hillesheim
- 137. Synthesis and biological activity of spiroindoline N-oxides. P. Maienfisch, R. S. Roberts, J. Cassayre, L. Molleyres, T. Winkler, E. Hillesheim
- 138. Effect of bedding material on air quality of bedded manure packs in livestock facilities. M. J. Spiehs, T. M. Brown-Brandl, D. N. Miller, D. B. Parker
- **139.** Flow characteristics of a dynamic flux chamber. **B. Woodbury**, D. Parker, R. Eigenberg, M. Spiehs
- **140.** Volatile organic compounds in pesticide formulations: Methods to estimate ozone formation potential. **L. L. McConnell**, M. Zeinali, C. J. Hapeman, A. Nguyen, W. F. Schmidt, C. J. Howard
- **141.** Atmospheric contributions of endosulfan to South Florida ecosystems. **C. J. Hapeman**, L. L. McConnell, T. Potter, B. Schaffer, R. Curry
- 142. Standardization of flux chambers and wind tunnels for area source emission measurements at animal feeding operations.
 D. B. Parker, B. L. Woodbury, S. L. Trabue, L. Cai, M. J. Spiehs, R. A. Eigenberg, T. M. Brown-Brandl, M. B. Rhoades, E. A. Caraway
- **143.** Modeling pesticides and their chemical transformation products. **R. Li**
- **144.** Monitoring of endocrine disrupting chemicals (EDCs)-suspected pesticide residues in orchard soils in Korea. **J. Lee**, H. Noh, K. Kang, K. Lee, H. Park, S. Choi, E. Lee, K. Kyung
- **145.** Search for neuraminidase inhibitors from Okinawan plants. **S. Tawata**, A. Upadhyay, J. Chompoo, T. Makise
- 146. Time-course residual characteristics of cyflufenamid and fluquinconazole in squash. K. Lee, H. Noh, K. Kang, J. Lee, H. Park, S. Choi, S. Yun, S. Shim, M. Anh, K. Kim, C. Jin, J. Ryu, S. Oh, K. Kyung
- **147.** Establishment of pre-harvest residue Ilmits (PHRL) of fungicide myclobutanil and dimethomorph in Korean melon under greenhouse condition. **J. Kim**, Y. Jeon, H. Kim, J. Hwang, J. Ahn, J. Kim
- **148.** Residual characteristics and estimated dietary intake of emamectin benzoate in leaf

- mustard. **S. Yun**, Y. Kim, S. Shim, K. Kim, C. Jin, S. Oh, J. Ryu, S. Park, H. Noh, K. Kyung
- 149. Monitoring of pesticide residues in leafy vegetables collected from wholesale and traditional markets in Korea. H. Noh, K. Kang, K. Lee, J. Lee, H. Park, S. Choi, E. Lee, K. Kyung
- **150.** Multiresidue analysis method for unregistered oragnophosphorus pesticides in Korea for imported agricultural products. **Y. Jeon**, H. Kim, J. Hwang, J. Do, M. Im, J. Lee, Y. Lee, J. Kim
- **151.** Estimation of the dietary intake of flusilazole and hexaconazole in squash at different sampling stage before harvest. **H. Noh**, K. Lee, J. Lee, K. Kang, H. Park, S. Choi, S. Yun, C. Jin, S. Oh, K. Kyung

DIVISION OF ENVIRONMENTAL CHEMISTRY

Veterinary Pharmaceuticals in the Environment Use and Modes of Action

Cosponsored by AGRO

Financially supported by USDA-Agricultural Research Service

G. P. Cobb, P. Smith, L. McConnell, *Organizers* B. Johnson, *Presiding*

ENVR Section B Sheraton Denver – Grand Ballroom 1

- 8:00 Introductory Remarks
- 8:10 ENVR 162. Mechanisms of anabolic steroidstimulated muscle growth. W. R. Dayton, M. E. White, M. R. Hathaway
- 8:40 ENVR 163. Interspecies comparison of the mechanisms of toxicity and effects of veterinary pharmaceuticals with estrogenic or androgenic activity: Are we really living in a sea of estrogens? L. E. Gray, Jr, V. S. Wilson, P. Hartig, G. Ankley
- 9:10 ENVR 164. Molecular target homology as a basis for species extrapolation to assess the ecological risk of veterinary drugs. C. A. LaLone, D. L. Villeneuve, L. Burgoon, C. L. Russom, J. E. Tietge, G. T. Ankley
- 9:40 Intermission
- 9:55 ENVR 165. In vitro assays for assessment of androgenic and estrogenic activity of defined mixtures and complex environmental samples. V. S. Wilson

- 10:25 ENVR 166. Application of steroidal implants in the U.S. beef cattle industry. J. L. Beckett, B. J. Johnson
- 10:55 ENVR 167. Overview of the U.S. Food and Drug Administration Center for Veterinary Medicine environmental risk assessment process for veterinary pharmaceuticals. H. M. Zahner, W. Hunter, E. Silberhorn, C. Eirkson

TUESDAY AFTERNOON

Endangered Species Act and Pesticide Regulation: Scientific and Process Improvements Policy and Process

Financially supported by CropLife America, Dow AgroSciences, and Intrinsik Environmental Sciences J. Johnston, J. Jenkins, K. Racke, T. Hall, S. Jackson, Organizers

J. Cowles, B. McGaughey, Organizers, Presiding

Section A Colorado Convention Center 710

- 1:30 Introductory Remarks
- 1:35 152. Regulatory improvements to the Endangered Species Act consultation process for pesticide registrations. Y. Li, J. Rylander, C. Kennedy
- 2:00 153. Application of the Endangered Species Act's best scientific data available standard.
 P. J. Donnelly, L. Bogert, L. R. Rhomberg
- 2:25 154. Producing food and fiber where endangered species live. H. Hansen
- 2:50 155. Endangered species pesticide protection programs in North Dakota: Past, present, and future. J. Johnson
- 3:15 Intermission
- 3:35 156. California's pesticide use reporting system. L. Wilhoit
- **4:00 157.** Role of state pesticide agencies in the endangered species assessment process: Examples from Florida. **M. Feken**
- 4:25 Panel Discussion: Policy and Process

Modern Agriculture and Biotechnology: Tools for Sustainability Sustainability Indicators

J. Van Emon, P. Rice, *Organizers* E. L. Arthur, P. Rice, *Organizers, Presiding*

Section B
Colorado Convention Center 712

- **1:30 158.** Bioenergy buffers: Creating sustainable agricultural landscapes. **D. Gustafson**
- 2:00 159. Ecosystem services framework for agricultural key performance indicators. S. Ozment
- 2:30 160. Measuring sustainability in the agri-food sector: Use and development of Eco-Efficiency Analysis. M. Gipmans, P. Saling, D. Voeste
- 3:00 Intermission
- 3:20 161. From isoprene to Taxol®: Modular architecture in terpenoid biosynthesis. M. Koksal
- 3:50 162. Sustainability initiatives in agriculture: The role of science. P. J. Rice, P. Rice, J. Van Emon, E. Arthur
- 4:20 Concluding Remarks

Advances in Protection of Agricultural Productivity, Public Health, and the Environment A. Barefoot, *Organizer, Presiding*

Section C
Colorado Convention Center 711

- 1:30 163. Regulating pesticide products used in the home: Comparison of biomonitoring data and exposures estimated with regulatory models. J. E. Johnston, X. Bi
- 1:50 164. Monitoring knockdown resistance in the human head louse populations using three molecular tools. K. S. Yoon, J. M. Clark, S. H. Lee, G. E. Aboelghar, D. H. Kwon, D. J. Previte, B. C. Poole
- 2:10 165. Resistance-breaking acetylcholinesterase inhibitors for the malaria mosquito, *Anopheles gambiae*. Q. Chen, D. M. Wong, J. M. Mutunga, F. Astha, J. Li, P. C. Lam, M. M. Totrov, J. R. Bloomquist, P. R. Carlier
- 2:30 166. Sarmentine as a bioherbicide. H. Huang, C. M. Morgan, R. N. Asolkar, M. E. Koivunen, P. G. Marrone
- 2:50 Intermission

- 3:05 167. Mp708 a maize (*Zea mays*) line resistant to herbivory constitutively releases (E)-β-caryophyllene. **A. E. Brown**, W. E. Crown Smith, R. Shivaji, W. P. Williams, D. S. Luthe, G. V. Sandoya, C. Smith
- **3:25 168.** Persistence and transferability of pyrethroid insecticides on urban concrete surfaces. **W. Jiang**, D. Haver, A. Soeprono, M. Rust, J. Gan
- 3:45 169. Sulfentrazone aquatic field dissipation study in Canada. A. W. Chen, D. Martens, M. Abetew
- 4:05 170. Spatial distribution of iodide concentrations in California groundwater. T.
 L. Negley, A. C. Newcombe, V. B. Houck, C. B. Meyer, C. Nordmark, J. Troiano
- **4:25 171.** Rice cultivation, pesticide load and water contamination. **T. Jindal**

DIVISION OF ENVIRONMENTAL CHEMISTRY

Veterinary Pharmaceuticals in the Environment Sampling Techniques and Chemical Analysis

Cosponsored by AGRO

Financially supported by USDA-Agricultural Research Service

G. P. Cobb, P. Smith, L. McConnell, *Organizers* W. Foreman, *Presiding*

ENVR Section B Sheraton Denver – Grand Ballroom 1

- 1:30 Introductory Remarks
- 1:35 ENVR 197. Quadrupole time-of-flight LC-MS analysis of veterinary drug residues in aquaculture samples. S. Turnipseed, S. Clark, J. Storey
- 1:55 ENVR 198. Liquid chromatography mass spectrometry: Analysis of veterinary growth promoters in airborne particulate matter. B. R. Blackwell, B. J. Johnson, M. Baker, M. D. Buser, G. P. Cobb, P. N. Smtih
- 2:15 ENVR 199. Analysis of steroids in newborn screening by LC-MS/MS. M. Fountain, D. Klein
- 2:35 ENVR 200. Deuterium exchange complicates isotope dilution methods for steroid hormones. W. T. Foreman, R. C. ReVello, J. L. Gray
- 2:55 Intermission

- 3:10 ENVR 201. Detection of tetracyclines and tetracycline resistant bacteria in soils under long-term swine effluent application. I. Popova, S. Deng, J. Hattey
- **3:30 ENVR 202.** Particulate matter emissions from animal feeding operations. **R. G. Maghirang**
- 3:50 ENVR 203. Particulate matter sampling strategies for agricultural operations. D. P. Whitelock, M. D. Buser, L. L. Wang
- **4:10 ENVR 204.** Growth promoters, wind, and human/ecological health: Preliminary feedyard PM analysis. **M. Buser**, B. Blackwell, P. Smith, G. Cobb, B. Smith
- 4:30 ENVR 205. Techniques for determining partial size distribution of particulate matter: Laser diffraction vs. electrical sensing zone. L. Wang Li, M. Buser, D. P. Whitelock, Z. Cao, Y. Zhang, C. Parnell

WEDNESDAY MORNING

Endangered Species Act and Pesticide Regulation: Scientific and Process Improvements Case Studies

Financially supported by CropLife America, Dow AgroSciences, and Intrinsik Environmental Sciences B. McGaughey, J. Jenkins, J. Cowles, S. Jackson, K. Racke, Organizers J. Johnston, T. Hall, Organizers, Presiding

Section A
Colorado Convention Center 710

- 8:30 Introductory Remarks
- 8:40 172. Endangered species assessments conducted under FIFRA: Fomesafen registration review case study. D. Campbell, M. Dixon, S. Wall, J. Overmyer
- 9:05 173. Fomesafen endangered species assessment: Novel approaches for assessment refinement. J. Overmyer, J. Bang, R. Brain, K. Henry, J. Perine, S. Wall
- 9:30 174. FIFRA Registration Review and the Endangered Species Act: Clomazone case study. A. Frank, B. McGaughey, G. Mitchell, J. Cummings, S. Longacre
- 9:55 Intermission
- 10:15 175. Invasive weed and endangered species interactions: Can herbicides facilitate a positive outcome? K. G. Beck, S. Nissen, J. Sebastian

- 10:40 176. Cranberry insect pest management and Karner Blue butterfly protection: A Wisconsin case study. K. D. Racke, L. G. Bowman, C. Carnes
- 11:05 177. Adaptive management of aquatic plants in the Sacramento-San Joaquin Delta in compliance with the Endangered Species Act: Applying lessons learned for strategic planning. L. W. Anderson
- 11:30 178. Vertebrate pesticides and the ESA. M. J. Bodenchuk

Agriculture and Air Quality: Emission Measurements and Models Pesticides and VOCs

S. Hafner, C. Howard, L. Mc Connell, R. Maghirang, Organizers

C. Hapeman, *Presiding*

Section B Colorado Convention Center 712

- 8:30 Introductory Remarks
- 8:40 179. Ten-years of pesticide volatilization monitoring. J. H. Prueger, T. J. Gish, L. G. McKee, W. P. Kustas, J. G. Alfieri, J. L. Hatfield, L. L. McConnell, C. J. Hapeman, C. J. Howard
- 9:00 180. New Investigator Award. Pesticide emission model: Evaluation of performance in predicting pesticide emissions from the Chesapeake Bay region. C. J. Howard, J. H. Prueger, T. J. Gish, C. J. Hapeman, L. L. McConnell, L. G. McKee
- 9:20 181. Reducing near-field agricultural fumigant emissions through efficacious changes in regional application practices. V. R. Hebert, D. Johnson, P. Hamm, D. Horneck
- 9:40 182. Predicting transport, fate, and pest control after fumigating soil with methyl iodide. L. Luo, S. Yates
- 10:00 183. Assessment of pesticide drift and deposition downwind of ground spray applications: A case study examining the impact of droplet size, boom height, and wind speed. R. J. Londergan, A. C. Newcombe, T. M. Wolf
- 10:20 Intermission
- 10:40 184. Volatile organic compound emissions from agriculture in Central Valley, California.
 C. Warneke, J. A. de Gouw, J. B. Nowak, J. Peischl

- 11:00 185. Speciation of VOCs from complex sources: Validation of reactivity-weighted emissions. P. G. Green
- 11:20 186. Mass balance evaluation of alcohol emission from cattle feed. S. D. Hafner, F. Montes, C. A. Rotz, C. Howard
- 11:40 187. Comparison of flux chamber devices for ammonia emission measurement. M. L. Hile, E. F. Wheeler, R. C. Brandt, P. A. Topper

Parameters for Pesticide QSAR and PBPK/PD Models

Chiral Isomers, Metabolism, GI, and Percutaneous Absorption

C. Timchalk, J. Knaak, R. Tornero-Velez, *Organizers* R. W. Gerlach, *Presiding*

Section C Colorado Convention Center 711

- 8:25 Introductory Remarks
- 8:30 188. Chiral chemistry and toxicity assessments for pyrethroid pesticides. R. W. Gerlach
- **8:55 189.** Direct chiral separation of pyrethroid isomers by HPLC with chiral stationary phases. **M. Okamoto**
- 9:20 190. Biotransformation and enzymatic reactions of pyrethroid insecticides in mammals. H. Kaneko
- 9:45 Intermission
- 10:00 191. Prediction and use of environmentallyand physiologically-relevant properties of pesticides. R. D. Clark, M. B. Bolger, J. Boyd
- 10:25 192. Characterization of potential agerelated differences in pyrethroid pharmacokinetics. J. V. Bruckner, T. G. Osimitz, S. Anand, D. Minnema, W. Schmitt
- 10:50 193. Fifteen steps to percutaneous penetration-man to animal: Why important?H. I. Maibach
- 11:15 194. On the estimation and use of dermal permeability coefficients. J. C. Kissel, A. L. Bunge
- **11:40 195.** Percutaneous absorption of pesticide formulations. **W. G. Reifenrath**

DIVISION OF ENVIRONMENTAL CHEMISTRY

Veterinary Pharmaceuticals in the Environment Occurrence Transport and Transformation of Veterinary Pharmaceuticals

Cosponsored by AGRO

Financially supported by USDA-Agricultural Research Service

G. P. Cobb, P. Smith, L. McConnell, *Organizers* P. Smith, *Presiding*

ENVR Section B Sheraton Denver – Grand Ballroom 1

- 8:00 Introductory Remarks
- 8:05 ENVR 229. Spatial variation in selected veterinary drugs across a cattle feedlot transect from barn to retention basin. C. P. Rice, K. Cook, A. Netthisinghe, B. Gilfillen, G. N. Guzmán
- 8:25 ENVR 230. Sorption and mineral-promoted transformation pathways of synthetic growth promoters in soil systems. S. Qu, E. P. Kolodziej, D. M. Cwiertny
- **8:45 ENVR 231.** Environmental assessment of the antibiotic florfenicol for use in a variety of aquaculture systems. **J. Staveley**, R. Endris
- 9:05 ENVR 232. Veterinary pharmaceuticals in sewage lagoons of a rural Canadian watershed: The role of phytoremediation for enhanced wastewater treatment. C. S. Wong, J. C. Carlson, J. E. Low, P. Cardinal, M. L. Hanson
- 9:25 Intermission
- 9:45 ENVR 233. Role of reduction-oxidation state on the degradation of synthetic growth promoters. E. P. Kolodziej, D. M. Cwiertny, J. Lee
- **10:05 ENVR 234.** Bioavailability of antimicrobial compounds in sediments. **J. R. Coats**
- 10:25 ENVR 235. Not tonight deer: Determination of an immunocontraceptive peptide in a wildlife vaccine formulation. D. A. Goldade, J. E. Kemp, L. A. Miller
- 10:45 ENVR 236. Risk assessment of steroid hormones in veterinary drugs at the U.S. Food and Drug Administration Center for Veterinary Medicine. H. M. Zahner, C. E. Eirkson, E. Silberhorn

DIVISION OF AGRICULTURE & FOOD CHEMISTRY

Future Agricultural Consumer Safety Demands for the Global Market

Cosponsored by AGRO
A. Loaiza, Organizer, Presiding

Section A Colorado Convention Center 505

- 8:30 Introductory Remarks
- 8:35 AGFD 122. Evaluation of the safety of crop products produced through biotechnology. W. Parrott
- 9:00 AGFD 123. Addressing the Safety of Crop Protection Products in a Global Market. W. Jones, R. McAllister, B. Glenn
- **9:25 AGFD 124.** Toxicological Safety Assessment of Biotech Crops. **C. A. Mathesius**
- 9:50 Intermission
- 10:05 AGFD 125. Allergenicity Evaluations of Proteins Introduced into Crop Products using Biotechnology. L. S. Privalle
- **10:30 AGFD 126.** Analytical Methods for Testing Biotechnology Products. **J. Chen**, P. Doyle
- 10:55 Concluding Remarks

WEDNESDAY AFTERNOON

Endangered Species Act and Pesticide Regulation: Scientific and Process Improvements Salmonid Case Studies

Financially supported by CropLife America, Dow AgroSciences, and Intrinsik Environmental Sciences B. McGaughey, J. Johnston, K. Racke, T. Hall, S. Jackson, Organizers J. Jenkins, J. Cowles, Organizers, Presiding

Section A Colorado Convention Center 710

- 1:25 Introductory Remarks
- 1:30 196. Pesticide aquatic exposure scenarios and modeling for juvenile Pacific salmonid floodplain habitat. N. Poletika, Z. Tang, S. Jackson
- 1:55 197. Spatial and temporal distributions of salmon and their prey: Implications for estimating their exposure to agricultural pesticides. S. Cramer, M. Teply, L. Dominguez

- 2:20 198. Modeling the exposure of salmon to agricultural pesticides. M. Teply, S. Cramer, N. Poletika
- 2:45 199. Modeling risk to aquatic species subject to realistic, dynamic exposures using a generalized form of Haber's Law. R. Reiss, K. Bogen
- 3:10 Intermission
- 3:30 200. Risks of pesticide mixtures to salmon in the Pacific Northwest. D. R. Moore, R. S. Teed
- 3:55 201. Application of a GIS-based approach to quantifying pesticide-use site proximity to salmonid habitat. M. F. Winchell, J. Bang, B. Patterson, K. A. Budreski, R. A. Brian, S. B. Wall
- **4:20 202.** Assessment of the potential risks of dimethoate to aquatic endangered species using the joint probability distribution analysis. **Q. Ma**, R. Reiss, C. Habig, P. Whatling
- 4:45 Panel Discussion: Case Studies

Agriculture and Air Quality: Emission Measurements and Models Animal Feeding Operation Emissions

C. Howard, L. Mc Connell, R. Maghirang, *Organizers* S. Hafner, *Organizer, Presiding*

Section B
Colorado Convention Center 712

- 1:30 203. Thermal reconstitution from sorbent tube odorant collections: Progress toward a robust, integrated strategy for capture, transport, archiving, and deferred "'re-play" of environmental odor events. **D. Wright**, F. Kuhrt, D. Eaton, J. Koziel
- 1:50 204. Optical fiber ammonia sensors for air quality monitoring. S. Tao, Y. Huang, L. Wieck
- 2:10 205. Comparison of VOC emissions from conventional and alternative biofuel crops. M. Graus, A. Eller, R. Fall, B. Yuan, Y. Qian, P. Westra, J. de Gouw, C. Warneke
- 2:30 206. Weather-based conditional sampling of ammonia near livestock operations using passive samplers. J. M. Ham, C. Williams, J. Stratton, T. Borch
- 2:50 207. Emissions from swine barns: Effects of slurry age. K. E. Jonassen
- 3:10 Intermission

- 3:30 208. Characterization of VOCs and odorants on PM from animal feeding operations. S. L. Trabue, D. Parker, R. Maghirang, L. L. McConnell
- 3:50 209. Interaction of urea hydrolysis, CO₂ emission, and pH on ammonia emission from dairy barn floors. F. Montes, S. D. Hafner, C. A. Rotz
- 4:10 210. Monthly, seasonal, and annual methane emissions from a beef cattle feedyard. R. W. Todd, N. A. Cole
- **4:30 211.** DairyGEM: A software tool for whole farm assessment of emission mitigation strategies. **C. A. Rotz**, F. Montes, S. D. Hafner

Parameters for Pesticide QSAR and PBPK/PD Models

Liver Tissues/Enzymes and NeurotoxicityC. Timchalk, J. Knaak, R. Tornero-Velez, *Organizers*E. Hodgson, *Presiding*

Section C Colorado Convention Center 711

- 1:30 212. Human metabolic interactions of pesticides: Induction and cytotoxicity. A. D. Wallace, E. Hodgson
- 1:55 213. Human metabolic interactions of pesticides: Inhibition. E. Hodgson, A. D. Wallace
- 2:20 214. In vitro and in vivo experimental data for pyrethroid pharmacokinetic models: The case of bifenthrin. M. F. Hughes, J. M. Starr, E. J. Scollon, M. J. DeVito
- 2:45 215. Paraoxonase 1 (PON1) status in risk assessment for organophosphate exposure and pharmacokinetics. C. E. Furlong, R. J. Richter, T. B. Cole, G. P. Jarvik, W. Li, K. E. Thummel, A. E. Rettie
- 3:10 Intermission
- **3:25 216.** Carboxylesterases: Dual roles in lipid and pesticide metabolism. **M. K. Ross**
- 3:50 217. Behavioral changes in young and adult rats: Indications of cholinesterase inhibition.
 V. C. Moser, P. M. Phillips, K. L. McDaniel, D. W. Herr
- 4:15 218. Comparison of esterase sensitivity, metabolic efficiency, and toxicity levels of two organophosphorus insecticides, parathion, and chlorpyrifos. J. E. Chambers, H. W. Chambers

DIVISION OF AGRICULTURE & FOOD CHEMISTRY

Future Agricultural Consumer Safety Demands for the Global Market

Cosponsored by AGRO

A. Loaiza, Organizer, Presiding

Section A
Colorado Convention Center 505

- 1:30 Introductory Remarks
- **1:35 AGFD 133.** Pesticide residues in food: The role of dietary risk assessment. M. G. Panek
- 2:00 AGFD 134. Secondary standards barrier or benefit? J. M. Stewart
- 2:25 AGFD 135. Remediation of fungicide residues on fresh produce using gaseous ozone. S. S. Walse
- 2:50 Intermission
- **3:05 AGFD 136.** Creating and Marketing More Sustainable Food Consumer Goods. C. Barcan
- 3:30 Panel Discussion
- 4:15 Concluding Remarks

WEDNESDAY EVENING

DIVISION OF ENVIRONMENTAL CHEMISTRY

Posters: Black Carbon and Biochar for Soil Fertility and Carbon Sequestration

Cosponsored by AGRO

C. Rostad, C. Hapeman, T. Potter, P. White, *Organizers*

D. Rutherford, Organizer, Presiding

ENVR Section E Colorado Convention Center Hall D

6:00 - 8:00

- **ENVR 316.** Biochar reference materials. **D. W. Rutherford**, C. E. Rostad, R. L. Wershaw, F.
 J. Calderon
- **ENVR 317.** Carbon isotopic fractionation as a function of charring temperature during the production of biochar. R. L. Wershaw, D. W. Rutherford, **C. E. Rostad**, N. M. Saad

- **ENVR 318.** Modeling the physical and chemical interactions of natural organic matter in soils: General principles. **R. L. Wershaw**, D. W. Rutherford, C. E. Rostad
- **ENVR 319.** Effects of biochar amendment in soil on bioenergy crop yield and biomass composition. **C. W. Edmunds**, N. Labbe, P. Kim, A. Johnson, M. Radosevich, T. Rials
- **ENVR 320.** Biochar effects on extractable NO₃⁻ and NH₄⁺ and greenhouse gas flux after biochar and fertilizer application to two temperate soils. **J. Zheng**, C. E. Stewart, M. Cotrufo
- **ENVR 321.** Distinct phosphorus leaching behaviors of poultry litter (PL) and PL Char. Y. Wang, P. T. Imhoff, M. Guo, **P. C. Chiu**
- **ENVR 322.** Ammonia removal using poultry litter and its biochar mixture. **N. Lovanh**, J. Loughrin
- **ENVR 323.** Characterization of biochars produced under different conditions by 1D and 2D solid-state ¹³C-NMR. **R. Hamdan**, A. R. Zimmerman, W. T. Cooper
- **ENVR 324.** Biochar for soil pH amelioration and improved crop yields. **J. L. Field**, F. Cotrufo
- **ENVR 325.** Thermo-chemical conversion of spent coffee to bio-oil and biochar. **B. K. Sharma**, W. Zheng, K. Witkin, N. Rajagopalan

THURSDAY MORNING

Endangered Species Act and Pesticide Regulation: Scientific and Process Improvements Scientific Advances

Financially supported by CropLife America, Dow AgroSciences, and Intrinsik Environmental Sciences J. Cowles, J. Jenkins, J. Johnston, S. Jackson, B. McGaughey, Organizers K. Racke, T. Hall, Organizers, Presiding

Section A
Colorado Convention Center 710

- 8:30 Introductory Remarks
- **8:40 219.** Advancements in Endangered Species Act effects determination for pesticide registration actions. **E. W. Odenkirchen**
- 9:05 220. Using GIS to assess pesticide exposure to threatened or endangered species for ecological risk assessment. J. Cowles

- 9:30 221. Development of a spatial-temporal cooccurrence index to evaluate pesticide risks to threatened and endangered species. G. Hoogeweg, D. Denton, R. S. Breuer, G. Hancock, P. TenBrook
- 9:55 Intermission
- 10:15 222. Access to NatureServe's best available data on the locations of endangered species. K. Maybury, L. Honey, S. Howie
- 10:40 223. DriftWatch.org: Pesticide sensitive crops and habitats registry implementation results. L. Hahn, L. Theller, A. Reimer, B. Engel
- 11:05 224. Use of risk-based spray drift buffers for protection of non-target areas. S. H. Jackson, M. Ledson
- 11:30 225. Development of a website (www.Pre-Serve.org) to help protect threatened and endangered plants near crop production. K.
 H. Carr, J. L. Honegger, S. R. Mortensen, D. I. Gustafson

Agriculture and Air Quality: Emission Measurements and Models Emission Measurement and Modeling S. Hafner, L. Mc Connell, R. Maghirang, *Organizers* C. Howard, *Organizer, Presiding*

Section B
Colorado Convention Center 712

- 9:00 226. Comparing two micrometeorological techniques for estimating trace gas emissions from distributed sources. K. S. Ro, M. H. Johnson, P. G. Hunt, T. Flesch
- 9:20 227. Source apportionment and tracing of agricultural and fossil fuel reactive N emissions using stable isotopic composition.
 J. D. Felix, E. M. Elliott, R. Maghirang, J. Briggs, L. McConnell, T. Gish, M. Hastings, D. Gay
- 9:40 228. Measurements of isocyanic acid (HNCO) from agricultural burning. J. M. Roberts, T. C. VandenBoer, S. B. Brown, W. P. Dube, N. Wagner, C. Young, C. A. Brock, A. Middlebrook, R. Bahreini, P. R. Veres, A. K. Cochran, C. Warneke, M. Graus, J. A. de Gouw, I. R. Burling, R. J. Yokelson
- 10:00 229. Residual carbaryl in treated pine bark and the presence of carbaryl in wood smoke.C. Peterson, S. Costello
- 10:20 Intermission

- 10:40 230. Detailed modeling of ozone formation from animal feed emissions in the San Joaquin Valley. J. Hu, C. J. Howard, P. G. Green, M. J. Kleeman
- 11:00 231. Airborne observations of ammonia emissions from agricultural sources and their implications for ammonium nitrate formation in California. J. B. Nowak, J. A. Neuman, R. Bahreini, A. Middlebrook, C. A. Brock, G. J. Frost, J. S. Holloway, S. A. McKeen, J. Peischl, I. B. Pollack, J. M. Roberts, T. B. Ryerson, M. Trainer, D. D. Parrish
- 11:20 232. Comparative study of observed and CMAQ modeled coarse particulate matter. R. Li, C. Wiedinmyer, M. P. Hannigan, K. R. Baker

Parameters for Pesticide QSAR and PBPK/PD Models

Neurotoxicity and QSAR

C. Timchalk, J. Knaak, R. Tornero-Velez, *Organizers* T. Shafer, *Presiding*

Section C Colorado Convention Center 711

- 9:00 233. Characterization of pyrethroid insecticide interactions with cloned human Na⁺ channels in high-throughput patch clamp. G. E. Kirsch, Y. A. Kuryshev
- 9:25 234. Pyrethroid actions on sodium channels: Isoform and species selectivity. D. M. Soderlund
- 9:50 235. Pyrethroid effects on sodium flux, calcium flux, and network activity assessed in cortical neurons. T. J. Shafer, Z. Cao, A. F. Johnstone, S. Losa, T. F. Murray
- 10:15 Intermission
- 10:30 236. Evaluating tools and models used for quantitative extrapolation of in vitro to in vivo data for neurotoxicants. M. Chan, M. J. DeVito, T. Shafer, M. F. Hughes
- 10:55 237. Structure-activity relationship models of human CYP450 and UGT metabolism. R. Fraczkiewicz, K. Enslein
- 11:20 238. Quantitative structure-activity relationships for organophosphate enzyme inhibition. C. Ruark, E. Hack, P. Robinson, P. Anderson, J. Gearhart

THURSDAY AFTERNOON

Endangered Species Act and Pesticide Regulation: Scientific and Process Improvements

Scientific Advances

Financially supported by CropLife America, Dow AgroSciences, and Intrinsik Environmental Sciences J. Cowles, J. Jenkins, J. Johnston, K. Racke, T. Hall, Organizers

S. Jackson, B. McGaughey, Organizers, Presiding

Section A
Colorado Convention Center 710

- 1:25 Introductory Remarks
- 1:30 239. Approach for the assessment of indirect effects to threatened and endangered terrestrial species exposed to herbicides: Glufosinate case study. R. S. Teed, D. R. Moore, T. Hall, G. Sabbagh, R. L. Breton
- 1:55 240. Demography and modeling to improve pesticide risk assessment of endangered species. J. D. Stark
- 2:20 241. Consideration of nontraditional endpoints in the assessment of ecological risk under the Endangered Species Act. N. H. Golden, G. Noguchi
- 2:45 Intermission
- **3:05 242.** Using causal analysis to evaluate stressor effects on endangered species. A. Fairbrother, N. W. Gard, C. A. Menzie
- **3:30 243.** Data quality and relevance standards for risk assessment. **A. T. Hall**, J. Gagne, B. McGaughey
- 3:55 Panel Discussion: Scientific Advances

Agriculture and Air Quality: Emission Measurements and Models Reducing Agricultural Emissions

S. Hafner, C. Howard, R. Maghirang, *Organizers* L. Mc Connell, *Organizer, Presiding*

Section B Colorado Convention Center 712

- 1:30 244. Methods for reducing ammonia emissions from poultry litter. P. A. Moore, Jr.
- 1:50 245. Amendments and feed-through additive for gas and odor emission reduction from dairy manure samples. E. F. Wheeler, R. C. Brandt, A. A. Adviento-Borbe, M. L. Hile, A. N. Hristov, P. A. Topper, H. A. Elliott, M. V. Bruns

- 2:10 246. Feeding tannins to dairy cows abates ammonia emissions from barns and soils. J. Powell, M. J. Aguerre, M. A. Wattiaux
- 2:30 247. Swine manure odor reduction efficacy of a humic amendment . R. C. Brandt, E. F. Wheeler, H. A. Elliott, R. E. Mikesell, Jr.
- 2:50 248. Reduction of odorous VOC in phenolics solutions and swine manure slurry using soybean peroxidase and hydrogen peroxide.

 D. B. Parker, L. Cai, M. Olsen
- 3:10 Concluding Remarks

Parameters for Pesticide QSAR and PBPK/PD Models

QSAR Models and PBPK/PD Models

C. Timchalk, J. Knaak, R. Tornero-Velez, *Organizers* D. Chang, J. Olson, *Presiding*

Section C Colorado Convention Center 711

1:30 – 249. In silico strategies for modeling stereoselective hydrolysis rates of pyrethroids. **D. T. Chang**, M. Goldsmith, R. Tornero-Velez, L. Chen, E. Ulrich, A. B. Lindstrom, C. C. Dary

- 1:55 250. Computational approaches for developing informative prior distributions for Bayesian calibration of PBPK models. J. L. Davis, R. Tornero-Velez, R. Setzer
- 2:20 251. Use of CYP-specific parameters and human biomarker data to develop a human PBPk/PD model for dermal chlorpyrifos exposure. J. R. Olson, C. A. Ellison, J. B. Knaak, R. McDougall, M. R. Bonner, P. J. Lein, F. M. Farahat, W. K. Anger
- 2:45 Intermission
- 3:00 252. Age-dependent, physiologically based pharmacokinetic/pharmacodynamic (PBPK/PD) modeling of organophosphorus (OP) insecticides in the preweanling rat: Implications of localized brain metabolism. C. Timchalk
- **3:25 253.** Bayesian calibration of carbaryl cholinesterase inhibition using physiologically-based pharmacokinetic and pharmacodynamic modeling. **A. Nong**, M. Yoon, H. J. Clewell
- 3:50 254. Use of in vitro data in PBPK models: An example of in vitro to in vivo extrapolation with carbaryl. M. Yoon, G. L. Kedderis, Y. Yang, B. C. Allen, Z. Yan, H. J. Clewell

AGRO DIVISION

AGRO 1

Use of 3D force field analysis as a tool for understanding molecular binding mechanisms

Scott H Jackson, scott.jackson@basf.com. Stewardship and Strategy, BASF Corporation, Research Triangle Park NC 27587

Scientists have worked to develop software which can accurately predict and model the behavior of molecules as they interact in the environment. A method is presented using molecular 3D interactions with clay lattice and organic matter structures by van der Waals and electrostatic forces. The method specifically allows the user to develop a detailed understanding of molecular binding mechanisms with clay lattice and organic structures that comprise soil. Preliminary results indicate that the method is capable of successfully predicting compound sorption/adsorption behavior using 3D force field methods based on the limited set of compounds evaluated.

AGRO 2

Effects of aging on retention, transport, and transformation of pesticides in soil

William C Koskinen, koskinen@umn.edu. Soil and Water Management Research Unit, USDA-Agricultural Research Service, St. Paul MN 55108

Aging has been shown to affect the sorption of pesticides in the soil which in turn can affect transport and transformation processes. Aging effects have been characterized by batch sequential extraction methods in which sorption coefficients (i.e., K_d) are determined for the chemical remaining after a given equilibration or incubation period. K_d 's have generally been shown to increase with aging time. Mechanisms that result in aging effects on sorption processes are unclear, but may be the result of decreased amounts of pesticide in the soil (when Freundlich 1/n < 1.0) or to changes in binding processes. Regardless of the mechanisms involved, aging may affect the prediction of pesticide transport and transformation processes and subsequent environmental risk. For instance, observed increases in sorption during pesticide aging should be taken into account during characterization of the sorption process for mathematical models of pesticide transport. Potential transport would be over predicted if fresh K_d 's were used to predict transport rather than aged K_d 's, resulting in a prediction of increased environmental risk. Possible aging affects on degradation is still unanswered. In spite of increased K_d 's, aging had no effect on some pesticide degradation by specific degrading microorganisms.

AGRO 3

Formation of soil- and sediment-bound residues of sulfonylurea herbicides and their relevance in environmental risk assessments: A case study

Richard Allen⁽¹⁾, richard.allen@valent.com; Reinhard Fischer⁽²⁾; David Judge⁽³⁾. (1) Valent Technical Center, Valent USA Corporation, Dublin CA 94568 (2) Environmental Safety, Bayer CropScience AG, Monheim 40789, Germany (3) Department of Natural Sciences, Gardner-Webb University, Boiling Springs NC 28017

The differential selectivity achieved with variation in chemical structure of sulfonylurea herbicides also influences their behavior in the environment. This presentation reviews differences in the formation of soil-and sediment-bound residues of sulfonvlurea herbicides and presents, as a casestudy, the investigations to understand formation of this fraction from foramsulfuron, which was shown in standard laboratory studies to form a soil-bound residue of greater than 90%. These studies demonstrated that the bound fraction was a consequence of microbial breakdown via a primary metabolite which became associated with the soil organic matter. Due to the significant formation of bound residues a compound-specific risk assessment was conducted that evaluated the potential effects on non-target organisms in soil and sediment. This in-depth study of the mechanism of formation and potential exposure and risk assessment demonstrated that no adverse effects would result from the bound residue formed from the degradation of foramsulfuron in the environment.

AGRO 4

¹⁵N-NMR studies on the reaction of aromatic amines with soil organic matter to form bound residues

Kevin A Thorn, kathorn@usgs.gov. Water Discipline, US Geological Survey, Denver CO 80225-0046

Aromatic amines result from chemical and microbial transformation of nitroaromatic munitions and several classes of pesticides. Covalent binding of aromatic amines to soil organic matter (SOM) has long been recognized as one of the pathways for the formation of bound residues. In laboratory reactions, solid and liquid state ¹⁵N-NMR spectroscopy has been used to determine the types of covalent bonds formed between SOM and $^{\rm 15}{\rm N\text{-}labeled}$ aromatic amines of varying nucleophilicity and substitution patterns under both noncatalyzed and enzyme- and metalcatalyzed conditions. Spectra have revealed differences in the distribution of condensation products for the various amines. Solid state ¹⁵N NMR spectroscopy has also been used in whole soil and compost studies to differentiate pathways of transformation and bound residue formation from mineralization and microbial immobilization. Incorporating the results from NMR studies into structure and reactivity and environmental fate models remains a future challenge.

How do laboratory assessments of S-metolachlor sorption and dissipation agree with field behavior?

Sharon K. Papiernik, sharon.papiernik@ars.usda.gov; Alegria Cabrera⁽²⁾; William C. Koskinen⁽³⁾. (1) North Central Agricultural Research Laboratory, USDA-Agricultural Research Service, Brookings SD 57006 (2) Institute for Natural Resources and Agrobiology, Sevilla, Spain (3) Soil and Water Management Research Unit, USDA-Agricultural Research Service, St. Paul MN 55108

Research has suggested that existing bonds become stronger with aging time, decreasing the extractability and bioavailability of some pesticides in soil. We found that using high-energy extraction conditions (elevated temperature and pressure in ASE) removed a higher proportion of sorbed Smetolachlor, which influenced calculated distribution coefficients and masked the aging effect. The difference in K_d values for manual extraction and ASE did not affect Smetolachlor dissipation rates. High-efficiency methods are advantageous from an analytical standpoint, but the significance of residues removed under harsh conditions in determining pesticide availability for mobility and biological uptake is unknown. The results of these laboratory tests are consistent with companion field studies. Together, they show that despite large differences in soil properties and sorption coefficients, dissipation proceeded at approximately the same rate (and weed control was the same) in soils from different landscape positions. Equilibrium processes may not drive dissipation and bioavailability under field conditions.

AGRO 6

Use of stable isotopes to predict HOC bioavailability in sediments

Laura I Delgado Moreno, Imoreno@ucr.edu; Jay Gan. Department of Environmental Science, University of California-Riverside, Riverside California 92521

Hydrophobic organic contaminants (HOCs) bioavailability is reflected in both the freely disolved concentration (Cfree) and what is available via desorption. Chemical methods for predicting HOC bioavailability in soils or sediments are based on partial extraction (mild solvent extraction, Tenax, cyclodextrin) or the measurement of Cfree at equilibrium (dialysis membranes, passive samplers). We explored the use of deuterated HOCs through isotope exchange to estimate the isotopically exchangeable pool (E) as an approximation of bioaccessibility. Bifenthrin and pyrene were selected as model HOCs. Sediments with different organic carbon content (0.8 - 4.5%) were considered. Results indicate that E values were significantly correlated (P < 0.05) with C_{free} measured by PDMS or the 6-h desorption measured by Tenax. HOCs bioaccumulation by Chironomus tentans was better estimated by the E values. In conclusion, the use of deuterated compounds overcomes shortcomings in the current estimation methods and expands our ability to predict HOC bioavailability in sediments.

Comparing pesticide distribution between formulated and natural sediments

Xinyi Cui⁽¹⁾, lizzyc@ucr.edu; Jeffrey M Giddings⁽²⁾; Jay Gan⁽¹⁾. (1) Department of Environmental Science, University of California-Riverside, Riverside California 92507 (2) Compliance Services International, Rochester MA 02770

Formulated sediments are recommended for toxicity testing of hydrophobic compounds in OECD guidelines. The organic carbon in peat may qualitatively differ from that in natural sediments, which may lead to different chemical distribution among the solid, dissolved organic matter (DOM), and water phases, and consequently, different toxicity effects. To test the validity of using formulated sediments in lieu of natural sediments, this study compared OECD formulated sediments with natural sediments in terms of (a) partitioning of 8 pyrethroids between sediment and water phases determined by batch adsorption; and (b) phase distribution of pyrethroids among the sediment phase, porewater, and overlaving water under conditions mimicking sediment toxicity tests. Solid-phase microextraction (SPME) was used to determine the freely dissolved concentration. Sediment properties of the 5 natural sediments and 3 formulated sediments were characterized and the characteristics were used for explaining differences observed in partition and phase distribution of pyrethroids in these sediments.

AGRO 8

AGRO 7

Use of passive sampling devices to estimate the bioavailability of pyrethroids

Kelly O'Neal, kloneal@ncsu.edu; Damian Shea. North Carolina State University, Department of Biology, Raleigh NC 27695-7617

Following the withdrawal of organophosphates there has been a significant shift towards the use of pyrethroid insecticides. With this increased usage, concern has arisen about the risks pyrethroids may pose to aquatic ecosystems especially with measured concentrations in surface waters often exceeding toxicity thresholds for aquatic invertebrates. However, we and others have found that these apparently toxic concentrations of pyrethroids often do not exhibit toxicity in the field. We will report on laboratory and field experiments demonstrating that one reason for this overestimation of field toxicity is the decreased bioavailability of pyrethroids. Our results also show that sorptive passive sampling devices (PSDs) provide a good estimate of the bioavailable fraction of cypermethrin and permethrin under most conditions. We will present a quantitative model of pyrethroid-organic carbon partitioning and its effect on bioavailability, and how PSDs can be used in the field to estimate chronic exposure to bioavailable pyrethroids.

Art of method development: Sensitive analytical methods for the trace residue analysis of crop protection chemicals in plant and environmental matrices using cutting edge technology

Manasi G Saha, manasi.saha@basf.com; Robert F Gooding; John E Jones. Chemistry, BASF Corporation, Research triangle Park North Carolina 27709

The tremendous demands for increasing sample throughput today driven by regulatory trends around the globe. Crop protection companies are continuously searching for new ways to improve the productivity and efficiency of residue analysis while simultaneously reducing the cost of these analyses. It is challenging, both from a time perspective and from technical constrains, to analyze thousands of samples collected from field dissipation and crop trial studies, using a sensitive, short, and rugged methods to quantitate multiple analytes. Automation and rapid analysis with high sample throughput can overcome the time challenge. Towards these goals, rugged analytical methods with limit of quantitation at 10 ppb were developed for several active ingredients and their relevant metabolites in soil, water, and plant. The state of the art technology for method development and associated challenges will be presented.

AGRO 10

Analyzing pesticide formulation adjuvants to assess their impact on pollinator health

Christopher A. Mullin, camullin@psu.edu; Timothy J. Ciarlo; Wanyi Zhu; Maryann T. Frazier; James L. Frazier. Department of Entomology, Center for Pollinator Research, The Pennsylvania State University, University Park PA 16803

Although we have found more than 130 different pesticides and metabolites in beehive samples, no individual pesticide amount correlates with recent bee declines. To examine if more generic formulation inerts that co-occur across classes of pesticides may be involved, we have identified, utilizing LC-MS, common adjuvants in pesticide formulations used around hives or where bees forage. Nonionic surfactants like Silwet L-77 and Triton X-100 were highly lethal to adult honey bees at 1% in artificial nectar while N-methyl-2pyrrolidone, although less toxic to adults, was more acutely toxic to the brood. The organosilicone Silwet L-77 at 0.1% significantly reduced learning performance of forager honey bees using the proboscis extension reflex assay. The impact of synergistic pesticidal blends on bees, which depend on plant nectars and pollens readily contaminated by pesticide treatments, cannot be fully understood without identification and risk assessment of formulation additives and other spray adjuvants.

AGRO 11

Mass spectrometry based, label-free proteomics: A case study for agricultural applications

Leah Riter, Isriter@monsanto.com; Pamela Jensen; Joan Ballam; Ewa Urbanczyk; Susan MacIsaac; Henry Valentin. Crop Analytics, Monsanto Company, Saint Louis MO 63167

The search for new crop protection chemicals with novel modes of action and improved safety profiles is a high priority in agrochemical research and development.

Proteomics, which may provide insights into mechanisms by examining changes in protein abundance, is an integral part of this endeavor. However, traditional gel-based, differential-quantitation methods dominate the plant proteomics literature, indicating that this method is still the core technology utilized in plant proteomics mode of action studies. This presentation will focus on our recent development of mass spectrometry based, label-free proteomics methods to characterize corn tissue. Data will be presented from work that examined the impact of numerous factors, including experimental design, data acquisition, and data processing on the analytical performance of this new method. The application of this method to biologically-relevant questions was tested; selected data will be shown.

AGRO 12

Analytical challenges for the analysis of pyrethroids at trace residue levels

Del A. Koch⁽¹⁾, kochd@abclabs.com; Kevin L. Clark⁽²⁾; Daniel M. Tessier⁽³⁾; Chung Lam⁽⁴⁾. (1) GLP & Synthesis Services, ABC Laboratories, Columbia MO 65202 (2) Morse Laboratories, LLC, Sacramento CA 95825 (3) Stine-Haskell Research Center, DuPont Crop Protection, Newark DE 19711 (4) Bayer CropScience, Stilwell KS 66085

Pyrethroid insecticides have unique characteristics which provide challenges in sampling, preservation, extraction/isolation, and analysis. They are currently being investigated because of reported detections in surface waters, waste water effluent and sediments, and associated biological activity. It is thus important to have a consensus between research groups regarding strengths and weaknesses of various analytical approaches. In order to best evaluate the effects of pyrethroids at low concentrations, methods which are sensitive, specific, rugged, and reproducible are necessary, especially for challenging matrices (e.g., sediment and sludge). Although water is often considered an easier matrix, very low water solubilities, and the tendency to adhere to surfaces, present sampling, and analytical challenges. The presentation will discuss different extraction/cleanup methods and instrumental approaches, with recommendation of basic analytical procedures meeting the desired criteria of high sensitivity/specificity, plus ruggedness/reproducibility. The talk will address opportunities for collaboration in the further development of recommended methodologies.

AGRO 13

Improved LC-MS/MS analysis of dicamba and its major metabolites in soy and cotton matrices

James E Foster, james.e.foster@monsanto.com; Chad E Wujcik. Environmental Sciences, Monsanto Company, St. Louis MO 63167

Early dicamba residue methods involved the use of hazardous methylating reagents to derivatize and convert metabolites to common chemophores for GC-ECD analysis. New methodologies developed at Monsanto avoided derivatization and, through acid hydrolysis, allowed for dicamba residues to be quantitated by direct analysis of dicamba, 5-hydroxydicamba, 3,6-dichlorosalicylic acid (DCSA) and 3,6-dichlorogentisic acid (DCGA) using LC-MS/MS. A significant degree of manual labor was still required for sample processing and cleanup which limited sample throughput and was more susceptible to human error. Further improvements to the methodology were

gained through more rigorous sample milling and homogenization which allowed for the procedure to be scaled down and processed in a more uniform automated format. These and other modifications led to a 3-fold increase in sample throughput with less manual-related effort as well as reductions in cost associated with materials and waste. Additionally, decreases in overall chromatographic run time have further increased the net method throughput.

AGRO 14

Analytical issues with ion suppression and enhancement in the quantitative analysis of small molecules in various matrices

Larry Mallis, Larry.Mallis@criticalpathservices.com; Connell Cunningham, Jr; Julie Eble. Analytical, Critical Path Services, LLC, Garnet Valley PA 19060

The use of LC in tandem with MS/MS continues to be a powerful tool in the quantitative analysis of pesticides and other small molecules. The much higher selectivity gained with this tool vis-a-vis LC/UV and GC approaches has allowed method development, validation, and analysis times to be dramatically reduced. Although the detection technique is extremely selective, substances present in the sample extract, while eluting unseen by the detector, can create mischief in the ionization source. These types of interferences, e.g., phospholipids, can lead to irreproducible results which can go undetected during method validation. Approaches to determining matrix effects will be discussed. Examples of suppression/enhancement will be presented along with possible analytical solutions including the use of stable-label isotopes.

AGRO 15

LC/MS/MS, GC/MS, and GC/MS/MS methods for the analysis of pesticides and their degradation products in air and water samples

Renata Raina, renata.raina@uregina.ca; Lina Sun; Michele Etter; Nicole Fergus; Erika Smith; Patricia Hall. Department of Chemistry and Biochemistry, University of Regina, Regina Saskatchewan S4S 0A2, Canada

New developments in LC/MS/MS, GC/MS, and GC/MS/MS methods for the analysis of a range of pesticides in air and water samples will be presented. Analytical methods have been developed for specific chemical classes of pesticides. Pesticides include organochlorines (OCs), organophosphorus pesticides (OPs), phenoxyacid herbicides, N-trihalomethyl fungicides, carbamates, phenylureas, triazoles, sulfonylureas, and other selected pesticides. The new LC/MS/MS methods have been developed to analyze pesticide active ingredients and their degradation products simultaneously for chemical classes including OPs, phenoxyacid herbicides, carbamates, and triazoles. New LC columns, mobile phase composition, and post-column reagent addition to improve selectivity of separation or MS sensitivity will be discussed. GC/MS methods also include use of large-volume, cold, on-column injection and PTV dirty matrix injection. Selected samples taken from air and water will be presented to illustrate capabilities of the various methods.

AGRO 16

High throughput analysis of glyphosate and aminomethylphosphonic acid in raw agricultural commodities

Nakia R. Smith, nakia.r.smith@monsanto.com; J. Mark Allan; Chad E. Wujcik. Department of Environmental Sciences Technology Center, Monsanto, St. Louis MO 63167

The direct quantitation of glyphosate, a non-selective herbicide, and its main degradation product aminomethylphosphonic acid (AMPA) in various raw agricultural commodities (RACs) has been complicated by the ionic nature of these analytes, the lack of sensitive and detectable structural moieties, and their propensity to interact strongly with stainless steel surfaces. Most analytical procedures involve derivatization and extensive sample cleanup. A simplified LC-MS/MS method has been developed that overcomes or minimizes many of these challenges while dramatically increasing sample preparation throughput. The optimization of sample homogenization was identified as a key component to enabling the scale-down of extraction and processing. The utilization of phosphoric acid as a sample extraction modifier was found to have supplemental benefits in minimizing the interactions with stainless steel surfaces that broaden peaks, increase tailing, and can affect injection carryover. This new methodology is capable of measuring underivatized glyphosate and AMPA down to 0.05 ppm in RAC samples.

AGRO 17

Aquatic exposure modelling for exposure assessment in support of the regulation of pest control products in the Canada

Greg Malis, greg.malis@hc-sc.gc.ca; Ian Kennedy; Lizanne Avon; Émilie Larivière. Environmental Assessment Directorate, Pest Management Regulatory Agency, Ottawa Ontario K1AOK9, Canada

Estimating concentrations of pesticides in water bodies is an integral part of the risk assessment process conducted by the Pest Management Regulatory Agency (PMRA). The PMRA has developed an approach for estimating pesticide concentrations in relationship to proposed and registered pesticide application practices across Canada. Pesticide concentrations in surface water and groundwater are estimated over a multi-year period for a series of agricultural scenarios that are typical of the major crop-growing areas in Canada utilizing regional meteorological data, characterisation of soils and crops, and chemistry and environmental fate data identified or calculated within the PMRA review process. For surface water, PMRA uses the linked models, PRZM (Pesticide Root Zone Model) and EXAMS (Exposure Analysis Modelling System) and for groundwater, PMRA uses the Leaching Estimation and Chemistry Model (LEACHM) model. These estimates are used to assess risks to human health and the environment in the context of regulatory decisions.

Spatially distributed pesticide exposure assessments in the Central Valley, California

Yuzhou Luo⁽¹⁾⁽²⁾, yluo@cdpr.ca.gov; Darren L. Ficklin⁽¹⁾; Eike Luedeling⁽¹⁾; Sarah E. Gatzke⁽¹⁾; Minghua Zhang⁽¹⁾. (1) Department of Land, Air, and Water Resources, University of California, Davis CA 95616 (2) Department of Pesticide Regulation, California Environmental Protection Agency, Davis CA 95616

A series of modeling studies have been conducted to evaluate the exposure and risk of organophosphate pesticides (OPs) in California's Central Valley, one of the most productive areas in the world. Spatiotemporal variability of pesticide distributions at both field and water scales are investigated with regards to their potential impacts on aquatic ecosystem and human health. Results provide strong evidences that surface runoff generation and pesticide application timing are the two influencing factors on the variability of OP sources from agricultural fields. By incorporating management-oriented sensitivity analysis, modeling results recommend structural best management practices for reducing soil erosion and sediment-transport capacity to be implemented in the study area. The resulting model is also used to assess the impact of climate change and to quantify the response of pesticide runoff on the variations of CO₂ concentration, temperature, and precipitation. The developed modeling framework is anticipated to facilitate watershed management and pesticide mitigation.

AGRO 19

Exploring approaches to Pesticide Aquatic Ecological Exposure Assessment: Issues in evaluating risk across the national landscape

Ronald D. Parker, parker.ronald@epa.gov; Michael R Barrett; Mohammed Ruhman. Office of Pesticide Programs, Environmental Fate and Effects Division, US Environmental Protection Agency, Washington DC 20460

The EPA Office of Pesticide Programs typically uses one or a few Pesticide Root Zone Model (PRZM) surrogate cropping scenarios to represent aquatic exposure for ecological risk assessment. Each surrogate scenario is used to represent all of the other sites on which a specific pesticide treated crop is grown. New modeling techniques will soon allow simulating most of the national agricultural landscape, possibly eliminating the need to rely on use of surrogate scenarios. These new capabilities will also pose new issues which will need to be addressed to assure the resulting risk assessment presents an accurate representation of national risk. This talk presents a variety of issues with the goal of stimulating that discussion. Issues addressed include land-to-water ratios, static versus flowing water, and addressing sediment exposure issues.

AGRO 20

Evaluation and refinements to Tier 2 US EPA drinking water risk assessments: Methods to improve modeling scenarios

Nathan Snyder⁽¹⁾, snydern@waterborne-env.com; Aldos Barefoot⁽²⁾. (1) Engineering, Waterborne Environmental Inc., Leesburg VA 20175 (2) Environmental Safety Assessment, Dupont Crop Protection, Newark DE

Evaluation of crop protection products for US registration requires the use of a standard modeling process that combines information about the environmental fate, anticipated use patterns, and toxicological data of a product. Implementing the modeling tools within the standard set of shells, while adequate for many products, may lead to assumptions that do not match the reality of actual use patterns for some products. Common short-comings can be overcome using the core models in their native forms and custom tools that allow refinements within the US EPA Tier 2 modeling framework. Methods to address multiple crop seasons and mixed application methods currently not available in the standard tools will be reviewed. In drinking water assessments, methods to address mixed major and minor crop can be shown to represent the mixed application dates and methods associated with minor crops in the United States.

AGRO 21

Meta-modeling of the pesticide fate model PRZM for aquatic risk assessment

Yuzhou Luo, yluo@cdpr.ca.gov; Frank Spurlock; Xin Deng; Sheryl Gill; Kean Goh. California Environmental Protection Agency, Department of Pesticide Regulation, Sacramento CA 95814

A simple use-exposure relationship is developed based on regression analysis of stochastic simulation results generated from the Pesticide Root-Zone Model (PRZM). The developed mathematical relationship estimates edge-of-field pesticide exposures from aerobic soil metabolism half-life, organic carbon-normalized soil sorption coefficient, and application rate. In a case study of California crop scenarios, the relationships explained 90 - 95% of the variances as predicted by PRZM simulations for a 30-year period. Koc was identified as the governing parameter in determining the relative magnitudes of pesticide exposures. The effects of chemical fate processes, such as partitioning and degradation, on pesticide exposure were similar among crop scenarios, while the cross-scenario variations were mainly associated with the landscape characteristics, such as organic carbon contents and curve numbers. With a minimum set of input data, the use-exposure relationships proposed in this study could be used in screening procedures for potential water quality impacts from the off-site movement of pesticides.

Use of modeling and monitoring in pesticide exposure assessments in a regulatory context

Michael R Barrett, barrett.michael@epa.gov; Ronald D Parker. Office of Pesticide Programs, Environmental Fate and Effects Division, US Environmental Protection Agency, Washington DC 20460

In the pesticide registration process, regulatory agencies typically rely on models to predict aquatic exposure informed by pesticide property and environmental fate data required for product registration. Monitoring data may be used to inform exposure assessments further, or the data may be used to evaluate, refine, or change predictive models. Accurate model prediction of exposure from ground or surface water sources in a regulatory context is complicated by the need to be conservative (protective) while dealing with uncertainties about future usage trends, local environmental factors, and multiple risk prevention goals. Use of monitoring data may be constrained by practical limits to sampling diversity and intensity and to the collection of contextual data crucial to interpretation of the significance of the sampling results. Examples of the dynamics of the use of monitoring and modeling results for risk assessments will be discussed.

AGRO 23

Prioritizing research and regulatory initiatives to minimize pesticide impacts on threatened and endangered species in California's Central Valley

Debra L. Denton⁽¹⁾, Denton.Debra@epamail.epa.gov; Richard S. Breuer⁽²⁾; W. Martin Williams⁽³⁾; Gerco Hoogeweg⁽³⁾; Minghua Zhang⁽⁴⁾. (1) Standards and TMDL Office, US Environmental Protection Agency, Region 9, Sacramento CA 95814 (2) California Department of Water Resources, Sacramento CA 95691 (3) Waterborne Environmental, Inc., Leesburg VA 20175 (4) Department of Land, Air, and Water Resources, University of California, Davis, Davis CA 95616

An ecological risk assessment was performed for California's Central Valley to rank the relative risk potential for pesticides to impact threatened or endangered species. The study utilized monitoring data, simulation modeling, and GIS to address the temporal and spatial co-occurrence of forty widely-used herbicides, fungicides, and insecticides to twelve aquatic and semi-aquatic species, including several species of Chinook salmon (Oncorhynchus tshawytscha), Central Valley steelhead (O. mykiss), southern North American green sturgeon (Acipenser medirostris), Delta smelt (Hypomesus transpacificus), striped bass (Morone saxatilis), San Francisco longfin smelt (Spirinchus thaleichthys), threadfin shad (Dorosoma petenense), California red-legged frog (Rana draytonii), and the California freshwater shrimp. Results are being used to improve decision making and to optimize resource spending across a number of federal, state, and regional water quality programs. The results can be used to identify and to rank areas of highest risk, to aid in placement of BMPs, and to support current and future monitoring programs, specifically strategic placement of sampling locations and frequency.

AGRO 24

Aquatic exposure modeling for registration of crop protection products in the European Union

Kristian W Paul⁽¹⁾, kristian.paul@usa.dupont.com; Neil Mackay⁽²⁾; Russell L Jones⁽³⁾; Aldos Barefoot⁽¹⁾. (1) DuPont Crop Protection, Newark Delaware 19714-0030 (2) DuPont (U.K.) Limited, Stevenage Hertfordshire, United Kingdom (3) Bayer CropScience, Stilwell Kansas 66085-9104

The regulatory requirements for performing aquatic exposure modeling for European Union and Member State approvals of crop protection products are well-defined. Nevertheless, the regulatory framework continues to evolve due to the adoption of newer scientific advances and increasingly stringent risk assessments. In this presentation, several key aspects of aquatic exposure modeling performed to register and to support crop protection products in the European Union for Annex I inclusion will be discussed. In particular, the various models and modeling frameworks used for Annex I inclusion will be examined. Mitigation options and strategies for reducing exposure via the entry routes spray drift and run-off will be explored, in conjunction with label language that can be used to support these various mitigation options.

AGRO 25

Evolving strategies in insecticide discovery: A career perspective

George P Lahm, george.p.lahm@usa.dupont.com. Crop Protection, Stine Haskell Research Center, E. I. DuPont, Wilmington DE

The strategies associated with the discovery of new insecticides have evolved over time. A constant theme has been the search for new leads through a variety of processes including traditional knowledge-based approaches as well as random screening in low and high volume screens, natural products, site-of-action assays, combinatorial chemistry, and other high volume chemistry sources. An evident result is that the application of synthetic organic chemistry and evolving synthetic methods have played a large role in the discovery process in combination with fundamental knowledge of agricultural chemistry and bioactivity principles. Specific current and historical examples relating to the discovery of new insecticides along with these evolving strategies will be discussed.

Diamide insecticides: New heterocyclic anthranilic derivatives

André Jeanguenat⁽¹⁾, andre.jeanguenat@syngenta.com, Schaffhauserstrasse, Stein Aargau 4332, Switzerland; Patricia Durieux⁽¹⁾; Andrew J. F. Edmunds⁽¹⁾; Roger G Hall⁽¹⁾; Livia van Innis⁽¹⁾; Olivier Loiseleur⁽¹⁾; Michel Mühlebach⁽¹⁾; Anthony O'Sullivan⁽¹⁾; Jagadish Pabba⁽²⁾; André Stoller⁽¹⁾; Stephan Trah⁽¹⁾; Jean Wenger⁽¹⁾; Ana C Dutton⁽³⁾. (1) Research Chemistry, Syngenta Crop Protection, Stein 4332, Switzerland (2) Research Chemistry, Syngenta Biosciences Private Limited, CORLIM ILHAS GOA Goa 403 110, India (3) Research Biology, Syngenta Crop Protection, Stein 4332, Switzerland

The anthranilic diamides, a new class of insecticides, are activators of the ryanodine receptors (Ca channels). They have excellent toxicity and ecotoxicity profiles due to specific interaction with insect receptors. Novel anthranilamides were prepared based on pharmacophore analysis. They have excellent *in vitro* activity and have showed a broad insecticidal spectrum *in vivo*, controlling lepidopteran, coleopteran, and hemipteran pests at low concentrations. The synthesis of heterocyclic anthranilic analogues and of sulfoximine derivatives will be presented as well as structure/activity trends.

AGRO 27

Design, synthesis, and properties of acyclic spiroindoline insecticides

Peter Maienfisch, peter.maienfisch@syngenta.com; Jerome Cassayre; Fredrick Cederbaum; Camilla Corsi; Louis-Pierre Molleyres; Thomas Pitterna; Elke Hillesheim. Crop Protection Research, Syngenta Crop Protection AG, Basel CH-4002, Switzerland

Spiroindolines are a recently discovered class of insecticides which originated from a weak screening hit. A initial optimization program led to the discovery of SYN876, a new exploratory insecticide for the control of lepidoptera. This talk will review the evolution of this area and focus specifically on the design, synthesis, insecticidal activity, and structure-activity trends of acyclic analogues of SYN876. This work resulted in the identification of SYN380 – a compound with improved activity against lepidopteran pests.

AGRO 28

Benzisothiazoles: A versatile source for new insecticide leads

Wolfgang von Deyn⁽¹⁾, wolfgang.deyn@basf.com; Sebastian Soergel⁽¹⁾; Vincent Salgado⁽²⁾; Barbara Wedel⁽²⁾. (1) BASF SE, Ludwigshafen 67056, Germany (2) BASF Corporation, Research Triangle Park NC 27709

1,2-Benzisothiazoles have been known as useful scaffolds in the field of crop protection for several years. A number of herbicide patents based on this structural element have been published. Recently it has been shown that 3-acetylamino-1,2-benzisothiazoles have the potential as insecticides for foliar and seed treatment use. However, the pest spectrum of these derivatives seemed to be limited to aphid species. Further evaluation of the benzisothiazole chemistry led to the discovery of novel structure types which

offer a broader scope of insecticidal activity. This shift in spectrum could be attributed to a different mode of action of the new analogs. Synthesis, biology, and structure-activity relationships of insecticidal 1,2-benzisothiazoles will be presented herein.

AGRO 29

Managing lands to retain and sustain biodiversity

Gwen Kittel, gwen_kittel@natureserve.org. Conservation Science, NatureServe, Boulder CO 80303

NatureServe provides the scientific basis for effective conservation action, enabling more informed management of species, lands, and natural resources. Our vision is to help people recognize and value the importance of biodiversity. For well over thirty years, NatureServe, along with its network of natural heritage programs throughout the western hemisphere, has tracked the health of rare and endangered species and ecosystems; we are seen as leaders in the area of conservation planning, ecosystem mapping, and watershed assessments. Our tools and expertise can be employed to help manage natural, agricultural, and forest lands for the highest biodiversity possible. Current activities include working with state and federal transportation agencies to plan for more effective and cost-efficient mitigation and with the forestry industry for sustainable certification of wood products. Better management of all lands can result in sustained health of our natural heritage which supports prosperous human communities for the benefit of current and future generations.

AGRO 30

Strategies for minimizing unintended effects of pesticides on biodiversity

Bernalyn McGaughey,

bmcgaughey@complianceservices.com; Larry Turner; Jim Gagne; Jeff Giddings. Department of Business Services, Compliance Services International, Lakewood WA 98499

Pesticide use is directed by the Federal label for a variety of agricultural and non-agricultural applications. To protect local, sensitive habitats or consider special local conditions, use of pesticides in agricultural settings is occasionally affected or further evaluated by state and local programs, and use in non-agricultural settings is often directly controlled by additional layers of regulation. Non-agricultural sites consist primarily of utility and other rights-of-way, e.g., roads, pipelines, industrial facilities, and railroads. To examine these strategies for further mitigation, local considerations involving diruon use or assessment will be examined. Separate from label requirements, certain limits exist on diuron usage at the Federal, state, county, and local levels, plus temporary limitations on diuron usage resulting from court orders and injunctions. Illustrations will show how the added regulatory programs address the local landscape and unique local programs.

Using herbicides to promote native plant communities

George Beck, George.Beck@Colostate.edu; Scott Nissen; James R Sebastian. Colorado State University

Invasive weeds are aggressive and displace native plants, especially forbs and shrubs. Herbicides decrease abundance of invasive weeds but concerns over disruption of native biodiversity sometimes preclude their use. In an experiment conducted in the foothills along Colorado's Front Range with aminocyclopyrachlor applied in late spring at 35, 70, and 140 g ha⁻¹, results showed that native forb and shrub richness decreased 22 to 44% and 33 to 75%, respectively. Cool- and warm-season grass richness did not change, although warm-season grass abundance increased up to 227%. In another experiment where aminocyclopyrachlor was used to decrease Russian knapweed (Acroptilon repens) abundance, 15 of 16 seeded native forbs, shrubs, and grasses successfully established compared to three species in non-treated control plots. These data show that herbicides can be used to decrease invasive weed abundance while providing native plant communities with an opportunity over time to recover and to conserve native biodiversity.

AGRO 32

Indirect effects of forest herbicides on wildlife: A literature review

Vickie L. Tatum⁽¹⁾, vtatum@src-ncasi.org; Gary J. Roloff⁽²⁾; Laurie A. Clark⁽³⁾; Larry L. Irwin⁽³⁾. (1) Southern Regional Center, National Council for Air and Stream Improvement, Newberry FL 32669 (2) Department of Fisheries and Wildlife, Michigan State University, East Lansing MI 48824 (3) Western Wildlife Program, National Council for Air and Stream Improvement, Tenmile OR 97481

Direct effects of contemporary herbicides on non-target biota are well documented. Comparatively little information exists on indirect effects on wildlife and their habitats. Our literature review indicated that: 1) general vegetation structure recovers ≤ 3 years following treatment, 2) generalized statements about wildlife response are inappropriate because vegetation and wildlife responses are site-, species-, and herbicide formulation-specific, 3) wildlife may be affected by altering forage species, 4) rate and extent of wildlife community response is implicitly linked to vegetation community dynamics, and 5) multiple vegetation control treatments may have greater indirect effects than single treatments. Information needs include: 1) long-term monitoring of biotic communities at multiple scales, 2) effects of herbicides (at field application rates) on habitats of sensitive wildlife taxa, 3) interactive effects of multiple and other silvicultural treatments, and 4) environmental effects (potentially synergistic) of evolving formulations, tank mixes, adjuvants, and surfactants.

AGRO 33

Biodiversity and landscape management in and around banana plantations in the humid tropics of Latin America

Peter John Edwards⁽¹⁾, peter.edwards@syngenta.com; Ronald Vargas⁽²⁾. (1) Environmental Safety, Syngenta, Bracknell Berkshire RG42 6EY, United Kingdom (2) P.O. Box 199-3017, Agriban, Heredia, Costa Rica

Bananas are the world's fourth most-valuable food crop with about 90% grown in tropical regions. Bananas, more than most agricultural crops, are affected by pests and diseases that require chemical control. The most important disease is Black Sigatoka (Mycosphaerella fijiensis) and requires about 20 - 40 aerial applications of fungicide each year. In addition, there are significant pesticide programs to manage weeds and nematodes. The history of banana cultivation is also controversial with respect to rainforest and its fragmentation. Syngenta funded work to support the banana industry in Latin America by an evaluation of biodiversity in banana plantations in Costa Rica and on the diversity and productivity of birds in rainforest fragments surrounding the plantations with the aim of producing management recommendations to growers. Much of the biodiversity in these plantations is associated with a network of channels draining the plantations into the river system. Some growers have planted indigenous species along these channels to improve bank integrity and biodiversity and to intercept fungicide. In the Syngenta study, litter degradation and invertebrate fauna associated with the degradation of banana plants were measured. Forest margins and adjacent rainforest fragments were censused for birds, and capture and colour marking were used to measure diversity and age structure of bird populations. Juvenile birds of most species were caught indicating these margins and fragments were breeding (source) habitats for many species. Soil respiration and banana plant litter degradation were active through the combination of microorganisms and a fauna of detritivores and associated predators including ants, spiders, lizards, and amphibians. Intelligent management in plantations through planting along canals and rivers with a view to improving connectivity is likely to improve biodiversity and help sustain many of the existing populations. The presentation with provide evidence and illustrate the findings and recommendations.

AGRO 34

Use of aquatic herbicides to enhance biological diversity in natural and managed ecosystems

Kurt Getsinger, Kurt.D.Getsinger@usace.army.mil. Research and Development Center, US Army Engineer, Vicksburg MS 39180

While much attention is placed on the risks and negative impacts of pesticide use on biodiversity, the alternative outcome of beneficial effects on ecosystems must also be considered. One emerging benefit is a method of herbicide application being used to control invasive plants selectively in natural and managed aquatic ecosystems. This species-selective approach can greatly reduce invasive plant populations, while allowing valuable native vegetation to thrive. Herbicide selectivity is driven by chemistry mode-of-action, application rate and techniques, and timing of treatments. For submersed plant control, herbicide-specific aqueous concentration and exposure time relationships are linked to phenological events of target and non-target

plants, matching this information with site-specific water exchange processes, and application technologies. When this prescriptive treatment approach is employed in the field, successful and selective control of invasive plants has been demonstrated – enhancing fish and wildlife habitat and overall biological diversity. In addition, habitat for endangered and threatened species has been improved and preserved using this operational strategy.

AGRO 35

Overview of issues in aquatic exposure modeling in the US EPA Office of Pesticide Programs, Environmental Fate and Effects Division (EFED)

Donald Brady, brady.donald@epa.gov. Environmental Fate and Effects Division, US Environmental Protection Agency, Office of Pesticide Programs, Washington DC 20460

In the globalized pesticide regulatory environment in which we increasingly find ourselves, we see that not only are there new challenges but even more there are new opportunities. We in the EPA Office of Pesticide Programs Environmental Fate and Effects Division (EFED) are exploring how we might use the newly available technologies and capabilities to meet the challenges of evolving international public policy in the arena in regulation of pesticides. As an organization, we need to continue to assure that both new and currently-registered pesticides continue to meet the statutory standard of no unreasonable adverse effects to human health and to the environment and to confirm that pesticidal products in the marketplace can be used safely. This talk describes how we see these new and evolving challenges and as well as the increasing opportunities and explores our possible responses to them.

AGRO 36

Integrating regulatory risk assessments, risk management, and best management practices to achieve the water quality objectives of the European Union: A long term initiative of the European Crop Protection Association (ECPA)

Richard Allen, richard.allen@valent.com. Valent Technical Center, Valent USA Corporation, Dublin CA 94568

The thematic strategy on the sustainable use of pesticides was adopted in 2006. ECPA considers this strategy and, together with the associated water framework directive, requires industry and regulators to develop an integrated approach to aquatic risk assessment, management, and promotion of best farming practices. A component of this initiative is to develop measures to reduce the potential for contamination of surface waters from diffuse sources, which can be implemented in regulatory decision making and become the basis for best management practices. The key drivers for evaluating the effectiveness of vegetative buffer strips have been integrated into the model VFSMOD-W. Scenarios and a tool to integrate into European surface water exposure methods used in aquatic risk assessments are in development. Existing spray drift reduction technology measures have been summarized in a database in order to broaden the adoption of these technologies in risk assessments and in practice throughout the region.

AGRO 37

Effects of input uncertainty on VFSMOD modeling of water, sediment, and pesticide trapping by vegetative filter strips

Solomon M Folle⁽¹⁾, solomon@stone-env.com; Michael F Winchell⁽¹⁾; Tammara L Estes⁽¹⁾; Katie A Budreski1⁽¹⁾; John P Hanzas⁽¹⁾; Roger L Breton⁽²⁾; Paul Whatling⁽³⁾. (1) Surface Water Analysis, Stone Environmental Inc., Montpelier VT (2) Ecological Risk Assessment, Intrinsik Environmental Science Inc., Ottawa ON, Canada (3) Agricultural Products, Cheminova Inc., Arlington VA

The Vegetative Filter Strip Model (VFSMOD) has shown promise as a tool for predicting the effectiveness of VFSs at reducing pesticides entering surface waters. Careful identification of sensitive and uncertain model input parameters is vital for establishing its standardized use in exposure risk assessments. In this study, a series of VFSMOD simulations were made to analyze the effects of input parameter uncertainty on predicted pesticide reduction efficiency. EPA PRZM/EXAMS model standard scenario simulations provided the daily runoff and sediment load inputs to VFSMOD. Two hypothetical pesticides with different mobility characteristics were analyzed, and the uncertainty of the sub-daily distribution of rainfall and runoff inputs, incoming sediment clay content, and vertical saturated conductivity was assessed. Our results highlight the variability in pesticide reduction efficiency due to input parameter uncertainty and provide suggestions on how to address these issues so as to enable the effective use of this model in exposure assessments.

AGRO 38

Effectiveness of buffers installed at targeted critical drainage areas in Minnesota

John P. Hanzas, Jr⁽¹⁾, jhanzas@stone-env.com; Ronald G. Struss⁽²⁾. (1) Agrochemical Fate and Exposure, Stone Environmental Inc., Montpelier VT 05602 (2) Department of Agriculture, Minnesota Department of Agriculture, St. Paul MN 55155

A paired watershed study is being conducted in Minnesota to assess the effectiveness of semi-circular 30-foot grass buffers, installed around critical drainage points from corn and soybean fields, in reducing herbicide residues, sediment, and nutrients in runoff water. These buffers are a voluntary Best Management Practice (BMP) recommended by the Minnesota Department of Agriculture (MDA). Previous research conducted by the University of Minnesota for the MDA using digital terrain analysis and SWAT modeling indicated that critical surface drainage points could be identified and that pollution reduction per land area placed in BMPs can be maximized. The study includes a single, yearly pre-emergent application of herbicide at a reduced rate (another Minnesota BMP) and measurement of rainfall, runoff flow, herbicide residue, sediment, and nutrients. Runoff events in 2010 yielded a strong statistical calibration between study watersheds. During the 2011 and 2012 field seasons, data will be collected to determine the effectiveness of this BMP.

Quantifying trapping efficiency of vegetative filter strips for pesticide registration

George J Sabbagh⁽¹⁾, george.sabbagh@bayer.com; Garey A Fox⁽²⁾; Rafael Muñoz-Carpena⁽³⁾; Dean Desmarteau⁽¹⁾. (1) ER, Bayer CropScience, Stilwell KS 66085 (2) Department of Biosystems and Agricultural Engineering, Oklahoma State University, Stillwater OK (3) Department of Biological and Agricultural Engineering, University of Florida, Gainesville FL United States

Vegetated filter strips (VFS) are often mandated for use of pesticides that do not pass higher-level environmental risk assessments. However, VFS performance in reducing pesticide loading with runoff water is not considered in risk assessments. This has been due to the lack of predictive tools that can explain the wide range of field-reported efficacies. Recently, a pesticide trapping equation has been linked with a numerical simulation model (VFSMOD) which is capable of predicting both runoff reduction (i.e., infiltration) and sediment trapping. The integrated model, called VFSMOD-W, is capable of simulating hydrology, sediment transport, and pesticide trapping through VFS in numerous hydrologic settings. Tools to integrate VFSMOD-W within current regulatory exposure assessments were developed, and strategies for adoption of the technology by regulators in the US and Europe are being pursued. Using two US EPA scenarios, this research demonstrates the influence of VFS on acute and chronic aquatic exposure concentrations of various pesticides including those with varying application dates, high and low organic-carbon sorption coefficients, and soil and water degradation rates.

AGRO 40

Key environmental and physicochemical parameters influencing PRZM-GW predicted groundwater concentrations

Timothy L Negley⁽¹⁾, timothy.negley@arcadis-us.com; Andrew C Newcombe⁽¹⁾; Dirk F Young⁽²⁾. (1) Risk Assessment and Ecological Sciences, ARCADIS US, Inc., Syracuse New York (2) Environmental Fate and Effects Division, US Environmental Protection Agency, Office of Pesticide Programs, Washington DC

The United States Environmental Protection Agency in collaboration with Canada's Pest Management Regulatory Agency has developed a draft Tier II modeling approach to predict pesticide transport to groundwater. This approach uses a modified version of the Pesticide Root Zone Model (PRZM) to predict groundwater concentrations (PRZM-GW) at a desired depth. To date, limited research has been undertaken regarding the sensitivity of PRZM-GW inputs on predicted pesticide concentrations in groundwater. This presentation provides a summary of PRZM-GW simulations and compares the influence of multiple environmental variables and physicochemical characteristics of the modeled pesticide on predicted groundwater concentrations. Key parameters accounting for variability in groundwater predictions were hydrolysis half-life, soil field capacity, and rainfall. The effect of simulation time was explored by extending the weather file to 100 years (increased from the standard 30 years) which allowed chemicals with high retardation factors (e.g., K_{oc}) to reach the aquifer.

AGRO 41

Estimation of reliable degradation kinetics parameters for complex metabolite pathways

Ishadeep Khanijo⁽¹⁾, khanijoi@waterborne-env.com; Neil Mackay⁽²⁾. (1) Waterborne Environmental Inc, Leesburg VA 20175 (2) DuPont (UK) Limited, Stevenage Hertfordshire SG1 4QN, United Kingdom

The degradation of chemicals in soil resulting in complex metabolite pathways have been encountered in recent studies. Representation of extended pathways with up to five metabolites in series and more than ten metabolites in total present numerous challenges. These may be increased because of constraints driven by minor occurrence / transience or emergence later in studies with consequently limited decline phases. Additional challenges include cases when mabolites transform into their precursors. Under such circumstances the estimation of reliable or statistically significant degradation rates and formation fractions of metabolites for such complex degradation pathways, using the EU FOCUS guidelines has proved challenging. A step-wise degradation kinetics approach using mini-pathway studies for a metabolite and metabolite applied as parent studies have been used for estimation of reliable metabolite parameters as a means of addressing kinetic uncertainties. Other suggested approaches that are being tested include Markov Chain Monte Carlo (MCMC) method and Iteratively Reweighted Least Squares (IRLS) method.

AGRO 42

Method for temporal analysis of exposure to residues of concern for a parent compound and degradates

Mohammed Ruhman, ruhman.mohammed@epa.gov; Michael R Barrett. Office of Pesticide Programs, Environmental Fate and Effects Division, US Environmental Protection Agency, Office of Pesticide Programs, Washington DC 20460

Exposure characterization conducted in support of pesticide regulatory decisions typically provides a quantitative analysis of the critical environmental fate and transport properties of the pesticide active ingredient. However, there are situations where metabolites occur in substantial amounts and/or are of substantial toxicological concern. In order to consider the temporal aspect of degradate(s) formation, a spreadsheet post processing method is devised to calculate Estimated Environmental Concentrations (EECs) for acute or chronic exposure from multiple Pesticide Root Zone Model / Exposure Analysis Modeling System runs. Specific methods will be discussed.

Tribal pesticide enforcement in the inland Northwest: Circuit rider approach

Eric Gjevre, egjevre@cdatribe-nsn.gov. Natural Resources Department, Coeur d'Alene Tribe, Plummer ID 83851

Since 1978, some federally recognized Indian Tribes have carried out pesticide enforcement programs under the Federal Insecticide Fungicide and Rodenticide Act, in cooperation with the US Environmental Protection Agency (EPA). More recently, the implementation of FIFRA circuit rider programs for tribes has provided a unique arrangement to pesticide enforcement where a multi-tribal approach is feasible. The Coeur d'Alene Tribe's pesticide enforcement program progressed from a single tribe program, starting in 1992, to a circuit rider program covering six tribes in northern Idaho and eastern Washington. An overview is presented on inspections and investigations conducted, as well as EPA case review/enforcement actions resulting from pesticide misuse across all participating circuit rider reservations.

AGRO 44

Analytical snapshot of agrochemicals associated with marijuana grow operations on the Colville Indian Reservation, Washington

Donald J. Hurst, Don.Hurst2@colvilletribes.com. Department of Environmental Trust, Colville Confederated Tribes, Nespelem WA 99155

In 2009, law enforcement agencies conducted raids on marijuana grow operation (MGO) sites within the Colville Indian Reservation (CIR). Cumulative capacity of the MGOs totaled ~21,000 plants. Tribal Police led field visits to six MGO sites where soil samples were obtained from areas of intense cultivation and refuse pits. Laboratory results documented azinphos methyl (AZM) in soil at concentrations significantly less than relevant cleanup standards and guidelines. AZM is a common organophosphate banned or phased out by US EPA on many food crops in Washington State, although it is registered for use on select crops and can be legally purchased. AZM is toxic to humans, birds, freshwater fish, and aquatic invertebrates. AZM breaks down quickly in the environment with studies citing AZM half-life of 2 - 5 days and ~90% AZM decomposition in soil within 30 days. An estimated 3 to 6 months transpired between AZM application and analysis.

AGRO 45

Pesticide application notification systems

Mark Aaron, mark.aaron@srpmic-nsn.gov. Tribal Pesticide Program Council, Salt River Pima-Maricopa Indian Community, Scottsdale Arizona

Pesticide applications on tribal lands often go unnoticed and unregulated because of the lack of environmental program capacity to oversee and to monitor applications, and to conduct use inspections as part of a tribal or federal pesticide inspection program. Several tribes in Arizona have implemented a pre-application notification system that is not a general permit system, but functions like a notice of intent where the applicator files a written notice with the appropriate office including information on date of

application, crop, harvest date, target pest, specific location, restricted entry interval, method of application, product, EPA registration number, active ingredient, rate, dilution, and total volume. Notice is also given for non-agricultural applications. Similar systems already exist in the States of Arizona and California. Notices allow tribes to collect information on pesticide applications, to monitor the use of restricted use pesticides (RUPs), and to use these notices to target inspections when and if necessary. Collecting the information electronically via a web interface allows collation and filtering of the data on the backend in a user-friendly, spreadsheet interface.

AGRO 46

Agricultural pesticide impacts on the health and culture of Maine's Native Americans

Fred E. Corey, fcorey@micmac-nsn.gov. Department of Environmental Health, Aroostook Band of Micmacs, Presque Isle ME 04769

The State of Maine is home to five-federally recognized Tribes who have relied for millennia upon Maine's abundant natural resources. For each of the Tribes, Tribal culture is inextricably linked to these resources, including the food, spiritual, medicinal, and recreational resources that are derived from the natural resources. However, chemical and pesticide impacts are affecting the ability of Maine's Tribes to practice their ancient cultures. In particular, both historic and contemporary pesticide-use in Maine is adversely affecting Tribal resources. DDT and its metabolites continue to bioaccumulate in fish, and herbicide applications have resulted in recent fish kills. These impacts and others have been exasperated by recent unusual climatological phenomena and could potentially be expected to increase in severity if additional climatological perturbations are observed. Along with discussing these specific impacts on Maine's Native Americans, other cultural factors that result in unique pesticide exposures and health risks will be discussed.

AGRO 47

Pesticides and the impact on traditional basketry

Diania Caudell, dicaudell@aol.com. California Indian Basketweavers Association, Escondido CA 92026

Native plants that are used for weaving traditional native baskets are sometimes exposed to pesticides that are sprayed over forests and fields and along rural highways. Basket weavers are not always aware if toxic sprays were used near the native plants that will be gathered. Most of the native plants that are gathered are not growing in special native gardens but in the vast forests and other open spaces either public or private. Native Plants will grow near golf courses and along rural roads, and these are areas that are usually sprayed more frequently. Educating the weavers and gatherers is an ongoing process with the California Indian Basketweavers Association (CIBA). Basket weavers use their mouth as a third hand while weaving and even though the material may have been washed before using sometimes this is not sufficient and the chemicals may be harmful to the weaver. CIBA has worked with the Tribal Pesticide Program Council and the US Environmental Protection Agency on a pamphlet explaining the dangers of pesticides and other toxic sprays while gathering.

Pesticide impacts on culturally-significant plants

Willie Keenan, williek@cskt.org. Pesticide Program, Confederated Salish and Kootenai Tribes. Pablo MT 59855

The Salish-Pend d'Oreille Tribes of the Flathead Reservation seeks to preserve, protect, and perpetuate the living culture and traditional ways of life of our people. Bitterroot, camas, and other traditional food plants along with medicinal plants are being subjected to pesticide exposure on range land where they are found and harvested. Noxious weed infestations are contributing to a decline in the abundance of cultural plants such as camas and bitterroot. Land managers are increasing the use of herbicides to suppress the spread of noxious weeds and preserve remnant native species and other desirable plants. Tordon, Escort, and Transline herbicides are used on an annual basis to control spotted knapweed and other noxious weeds on sites that were traditionally and continue to be used by implementing the diets and cultural ways of native people.

AGRO 49

Progress toward control of Eurasian watermilfoil and an invasive hybrid milfoil in Coeur d'Alene Lake Tribal Waters by the Coeur d'Alene Tribe

David S. Lamb, dlamb@cdatribe-nsn.gov Lake Management Department, Coeur d'Alene Tribe, Plummer ID 83851

Eurasian milfoil (Myriophyllum spicatum) was first documented in Coeur d'Alene Lake, Idaho in 2004 through aquatic vegetation survey efforts of the Coeur d'Alene Tribe. In 2006, the Tribe began an integrated program of milfoil surveys, control treatments, and related water monitoring. Under this program, diver and rake surveys coupled with GIS mapping provided guidance for herbicide, diver dredging, diver hand removal, and bottom barrier treatments from 2006 through 2010. Modifications in treatment (especially herbicide application) protocols were made during these years to try to overcome low efficacies in some areas. The net results of various treatments over almost 2,000 acres of Tribal waters was the overall reduction in density of the milfoil infestation but an increase in the distribution of the weed. Protection and testing of the culturally important wetland plant Water Potato (Sagitaria latifolia) was an important aspect of this work.

AGRO 50

Pesticide applications near well heads

Mark Aaron, mark.aaron@srpmic-nsn.gov. Tribal Pesticide Program Council, Salt River Pima-Maricopa Indian Community, Scottsdale AZ

Many tribal communities utilize land for agricultural lease and development and for developing home sites on these allotted lands. Agricultural uses can include pesticide applications in close proximity to a community's or homeowner's well head, usually the primary source for drinking water. Groundwater protection and aquifer protection programs are not often in place in tribal communities; although, access to clean water is of primary importance to these peoples. Cultivating awareness with

community outreach to growers and applicators is the first step in protection development.

AGRO 51

Integrated pest management on tribal lands

Mark Aaron, mark.aaron@srpmic-nsn.gov. Tribal Pesticide Program Council, Salt River Pima-Maricopa Indian Community, Scottsdale AZ

Several Tribal pesticide programs are implementing integrated pest management (IPM) programs based on community values and techniques inherent within their people and communities, and by working within a network that includes members of the Tribal Pesticide Program Council (TPPC) and regional IPM centers. These pesticide program specialists have conducted outreach and needs assessments and have organized pilot trainings and practicums. Programs are now being developed to utilize tribal personnel to teach IPM practices to students, school, and facility personnel, and to involve the tribal community, farmers, and land managers in the processes on Tribal lands by using natural processes and monitoring focused on long-term prevention.

AGRO 52

Insecticide runoff from urban hard surfaces during simulated and natural rainfalls

Weiying Jiang⁽¹⁾, wjian001@ucr.edu; Darren Haver⁽²⁾; Andrew Soeprono⁽³⁾; Michael Rust⁽³⁾; Jay Gan⁽¹⁾. (1) Department of Environmental Sciences, University of California-Riverside, Riverside CA 92521 (2) University of California South Coast and Extension Center, Irvine CA 92618 (3) Department of Entomology, University of California, Riverside CA 92521

Intensive urban insecticide use has resulted in their offsite transport through irrigation/rainfall-induced runoff and in contamination of urban waterway. However, the runoff patterns of insecticides from residential areas are not well understood, and factors influencing their runoff potential are not clearly characterized. In this study, runoff potentials of fipronil and pyrethroids in professional formulations from concrete were measured following simulated precipitations or natural rainfall events. All insecticides displayed an initial rapid decrease in pesticide runoff potential, with less than 5% of the applied amount was detected in the 1-d runoff. However, after 89-d outdoor exposure and 4-time repeated wash-off, insecticide residues were still detectable in the runoff water, indicating their extended persistence on concrete and sustained transferability. The long insecticide persistence on concrete was also evident from occurrence of pesticides in runoff generated by winter rain events. Insecticides were detected in the rain runoff after 7 months from pesticide treatment.

Degradation of saflufenacil as affected by moisture content and soil characteristics

Edinalvo Camargo⁽¹⁾⁽²⁾, edinalvo_camargo@yahoo.com.br; Scott Senseman⁽¹⁾⁽³⁾; Rick Haney⁽⁴⁾; John Brad Guice⁽⁵⁾; Garry McCauley⁽³⁾. (1) Department of Soil and Crop Sciences, Texas A&M University, College Station TX 77843-2474 (2) Conselho Nacional de Desenvolvimento Científico e Tecnológico, College Station TX 77843-2474 (3) Texas AgriLife Research, College Station TX 77843-2474 (4) Grassland Soil and Water Research Laboratory, USDA-Agricultural Research Service, Temple TX (5) BASF Corporation

The objective of this study was to evaluate saflufenacil persistence and degradation in soils from rice regions under flooded and non-flooded conditions. Soil samples from 4 locations were used in the study. Saflufenacil dissolved in acetonitrile was added into pre-incubated samples at the rate of 2000 g ha⁻¹. Amount of water added in the field capacity and saturation treatments was determined using a water retention curve. Samples were incubated at 24.8 °C in the dark for 0, 1, 3, 7, 14, 21, 30, and 45 days. An accelerated solvent extraction method was developed and used to extract saflufenacil from soil samples. Microbial respiration was determined hourly for 30 days. Carbon mineralization was higher under field capacity conditions. Half-life averaged among soils was 59 and 38 days for saturated and field capacity, respectively. Results indicated that saflufenacil persistence in the environment would be 2 to 3 times longer under flooded conditions.

AGRO 54

DDA, a new water-soluble degradation product and biomarker of DDT in the Los Angeles Bight

Zhenshan Chen⁽¹⁾, zchen009@ucr.edu; Li Chen⁽¹⁾; Yu Liu⁽¹⁾; Chi-Li Tang⁽²⁾; Helen Vega⁽¹⁾; Robert I Krieger⁽¹⁾. (1) Personal Chemical Exposure Program, Department of Entomology, Environmental Toxicology Graduate Program, University of California-Riverside, Riverside CA 92521 (2) Sanitation Districts of Los Angeles County, Whittier CA 90607

The Los Angeles Bight is highly contaminated with DDT, but the available mass balance accounts for ~10% of total DDT discharged (p,p'- and o,p'-DDT, DDD, DDE). DDA, a water soluble DDT metabolite, was not previously detected. Soxhlet extraction of sediment demonstrated DDE dominance in the LA Bight. Alkaline hydrolysis and dichloromethane extraction of those soxhlet-extracted samples revealed DDA in the sediment extract. The study site 8C at the DDT outfall contained the highest DDA (76 ug/kg dry matter). DDT (25,000 ug/kg) and DDD (186,000 ug/kg) levels were also high at 8C. Sediment DDT and DDD could be sources of continuing DDA formation. DDA might play an important role in natural recovery of DDT in the LA Bight. Meanwhile, lack of the DDA biomarker and dominance of DDE in brown pelican and sea gull feces indicated no recent DDT exposure occurred in wildlife in the LA Bight.

AGRO 55

Decomposition of pharmaceuticals by manganese oxide molecular octahedral sieves

Xiao Xiao, xx42@cornell.edu; Ann T Lemley. Graduate Field of Environmental Toxicology, Cornell University, Ithaca New York 14850

The wide presence of pharmaceuticals in the aquatic environment has become a growing concern due to undesirable biological effects and continuous release. While traditional wastewater treatment methods are not designed specifically for treating such compounds, advanced oxidation technology has gained interest as a good candidate. Decomposition of pharmaceuticals (ciprofloxacin, sulfamethazine, and carbamezapine) was studied in aqueous solution at room temperature using several mixed valent manganese oxides. These oxides belong to a family of porous manganese oxides with a cryptomelane-type structure. Two transition metals, vanadium and molybduem, were used to dope the manganese oxides to increase their activity. Different sources of strong oxidants, t-butyl peroxide and persulfate, were used to develop an efficient treatment system. Effects of solution conditions such as pH and cations on the degradation processe were investigated. Structures of these manganese oxides were characterized by XRD, FTIR, and Raman spectroscopy. All results will be discussed.

AGRO 56

Environmental fate of the transgenic insecticidal protein Cry1Ab in water within a Bt maize agricultural ecosystem

Sara Mueting, mueting@siu.edu; Michael Lydy. Department of Zoology, Southern Illinois University, Carbondale IL 62901

Fate of transgenic, insecticidal proteins in the environment is a relatively new scientific endeavor. The goal of this project was to investigate the fate of Cry1Ab proteins in water within a transgenic-maize agroecosystem. We measured concentrations of Cry1Ab in runoff water, soil pore water, and groundwater within a 36.4 ha area divided into separate non-Bt and Bt fields at several time points during the growing season. A method detection limit (MDL) of 3.2 ng/L was achieved using a centrifugal filter device and ELISA plates. Thirty-six of 54 runoff samples, six of 63 soil pore water samples, and five of 20 groundwater samples had detectable Cry1Ab concentrations. Concentrations of Cry1Ab decreased over time in the runoff water from 11.7 ng/L in June to 5.8 ng/L in September. This experiment will continue over the next two years to increase the understanding of the fate of this protein in the environment.

AGRO 57

Oxidation of bisphenol F (BPF) by manganese dioxide

Zhijiang Lu, zlu004@ucr.edu; Jay Gan. Department of Environmental Sciences, University of California-Riverside, Riverside CA 92521

Bisphenol F (BPF), an environmental estrogen, is used as a monomer in plastic industry and its environmental fate and decontamination is an emerging concern. This study focused on the kinetics, influencing factors, and pathways of its oxidation by MnO₂. At pH 5.5, about 90% of BPF was oxidized in 20 min in a solution containing 100 μ M MnO₂ and 4.4 μ M BPF. The reaction was pH dependent, following an order of pH 4.5 > pH 5.5 > pH 8.6 > pH 7.5 > pH 6.5 > pH 9.6. Humic acids inhibited the reaction at low (\leq 5.5) and

high pH (\geq 8.6) at high concentrations. In addition, metal ions and anions also suppressed the reaction, following the order Mn²⁺ > Ca²⁺ > Mg²⁺ > Na⁺ and HPO₄²⁻ > Cl⁻ > NO₃⁻ » SO₄²⁻. A total of 5 reaction intermediates were identified from which a tentative pathway was proposed.

AGRO 58

Assessing bioavailability and toxicity of permethrin and p,p'-DDT in sediment using matrix solid phase microextraction

Yuping Ding⁽¹⁾, dingyuping80@yahoo.com; Peter F Landrum⁽¹⁾; Jing You⁽²⁾; Michael J Lydy⁽¹⁾. (1) Department of Zoology, Fisheries, and Illinois Aquaculture Center, Southern Illinois University, Carbondale Illinois 62901 (2) State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Guangzhou Guangdong 510640, China

Matrix solid phase microextraction (SPME) was evaluated as a surrogate to estimate bioavailability and toxicity of permethrin and $p_i p'$ -DDT in laboratory-spiked sediments. Sediments were incubated for 7, 28, and 90 d at room temperature to characterize the effect of sequestration on toxicity and bioavailability. Ten-day sediment toxicity was determined by exposing two freshwater invertebrates, the midge Chironomus dilutus and the amphipod Hyalella azteca. Disposable polydimethylsiloxane (PDMS) fibers were simultaneously exposed with organisms via direct burial within the sediment, to absorb the freely dissolved pesticides in porewater. The fiber concentrations were measured at the end of the exposure and after attaining equilibrium. The study showed a good correlation between uptake of pesticides in the organisms and SPME fibers in sediments. The fiber concentrations for both pesticides substantially decreased with sequestration time. Matrix-SPME mimics bioaccumulation of organisms and enables estimation of body residues and prediction of sediment toxicity.

AGRO 59

Development of an in vitro method to determine the bioavailability of xenoestrogens in soil

Katherine Neafsey Engler, kjn23@cornell.edu; Ann T. Lemley. Graduate Field of Environmental Toxicology, Cornell University, Ithaca New York 14853

Biosolids applied to agricultural fields, parks, and other areas represent significant sources of the estrogen-like endocrinedisrupting compound (EEDC) inputs to soil. It is important to determine EEDC bioavailability in soil in order to conduct risk assessments concerning their presence in the environment. The development of an in vitro bioavailability method that is as effective as a traditional in vivo method and that accurately describes the effective estrogenicity of the soil will decrease time, expenses, and use of solvents in future analyses. In this research, a thin-film solid phase microextraction method for determining the bioavailability of EEDCs detected in biosolids was developed and compared with one employing the terrestrial organism Eisenia fetida. The efficacy of SPME to predict the bioavailability of EEDCs in soil will be discussed. Future research will focus on the effects of EEDC mixtures on bioavailability and estrogenicity, the latter being quantified with a fluorescent polarization competitive binding assay.

AGRO 60

Effect of exposure method on SPME-based bioavailability estimates for hydrophobic compounds

Amanda D Harwood, amandaharwood@gmail.com; Michael J Lydy. Fisheries and Illinois Aquaculture Center, Department of Zoology, Southern Illinois University, Carbondale IL 62901

The ability of polydimethlysiloxane-coated solid-phase microextraction (SPME) fibers to predict bioavailability has been well documented. However, factors such as exposure regimen could affect fiber concentrations. Therefore, the objective of this study was to examine the effects of exposure method on SPME fiber concentrations of permethrin and DDE. The SPME fibers were placed in laboratory-spiked sediment under four conditions. For each treatment, the time for the fiber to reach 90% of equilibrium, the concentration on the fiber at equilibrium, fiber uptake and desorption rates were calculated. These estimates were affected by exposure treatment. This difference between estimates could affect the accuracy of bioavailability estimates and limit comparability among data sets. It also demonstrates that animals may influence their own exposure conditions. This is further evidence that a standardized SPME technique is necessary. However, the impact of these differences on tissue residue predictions requires further consideration.

AGRO 61

Predicting the toxicity of permethrin to *Daphnia* magna in water using SPME fibers

Amanda D Harwood⁽¹⁾, amandaharwood@gmail.com; Aubrey R Bunch⁽¹⁾; Jing You⁽²⁾; Michael J Lydy⁽¹⁾. (1) Fisheries and Illinois Aquaculture Center and Department of Zoology, Southern Illinois University, Carbondale IL 62901 (2) State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Science, Guangzhou, China

The current study examined the potential use of solid-phase microextraction (SPME) fibers to predict the toxicity of permethrin to Daphnia magna across various water sources including a laboratory reconstituted water, two natural waters, and a modified natural water. Water source strongly affected the toxicity of permethrin as well as the concentration response relationships. While permethrin concentrations in the water could predict toxicity to D. magna for individual water sources, there was no relationship between permethrin concentrations among water sources and mortality. This indicates that subtle differences in suspended materials among water sources can greatly influence toxicity. Additionally, while tissue residues could predict mortality for individual waters, the correlation among waters was not as clear. Finally, both 48-h and equilibrium-based SPME fiber concentrations could adequately predict toxicity independent of water properties. This demonstrates that bioavailability-based estimates provide a more accurate prediction of toxicity than a water concentration.

Cotton socks monitor the indoor distribution, fate, and persistence of fipronil following Frontline® application to companion animals

Yu Liu, liuyucau@gmail.com; Li Chen; Zhenshan Chen; Melinda Bigelow Dyk; Helen Vega; Robert Krieger. Department of Entomology, University of California, Riverside CA 92507

Prevention, control, and/or eradication of fleas and other pests of companion animals using pesticides introduce residues into residences. Frontline® products containing fipronil are the leading flea and tick treatments. Cotton socks were used as a dosimeter to estimate the distribution and persistence of indoor surface residues of fipronil transferred from pets in an observational study. Socks worn by participants after Frontline application to companion animals were collected and analyzed in 2009, 2010, and 2011. Fipronil and its environmental metabolites desulfinylfipronil, fipronil sulfonem, and fipronil sulfide were observed in most samples. A first-order decay in fipronil was observed. The lowest and highest sock levels in µg/pair-h were 0.4 - 220 (4w; 2009); 2.3 - 109 (4w; 2010); 1.4 - 6.3 (8w; 2011). The average indoor half life of fipronil was about 4.7w. Percent applied to animals recovered from socks ranged from 0.02 - 2.5% after 4w. Surface residue will be of greatest significance following direct skin contact or hand-tomouth transfer and ingestion.

AGRO 63

Surrogate system using rubber latex gloves to assess contact transfer and accumulation of surface pesticide residues

Terry E Lopez⁽¹⁾⁽²⁾, terry.lopez@email.ucr.edu; Li Chen⁽²⁾; Zhenshan Chen⁽¹⁾⁽²⁾; Li Cui⁽²⁾; Yu Liu⁽²⁾; Phuong J Nguyen⁽²⁾; Gayatri Sankaran⁽¹⁾⁽²⁾; Loi T Tang⁽²⁾; Helen Vega⁽²⁾; Robert I Krieger⁽¹⁾⁽²⁾. (1) Department of Entomology, Environmental Toxicology Graduate Program, University of California-Riverside, Riverside CA. 92521 (2) Department of Entomology. Personal Chemical Exposure Program, University of California-Riverside, Riverside CA. 92521

The use of light rubber latex gloves as PPE (personal protective equipment) in agricultural settings has been shown to accumulate multiple pesticide surface residues. A surrogate model system, the Brinkmann Transfer Unit (BTU) developed at UCR, was designed to measure contact transfer of surface pesticide residues from treated turf in controlled studies performed at UC Riverside's Turfgrass Research Facility. The BTU is a modified cart fitted with 3 mannequin hands that allows for the use and sampling using rubber latex gloves. Applications of malathion and fenpropathrin at a rate of 2.24 kg/ha on turf have shown a range of residue accumulation of 0.14 - 308 µg/glove for malathion and 0.5 -146 µg/glove for fenpropathrin. Glove accumulation is dependent on the extent of mannequin hand contact of treated turf. Variability (CV) is < 50% hand-to-hand and run-to-run during the 13 d study periods. Gloves may be a useful direct dosimeter for human exposure assessment.

AGRO 64

Rubber latex gloves as a potential direct dosimeter to estimate pesticide exposure in strawberry harvesters

Gayatri Sankaran⁽¹⁾⁽²⁾, gsank001@ucr.edu; Li Chen⁽²⁾; Zhenshan Chen⁽¹⁾⁽²⁾; Yu Liu⁽²⁾; Terry Lopez⁽¹⁾⁽²⁾; Helen Vega⁽²⁾; Robert I Krieger⁽¹⁾⁽²⁾. (1) Department of Entomology, Environmental Toxicology Program, University of California-Riverside, Riverside CA 92521 (2) Department of Entomology, Personal Chemical Exposure Program, University of California-Riverside, Riverside CA 92521

When harvesters wear rubber latex gloves as required PPE (personal protective equipment) at DB Specialty Farms, Santa Maria, CA, it creates an opportunity to use the gloves as a direct exposure dosimeter. Pesticide Glove Residues (PGR) are the part of Dislodgeable Foliar Residues (DFR) accumulated during harvesting. Malathion (M) and fenpropathrin (F) insecticides were sprayed at 1.12 kg/ha. Both total leaf surface residues (µg/cm²; M: 0.38 to 0.006, F: 0.03 to 0.012) and accumulated glove residues (ug/pair; M: 900 to 15, F: 1300 to 120) follow an exponential decay for 2 to 3 w (p < 0.05). Glove dosimetry enables the estimation of multiple pesticide residues, represents complete coverage of the hands, and utilizes a clean, noninvasive dosimeter that can be conveniently replaced. An empirical glove transfer coefficient relates PGR to DFR (cm²/hr; M: 3,500 - 29,000, F: 2,300 - 45,000). A dermalbased exposure model using glove dosimetry is particularly attractive for harvester exposure assessment.

AGRO 65

Enzyme kinetic analysis of allosteric solvent effects when screening mosquito-selective carbamates against *Anopheles gambiae*

Daniel Swale⁽¹⁾, dswale@gmail.com; Paul Carier⁽²⁾; Ming Ma⁽²⁾; Josh Hartsel⁽²⁾; Maxim Totrov⁽³⁾; Jeffrey Bloomquist⁽¹⁾. (1) Department of Nematology and Entomology, University of Florida, Gainesville FL 32602 (2) Department of Chemistry, Virginia Tech, Blacksburg VA 24061 (3) Molsoft LLC, LaJolla CA 92037

To control the malaria vector, Anopheles gambiae (Ag), we have developed several phenyl substituted Nmethylcarbamates that display high selectivity ratios (≥ 500-fold) over human acetylcholinesterase (AChE). Screening of these carbamates in the presence of 0.1% DMSO (v/v), versus EtOH, yielded higher IC₅₀'s for AgAChE, thus reducing the AgAChE-selectivity. Enzyme kinetic analyses were performed to determine interactions between 0.1% DMSO and the carbamoylation reaction of AgAChE. In the presence of 0.1% DMSO, the bimolecular rate constant (k_i) of the experimental carbamates, exposed to AgAChE, decreased by approximately 3 fold when compared to 10⁻⁵% DMSO. However, this effect was not observed for nonselective carbamates or for human AChE. These results correspond to the IC₅₀ data. Secondly, 0.1% DMSO displayed a small (17%) increase in V_{max} and a 53% increase in K_m of the enzyme substrate acetylthiocholine (ACTh), indicating little influence on the binding/hydrolysis of ACTh. Molecular models supporting these observations will be presented.

Extensive permethrin resistance in North American head louse populations detected by quantitative sequencing and serial invasive signal amplification reactions

Domenic J Previte⁽¹⁾, prev23@gmail.com; Bryan C Poole⁽²⁾; Kyong Sup Yoon⁽²⁾; Gamal E Abo El-Ghar⁽³⁾; Deok Ho Kwon⁽⁴⁾; Si Hyeock Lee⁽⁴⁾; J. Marshall Clark⁽¹⁾⁽²⁾. (1) Molecular and Cellular Biology Program, University of Massachusetts, Amherst, Amherst MA 01003 (2) Department of Veterinary and Animal Science, University of Massachusetts, Amherst, Amherst MA 01003 (3) Department of Pesticides, Menoufiya University, Egypt (4) Department of Agriculture Biotech, Seoul National University, Seoul 151-742, Republic of Korea

Three point mutations (M8151, T9171, and L920F) in the para-orthologous voltage-sensitive sodium channel a-subunit gene of the head louse are associated with resistance to pyrethrins and pyrethroid-based insecticides due to target site insensitivity known as knockdown resistance (kdr). Quantitative sequencing (QS) and serial invasive signal amplification reactions (SISAR) and have been developed to detect kdr and serve as resistance monitoring tools. The current study focuses on North American populations collected from 12 American states and 3 Canadian provinces. QS and SISAR results indicate kdr alleles are wide spread with total resistant allele frequencies of 98.4% and 89.7%, respectively. Access to over-the-counter pyrethroids and overuse of these pediculicidal products in these highlydeveloped nations have led to high instances of kdr. Kdr alleles are the likely cause of increased pediculosis and failure of permethrin-based pediculicides in the United States.

AGRO 67

High-throughput screening of terpenoid compounds at the American cockroach octopamine receptor to determine structure-activity relationships

Aaron D. Gross⁽¹⁾, adgross@iastate.edu; Michael J. Kimber⁽²⁾; Paula Ribeiro⁽³⁾; Joel R. Coats⁽¹⁾. (1) Deparment of Entomology, Iowa State University of Science and Technology, Ames IA 50011 (2) Department of Biomedical Science, Iowa State University of Science and Technology, Ames Iowa 50011 (3) Institute of Parasitology, McGill University, Ste. Anne de Bellevue Quebec H9X 3V9, Canada

Natural products have emerged as potential insecticides/acaracides because of their lower mammalian and environmental toxicity. Octopamine is a vital neurotransmitter, neurohormone, and neuromodulator in invertebrates and an under-utilized target for insect/tick control. The presented research will focus on the ligandindependent expression of the a-adrenergic-like octopamine receptor from the American cockroach (Periplaneta americana) in a genetically engineered yeast cell line, which results in a high-throughput screening platform. Various terpenoid structures are screened against this constitutively active octopamine receptor. Quantitative structure-activity relationships (QSAR) give insight on the important physicochemical properties of a compound that influence the activity of that naturally occurring terpenoid compound that are important to octopaminergic activity.

AGRO 68

Differential potency and substrate kinetics of acetylcholinesterase peripheral site ligands: The molecular basis of selectivity for *Anopheles gambiae* mosquitoes

James M Mutunga⁽¹⁾, jmutunga@vt.edu; Dawn M Wong⁽²⁾; Ming Ma⁽²⁾; Polo C.-H Lam⁽³⁾; Max Totrov⁽³⁾; Li Jianhong⁽⁴⁾; Paul R Carlier⁽²⁾; Jeffrey R Bloomquist⁽⁵⁾. (1) Department of Entomology, Virginia Polytechnic Institute and State University, Blacksburg VA 24061 (2) Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg VA 24061 (3) Molsoft L.L.C., San Diego CA 92121 (4) Department of Biochemistry, Virginia Polytechnic Institute and State University, Blacksburg VA 24061 (5) Department of Entomology and Nematology, Emerging Pathogens Institute, University of Florida, Gainesville FL 32610

Recent molecular modeling of a piperidine-bearing peripheral site ligand (PRC 472) suggests that its selectivity to Anopheles gambiae acetylcholinesterase (AgAChE) was due to preferential interactions with 170 in the mosquito, which is Y70 in HuAChE. In order to test this model, a mosquito recombinant-enzyme I70Y-AqAChE and chicken and human AChEs were tested against known non-selective peripheral site ligands, propidium, BW284c51, and ethidium, as well as PRC 472. AChE gorge mapping with tacrine dimers and substrate kinetics with acetylthiocholine and butyrylthiocholine were also evaluated. AChE gorge mapping showed that gorge geometry for I70Y-AgAChE and HuAChE were similar. Potency of PRC 472 to AgACHE-I70Y decreased significantly (40-fold) compared to WT AgAChE unlike other nonselective inhibitors. Enzyme kinetics showed a K_m of AgAChE-I70Y and HuAChE were both significantly different from that of AgAChE-WT. All indices are in support of the proposed model of PRC 472 selectivity to mosquito AChE.

AGRO 69

Deltamethrin increases peak current and slows deactivation kinetics of the voltage-gated calcium channel ($\text{Ca}_{\text{V}}2.2$) from rat brain following PKC dependent phosphorylation

Anna-Maria Alves⁽¹⁾, aalves@mcb.umass.edu; Steven Symington⁽²⁾; John Clark⁽³⁾. (1) Molecular and Cellular Biology Program, University of Massachusetts, Amherst, Amherst MA 01003 (2) Department of Biology, Salve Regina University, Newport RI 02840 (3) Department of Veterinary and Animal Sciences, University of Massachusetts, Amherst, Amherst MA 01003

Pyrethroids are insecticides used since the 1970s. They are favored for their low mammalian toxicity, improved environmental stability, and insecticidal potency. Voltagegated sodium channels (VGSCs) are a known target but in *vitro* evidence indicates that voltage-gated calcium channels (VGCCs) are also targets. Site-directed mutagenesis of Ca_v2.2 (N-type), altering threonine 422 to glutamate (T422E), produces a mutant channel that acts as if permanently phosphorylated. Deltamethrin increases peak current of T422E Ca_v2.2 compared to its antagonistic action on wild type Ca_v2.2 when expressed in *Xenopus* oocytes. Phosphorylation of wild type Ca_V2.2 is evoked by the phorbol ester PMA by activating endogenous protein kinase C (PKC) in oocytes. Under steady-state conditions, deltamethrin increases transient peak current and reduces deactivation kinetics of the PKC phosphorylated channel that slows channel closure, increasing Ca2+ influx and neurotransmitter release. Conversely, deltamethrin treatment resulted in no

effect on the deactivation kinetics of the unphosphorylated or T422E channels.

AGRO 70

Evaluating the mode of action of terpenoids as insecticides: Evidence for membrane interaction

Jonathan W Childress, jonchild@iastate.edu; Joel R Coats. Department of Entomology, Iowa State University, Ames IA 50011-3140

Terpenoids (isoprenoids) are a class of compounds readily found in nature and are commonly extracted from plants. Terpenoids have been explored as insecticides and show promise due to: low mammalian toxicity, absence of resistance in insect pests, and environmental biodegradability. Though terpenoids are insecticidal, their mechanism of action is still not well understood. This research evaluates cellular membrane disruption as a possible mode of action of terpenoids. Synthetic lecithin liposomes were prepared, with and without cholesterol, and treated with various concentrations of the terpenoids carvacrol, eugenol, menthol, nerolidol, and thymol. The size of the liposomes can be an indicator of the permeability of the liposome membranes. The effects of monoterpenoids on liposome size were determined via sizeexclusion chromatography and membrane interaction/disruption was determined by comparing the average size of control liposomes to the average size of treated liposomes. Effects of including various concentrations of cholesterol were also evaluated.

AGRO 71

Preformed biomarkers in produce may confound biomonitoring in pesticide exposure and risk assessment

Li Chen, chenli134134@163.com; Zhenshan Chen; Yu Liu; Terry Lopez; Gayatri Sankaran; Helen Vega; Robert Krieger. Department of Entomology, University of California-Riverside, Riverside CA 92521

Trace levels of pesticides used in conventional or organic crop protection and their degradation products may occur in produce. The absorption and excretion of preformed biomarkers by consumers would falsely indicate human pesticide exposure. To investigate the formation of potential urine biomarkers in produce, malathion monoacid, malathion diacid, tetrahydrophalimide (captan) and 3-phenoxybenzoic acid (pyrethroids) were measured in 84 produce samples. Potential biomarkers were present in 79 samples. More samples (47 of 84) contained more biomarker than parent pesticide. To demonstrate that those biomarkers are absorbed and excreted in urine of consumers, the disposition of biomarkers is being studied in rats. Rats dosed orally with malathion diacid (20 and 40 mg/kg b.w., respectively) excreted the diacid primarily in urine. Biomarkers present in produce may be absorbed and excreted in urine.

AGRO 72

Adduct identification from reactions of phenoxy/propanoic herbicides with DNA in plants

David R Hall, U_Dhall@umassd.edu; Donald Boerth. Department of Biochemistry and Chemistry, University of Massachusetts, Dartmouth, North Dartmouth MA 01524

Previous studies indicate that pesticides used in crop production pose risks to agricultural plants, including stress to the plant from lipid peroxidation and alterations of the genome. Methods developed in our laboratories have been used to study 2,4-dichlorophenoxyacetic acid (2,4-D), 4chloro-2-methylphenoxyacetic acid (MCPA), diclofop, and related aryloxycarboxylic acid herbicides and their interactions with DNA in a variety of crop plants, including wheat, barley, soybeans, bush beans, and corn. DNA extracted from treated plants has been subjected to $^{\rm 32}{\rm P}$ postlabeling studies, yielding evidence of adduct formation with nucleotide bases from pesticides or their metabolites, as well as from products of peroxidation. Direct in vitro reactions of several herbicides with guanosine gave adducts which have been identified by HPLC chromatography. Structure determination has been pursued by electrospray LC-MS and MS/MS spectroscopy. Computational modeling at the B3LYP-6-31G* level is used to relate energetics of adduct formation with experimental herbicide reactivity.

AGRO 73

Lignocellulosic biomass as a carbon source for biofuels production from oleaginous yeast

Miriam L Revellame⁽¹⁾, mlr305@msstate.edu; Renuka Shivaji⁽¹⁾; Rafael Hernandez⁽²⁾; Darrell Sparks⁽¹⁾; Ashli Brown⁽¹⁾. (1) Department of Biochemistry, Molecular Biology, Entomology, and Plant Pathology, Mississippi State University, Mississippi State MS 39762 (2) Dave C. Swalm School of Chemical Engineering, Mississippi State University, Mississippi State MS 39762

Rhodotorula glutinis is a yeast that has shown to be capable of consuming lignocellulosic biomass directly. Additionally, R. *glutinis* is an oleaginous microorganism that can accumulate oil, which can be used for the production of biofuels and biobased products. This study focused on the elucidation of the mechanism by which R. glutinis utilizes lignocellulosic biomass. Rhodotorula glutinis was cultivated using cellulosic material (cellobiose) as a carbon source, and its capability to hydrolyze the substrate was evaluated. Using HPLC analysis and Nelson-Somogyi assay, the consumption of the cellobiose and activity of sodium carboxymethyl cellulase (NaCMCase) was determined, respectively. After seven days of cultivation, the cellobiose was reduced to as much as half of the original concentration, indicating that the microorganism has the capability of degrading the disaccharide and producing the necessary enzyme. The cellulase activity of R. glutinis was determined to be 0.1 U (glucose) per milliliter of the culture medium.

AGRO 74

Isolation of cellulolytic organisms in the gastrointestinal tract of the giant panda and their potential use in the generation of lignocellulosic-based biofuels

Candace Williams⁽¹⁾, clw224@msstate.edu; William Holmes⁽²⁾; J. Fields Falcone⁽³⁾; Darrell Sparks⁽¹⁾; Carol L Williams⁽⁴⁾; Andrew Kouba⁽³⁾; Scott Willard⁽¹⁾; Ashli Brown⁽¹⁾. (1) Department of Biochemistry, Molecular Biology, Entomology and Plant Pathology, Mississippi State University, Mississippi State MS 39762 (2) Dave C. Swalm School of Chemical Engineering, Mississippi State University, Mississippi State MS 39762 (3) Department of Conservation and Research, Memphis Zoological Society, Memphis TN 38112 (4) Mississippi State Chemical Laboratory, Mississippi State MS 39762

Lignocellulosic biomass is a renewable resource that can be used for biofuel production with the assistance of cellulolytic anaerobic organisms from fecal material. The ability of fecal material to degrade was shown by the treatment of biomass with giant panda (*Ailuropoda melanoleuca*) feces, indicating

that gut flora may reduce biomass. In our study, eight bacterial groups were enumerated monthly over a fourteenmonth sampling of the giant pandas to characterize the gastrointestinal flora. Colony forming units per gram fecal material for *Bacteroides* spp. ranged in the male and female panda from 10² to 10⁴, values for *Clostridium* spp. ranged from 10² to 10⁵. The previously unidentified *Bacteroides* spp. in the giant panda and *Clostridium* spp. may be useful in the degradation of lignocellulosic biomass and its conversion to biofuels. Further work must be conducted to identify species and to isolate cellulase genes in these organisms; metagenomic work is underway to accomplish these tasks.

AGRO 75

Mosquito cell lines as an economical platform for discovery of new insecticides to control malaria

Lacey J Jenson, Ijenson@ufl.edu; Dmitry Diykov; Jeffrey R Bloomquist. Department of Entomology and Nematology, University of Florida, Gainesville FL 32611

This research evaluated the presence of insecticide target proteins from undifferentiated insect cell lines, which could lead to new high throughput screening methods. We used cultures of Anopheles gambiae (Sua1B) insect cells and evaluated insecticidal compounds to detect expression of target proteins. Sua1B cells showed no growth effect from exposure to veratridine alone, but when applied in combination with the pyrethroid, fenvalerate, there was inhibition of cell growth that was fit by a two-site binding model. This effect was inhibited in the presence of one micromolar tetrodotoxin, a specific sodium channel blocker. Patch clamp studies identified a class of voltage-sensitive chloride channel, but not currents typical of fast inactivating sodium channels. However, we did observe effects of fenvalerate indicative of "electrically-silent" sodium channels previously observed in vertebrate C9 cells. The presence of ion channels and receptors in these cells will potentially accelerate high throughput screening for new insecticides.

AGRO 76

Biological stability and delivery studies to elucidate the role of thickener solid particles on water-in-oil emulsion containing microalgae

Lorena Elizabeth Fernandez (1)(2),

Iefernandez@ucdavis.edu; Hongyun Guo⁽¹⁾; Herbert Scher⁽¹⁾; Jean S VanderGheynst⁽¹⁾. (1) Department of Biological and Agricultural Engineering, University of California Davis, Davis CA 95616 (2) Agricultural and Environmental Chemistry Group, University of California Davis, Davis CA 95616

The production of bioenergy from renewable biomass could prove to be a solution for global warming and provide an alternative fuel source for petroleum. Producing oil from microalgae is feasible, but, because of high production costs, it is still not economically viable. Contributing costs include those associated with algae storage to maintain biological activity and transportation. Water-in-oil emulsions allow algae to be produced off-site by an independent "seed" producer, stored until purchased, and then delivered to the grower. In this study emulsions were prepared with different oil dispersible surface modified particles in order to investigate release kinetics and improve storage stability. We found that emulsions containing Aerosil R974, Bentone 38, and Bentone 150 were physically stable up to 365 days of storage at room temperature. The concentration of particles in the continuous phase had a significant effect on the stability and cell viability of the W/O emulsion.

AGRO 77

Raman microscopic analysis of PM₁₀ for assessing source distributions from agricultural operations

Qiang Huang⁽¹⁾, jizaiqiang@gmail.com; Walter F Schmidt⁽²⁾; Edna Razote⁽³⁾; Laura L McConnell⁽²⁾; Cathleen J Hapeman⁽²⁾; Alba Torrents⁽¹⁾; Ronaldo Maghirang⁽³⁾; Steven L Trabue⁽⁴⁾. (1) Department of Civil and Environmental Engineering, University of Maryland, College Park MD 20742 (2) USDA-Agricultural Research Service, Beltsville MD 20705 (3) Biological and Agricultural Engineering, Kansas State University, Manhattan KS 66506 (4) National Laboratory for Agriculture and the Environment, USDA-Agricultural Research Service, Ames IA 50011

Emission of particulate matter (PM) from animal feeding operations (AFOs), including open beef cattle feedlots and dairies, is a major air quality concern. Fine PM, typically those with equivalent aerodynamic diameter of 10 µm or less (PM₁₀), can penetrate deep into the lungs and cause serious health problems. Knowledge of the physical and chemical characteristics of PM emissions is important in investigating their fate and transport mechanisms, and new tools are needed to clearly identify sources of PM. This work is aimed at the development of spectroscopic techniques to determine the distribution of source materials contributing to PM₁₀ particles collected downwind from agricultural operations. As part of a larger project to examine emissions from cattle feedlots, source materials for PM₁₀ were collected and were analyzed with Raman microscopy. While some sources are quite heterogeneous in nature, unique Raman shifts in the spectra are expected to serve as markers for essential materials/chemicals that could be used to identify PM sources (i.e., pen surface material, unpaved road, manure, cattle feed, feed mill, and vehicle exhaust). A spectral library that includes hundreds of individual spectra of single particles from different source materials is under development. This library will be used with advanced statistical methods to characterize the distribution of source materials contributing to PM₁₀ particles collected downwind from the feedlot. This work will serve as proof of concept and can be expanded for use in evaluation of best management practices to minimize PM₁₀ emissions from AFOs.

AGRO 78

Optical fiber ammonia gas sensor using a dual layer poly(methyl methacrylate)/chlorophenol red coating

Yu Huang, yhuang2@buffs.wtamu.edu; Shiquan Tao. Mathematics, Chemistry, and Physics, West Texas A&M University, Canyon TX 79016

An optical fiber ammonia sensor has been developed using chlorophenol red (CPR) as a sensing reagent. The transducer of the sensor is a bent optical fiber probe, which is first coated with a thin layer of poly(methyl methacrylate) (PMMA). A thin layer of CPR is then coated on the surface of the PMMA membrane. The exposure of this bent optical fiber probe to trace $\rm NH_3$ in an air sample causes an optical absorption spectrum with peak absorption wavelength at around 590 nm. This sensor is reversible and sensitive; it can detect $\rm NH_3$ in air down to 2.0 ppbv. The response time of the sensor is 15 minutes. The effects of moisture and $\rm CO_2$ in air on sensor function for detecting trace $\rm NH_3$ in air have been investigated. Potential applications of this sensor in air quality monitoring will be discussed.

Piperidine thiazole fungicides

Mary Ann Hanaga, mary-ann.hanagan@usa.dupont.com; Robert J Pasteris; Rafael Shapiro; Yewande Henry; Boris Klyashchitsky. Crop Protection, E I DuPont, Newark DE 19714

The control of plant diseases caused by fungal plant pathogens is extremely important in preventing crop damage and obtaining high yields. Many products are available for these purposes, but the need continues for new compounds which are more effective and have new modes of action. The synthesis of a new class of fungicides for the control of oomycetes will be discussed.

AGRO 80

Sedaxane: A new broad-spectrum seed treatment fungicide

Harald Walter⁽¹⁾, harald.walter@syngenta.com; Camilla Corsi⁽¹⁾; Michael Oostendorp⁽²⁾; Gabriel Scalliet⁽³⁾; Ronald Zeun⁽³⁾. (1) Research Chemistry, Syngenta Crop Protection AG, Stein Aargau 4332, Switzerland (2) Product Biology Seed Care, Syngenta Crop Protection AG, Basel Basel-Stadt 4058, Switzerland (3) Research Biology, Syngenta Crop Protection AG, Stein Aargau 4332, Switzerland

Sedaxane (SDX) is a broad spectrum pyrazole carboxamide fungicide which originates from the *bis*-cyclopropylphenyl amide subclass. SDX inhibits succinate dehydrogenase (SDH), a well known fungicidal mode of action. Syngenta entered the SDHI area in 1998 and one of the priority goals was to find a broad-spectrum seed treatment compound which controls *Ustilago nuda* as a key disease. Starting from various structures, including carboxin (figure 1), the broad-spectrum seed treatment SDHI sedaxane was discovered in 2002. Sedaxane has a unique structure which contains an orthobiscyclopropylphenyl moiety. The interesting chemistry of SDX as well as biological and mode of action aspects will be discussed.

AGRO 81

From pyridines to pyrazoles: The discovery of $Xemium^{\circ}$

Jochen Dietz⁽¹⁾, jochen.dietz@basf.com, Carl-Bosch-Str. 38, Ludwigshafen Rheinland-Pfalz, Germany; Thomas Grote⁽¹⁾; Siegfried Strathmann⁽²⁾. (1) BASF SE, Ludwigshafen 67056, Germany (2) BASF SE, Limburgerhof 67114, Germany

Xemium[®] is BASF's newest fungicide innovation. This novel SDH inhibitor was discovered by exploiting hits from BASF's proprietary library assisted by key learnings from BASF's Boscalid optimization program. The presentation covers topics of the Xemium[®] discovery process.

AGRO 82

Fused pyrazole kinase inhibitors as broad-spectrum fungicides

Thomas M. Stevenson,

thomas.m.stevenson@usa.dupont.com; Andrew E Taggi; A. Don Crews; Michael H. Howard; John J. Bisaha; Courtney J. Megatulski; Teodorica M. Cenizal; Patrick R. Kovacs; Paula L. Sharpe; John Andreassi. Crop Protection, DuPont, Newark DE 19711

A series of fused pyrazoles was synthesized by the reaction of bicyclic sydnones with alkynes. High levels of fungicidal activity were found for compounds with 2-alkylamino-pyrimid-4-yl substituents at the 4-position of the pyrazole ring. Optimization of this system provided compounds with broad spectrum activity at low application rates. Synthesis, structure-activity relationships, and site of action studies for this class will be detailed.

AGRO 83

Pyrimidinone methylsulfonylisoxazolines: Novel herbicidal inhibitors of very long chain fatty acid biosynthesis

Thomas P Selby, thomas.p.selby@usa.dupont.com; Brenton T Smith; Andy Travis; David A Clark; Stephen Bolgunas; Richard Crosswicks; Marc Ruggiero; Michael McComrick; Christian T Pedersen; Steven Gutteridge. Crop Protection, DuPont, Newark DE 19714

Discovered at Kumiai, pyroxasulfone is a substituted pyrazolyl methylsulfonylisoxazoline herbicide in development for preemergent weed control in corn, soybeans, and cereals. The compound is representative of a new class of potent very long chain fatty acid (VLCFA) biosynthesis inhibitors that have a much lower use rate and broader activity spectrum than older acetanilide-based products with this mode-of-action. In our search for a novel chemotype from this area of chemistry, we discovered that pyrimidinone substituted methylsulfonylisoxazolines also expressed very high levels of herbicidal activity. A substantial optimization effort followed with many heterocyclic variations explored. DPX-Q6K47 was found to provide optimum levels of weed control with impressive safety to corn, soybeans, and wheat. Extensive global field trails were conducted on DPX-Q6K47 in both warm and cool season crops. Here, we report on the synthesis, biology, and structure-activity relationships of pyrimidinone methylsulfonylisoxazolines as well as some other heterocyclic modifications.

AGRO 84

Indaziflam: A new low-dose, non-selective solution for broad-spectrum weed control

Hartmut Ahrens, hartmut.ahrens@bayer.com; Hansjoerg Dietrich; Klemens Minn; Thomas Auler; Mark Ford; Erwin Hacker; Eckhard Rose; Hermann Bieringer; Martin Hills; Hubert Menne; Heinz Kehne. Department of Research Weed Control, Bayer CropScience AG, Frankfurt am Main 65926, Germany

Indaziflam is the new, innovative, active ingredient of Specticle™ (first registered in 2010 in the United States) and Alion® (expected to be registered in 2011) by Bayer CropScience. The new compound belongs to the alkylazine chemical class and acts via inhibition of plant-specific cellulose biosynthesis. It provides excellent long-lasting action combined with highly efficient control of a broad spectrum of weeds. The discovery process and the

optimization of the alkylazine class which led to indaziflam, including biological profiles and the resulting Structure-Activity-Relationships, will be presented.

AGRO 85

Innovation in agrochemical research: The role of paradigms

Axel Kleemann, axel.kleemann@basf.com. Global Research Crop Protection, BASF SE, Ludwigshafen RP D-67056, Germany

Varying agricultural commodity prizes, slowly growing markets, generic competition, and heightened regulatory standards are trends that constantly increase R&D challenges. Thus, the constant need for innovation is not new. Ever since the introduction of chemical crop protection, many new approaches have been tried with strategies and tools that particularly in recent decades have been made available by the rapid development in chemistry, biochemistry, and molecular biology. However, examples for success are rare and not all of the recent technology advances have yet come to fruition or have justified the sometimes huge investments. Why is it that many of those appealing and smart approaches have so far not lived up to the expectations? Have the low-hanging fruits already been picked, leaving current and future generations of scientists in the field with ever growing costs, risks, and uncertainties? Lead identification and optimization require multidisciplinary approaches, and the routes to successful product discoveries are now multidimensional endeavours. Factors such as chemical library design, target selection, screening, and validation strategies are as important than clever test design and set-up for in vivo testing. Understanding of the required properties of a chemical structure and suitable tools to predict their behaviour in complex systems (biology, regulatory) has also increased and is/should be used broadly to influence and to steer discovery work as early as possible. Included are better understanding of phenomena such as uptake, stability, and metabolism early on. Agrochemical research has certain strengths over related disciplines that sometimes seem to have been forgotten. Although the research's business model has frequently been discussed in the past, there are still ways to innovation that do not always require high-tech but also a sound understanding of relevant factors, creativity, passion, and, of course, luck.

AGRO 86

Forest herbicides: Effective tools for intensive management and sustainable forestry

Darren A. Miller⁽¹⁾, darren.miller@weyerhaeuser.com; Raymond B. Iglay⁽²⁾; Vanessa R. Lane⁽³⁾; Phillip D. Jones⁽²⁾; Stephen Demarais⁽²⁾; Steven B. Castleberry⁽³⁾; Karl V. Miller⁽³⁾; T. B. Wigley⁽⁴⁾. (1) Southern Environmental Research, Weyerhaeuser NR Company, Columbus MS 39704 (2) Department of Wildlife, Fisheries, and Aquaculture, Mississippi State University, Mississippi State MS 39762 (3) Warnell School of Forestry and Natural Resources, University of Georgia, Athens GA 30602 (4) National Council for Air and Stream Improvement, Inc., Clemson SC 29634

Forest herbicides are used to control competing vegetation in intensive management of loblolly pine (*Pinus taeda*) and indirectly impact wildlife by altering vegetation structure and succession. Three recent studies (MS and NC) have documented wildlife responses to herbicide use during early and mid-rotation. Woody plant suppression via chemical site preparation and mid-rotation release, with or without additional treatments (e.g., mechanical site preparation, row spacing, mid-rotation prescribed fire), promoted herbaceous

plants including quality white-tailed deer (*Odocoileaus virginianus*) forages. However, site-specific conditions influenced understory responses. Mid-rotation herbicide application, particularly when combined with fire, promoted forest structure similar to natural pine-grasslands. Avian species of conservation concern responded most to herbicide treatments at site preparation and mid-rotation. Small mammal response was short-term and species-specific. Herpetofauna and carabid beetles had limited responses at mid-rotation. Our results suggest a positive role of forestry herbicides for meeting forest productivity and biodiversity goals within southeastern pine plantations.

AGRO 87

Operation pollinator: Positive action for pollinators

Jeff Peters⁽¹⁾, jeff.peters@syngenta.com; Neal Williams⁽²⁾; Rufus Isaacs⁽³⁾; Jamie Ellis⁽⁴⁾; Donn Waage⁽⁵⁾; Julianna Tuell⁽³⁾; Akers Pence⁽⁴⁾; Kimora Ward⁽²⁾; Diane Wilson⁽⁶⁾; Jaret Daniels⁽⁴⁾. (1) Sustainability, Syngenta Crop Protection, Greensboro NC 27409 (2) Department of Entomology, University of California-Davis, Davis CA 95616 (3) Department of Entomology, Michigan State University, East Lansing MI 49060 (4) Department of Entomology, University of Florida, Gainesville FL 32611 (5) National Fish and Wildlife Foundation, Washington DC 20005 (6) Applewood Seed Company, Arvada CO 80002

Pollinating insects are essential for the production of many food crops and the health of the natural environment; as such, development of science-based conservation practices that enhance their habitat is a priority. Operation Pollinator is a global initiative launched by Syngenta that includes research and implementation in California, Florida, and Michigan—key horticultural areas in the United States. This collaborative effort involves a diverse group of stakeholders whose goal is to develop a conservation program which growers can integrate into their farm landscapes. This program will evaluate the provision of additional foraging habitat and nesting sites for native pollinators on nonproduction areas of the farm. Through research, a set of economically-viable management practices will be developed with the agricultural community. Through Operation Pollinator, the agribusiness community will see first-hand, how sustainable agriculture and science-based solutions can work together to enhance pollinator biodiversity and feed a growing world.

AGRO 88

Acute toxicity of forestry herbicide mixtures to aquatic organisms

Vickie L. Tatum⁽¹⁾, vtatum@ncasi.org; Dennis L. Borton⁽²⁾; William R. Streblow⁽²⁾; Jeffrey Louch⁽³⁾; James P. Shepard⁽⁴⁾. (1) NCASI, Newberry FL 32669 (2) NCASI, New Bern NC 28561 (3) NCASI, Corvallis OR 97339 (4) Forest Biology and Ecology, Auburn University, Auburn AL 36849

Because many herbicides selectively target specific species or types of vegetation, they are often applied as mixtures in order to achieve better control. When herbicides are applied in forest ecosystems, streams, ponds, and other bodies of water, they are typically protected by no-spray buffer zones. In some landscapes, small wetlands and streams are difficult to see and avoid, thus the potential acute toxicity of herbicide mixtures to aquatic organisms is of interest, yet is not well-studied. Of particular concern is synergistic mixture toxicity, in which the toxicity of mixtures is greater than anticipated based on individual component toxicity. The results of a recent study of the acute toxicity of 23 herbicide mixtures to *Ceriodaphnia dubia* and *Pimephales promelas*

were consistent with other studies that found when acute toxicity was observed, it was usually additive or antagonistic (less than expected). In the few mixtures showing synergistic toxicity, synergism was slight.

AGRO 89

Vertebrate pest management: Case studies in pesticides and the management of biodiversity

Michael J Bodenchuk,

michael.j.bodenchuk@aphis.usda.gov. Texas Wildlife Services, USDA-Animal and Plant Health Inspection Service, San Antonio TX 78249

Vertebrate pests pose a unique problem for agriculture and managed ecosystems. Invasive vertebrates such as feral swine (Sus scrofa), European starlings (Sturnus vulgaris), and Indian mongoose (Herpestes javanicus) affect native species through habitat destruction, competition, and direct predation. Even native species can require management to avoid ecosystem-level impacts. Vertebrate pest management differs from Integrated Pest Management (IPM) in that the native pest species may also serve a positive ecological role. Management in these cases must balance ecological and social values. This paper presents integrated wildlife damage management as a type of IPM, describes the ecological trade off necessary to meet sometimes mutually exclusive goals, and provides case histories of management programs designed to enhance biodiversity through judicious use of pesticides.

AGRO 90

Impact of farming practices, pesticides, and landscape management on farmland birds in Europe and the role of Cross Compliance and Agri-Environmental Schemes

Peter John Edwards⁽¹⁾, peter edwards@syngenta.com; Gavin Siriwardena⁽²⁾. (1) Environmental Safety, Syngenta, Bracknell Berkshire RG42 6EY, United Kingdom (2) British Trust for Ornithology, Thetford Norfolk IP24 2PU, United Kingdom

Long-term monitoring of bird populations in Europe, especially in the United Kingdom by the British Trust for Ornithology's Common Birds Census Scheme, provided the first evidence of declines in some farmland bird species. A host of changes in farming practices and landscape management have contributed to these changes, including the indirect effects of pesticides on bird food supplies. The Common Agricultural Policy (CAP) recognised the need to take account of this and other environment issues and changed the financial incentives in 2003 from production to environment. The CAP has an annual budget of €50 billion to provide incentives to farmers through single area payments (SAP) and by modulation for rural development as agrienvironmental schemes (AES). To receive payments, farmers must comply with guidance. AES guidance, defined by member states (MS), has the option to make refinements to fit rural development targets. In the UK, farmland birds have been used as one indicator of the success of AES and a range of 'options' within the schemes have been designed specifically to benefit bird populations. To-date, the farmland bird response has been disappointing at the MS scale, probably because the best balance of options for birds within the schemes has not been taken up by farmers and options not optimally implemented. A lag in population responses at the MS scale may also be a factor. There have, however, been many successful examples where combinations of targeted management practices, applied at a small/local scale, have had the desired positive effects. A lack of a positive response at the MS level may threaten long term

payments to farmers. The presentation will discuss and illustrate options for combining specific management options in an optimal way with other biodiversity and sustainable farming practices to maximise the chances of success in improving farmland bird populations.

AGRO 91

Contribution of zero tillage to sustainability in Brazil's tropics

John N Landers, john.landers@uol.com.br. SMDB, Associacao de Plantio Direto no Cerrado, Uberlandia-MG Minas Gerais 38408.032, Brazil

Zero tillage (ZT) is one of the most important revolutions in sustainable crop production ever developed, especially in the tropics, and represented 106 million ha worldwide in 2006. On erosion-prone soils, tropical ZT has averted an ecological disaster. In 1992, when the economics started to favour ZT over conventional tillage (CT), it expanded rapidly to 30 million ha in 2010 of which 14 million ha were in the new Cerrado and pre-Amazon regions. Benefits are reduced water and wind erosion, leaching, drought stress, and irrigation, and increased soil carbon sequestration, albedo, rainfall infiltration, microbial activity and fauna, all leading to the potential for sustainable land intensification (LUI) and therefore less pressure on de-forestation. This has increased farmer respect for on-farm reserves (at least 20% of farm in the Cerrado, 35% Pre-Amazon) totaling 95 million hectares in Brazil. Higher sustainable yields per unit of fertilizer and water has led to cheaper food with lower capital investment per hectare. De-forestation has reached 48% of the Cerrado biome but only 15-17% of the Amazon. To stop deforestation, land use intensification (LUI) is required. Yield gains in soybeans and corn have been impressive, but their future LUI impact is small compared to pasture renovation, with a de-forestation mitigation potential (DMP) of up to 3 ha ha-1 with tropical rainfed ley farming systems, or up to 8 ha ha 1 for pasture renovation. The trader-imposed Soybean Moratorium banned purchase of soybeans from Amazon lands cleared after 2006, but beef cattle are the major direct driver and there is now also a Beef Moratorium. The Round Table on Responsible Soy has a certification system including a moratorium on forest clearing. Current challenges for ZT, crop protection and de-forestations will be discussed. Brazilian farmers have solutions for LUI but they cost more, and who is willing to pay?

AGRO 92

Watershed regressions for pesticides (WARP) for predicting atrazine concentrations in corn belt streams

Wesley Stone, wwstone@usgs.gov; Robert Gilliom. National Water Quality Assessment, US Geological Survey, Indianapolis IN 46278

Corn Belt WARP (WARP-CB) models were developed for predicting annual atrazine concentration statistics for streams within areas of the corn belt region that have high intensities of atrazine use. The models accounted for 53 - 62% of the variability in the various concentration statistics among the sites used for model development. WARP-CB model predictions for development sites were within a factor of 5 of the observed concentration statistic for more than 90% of the site and year combinations. WARP-CB predictions for model development sites had smaller overall residual error and reduced uncertainty compared to the National WARP model predictions for the same sites. WARP-CB model predictions can be used to estimate the probable concentrations of atrazine for comparison to specific water-

quality benchmarks. Sites with a high probability of exceeding a benchmark for human health or aquatic life can be identified and prioritized for monitoring.

AGRO 93

Analysis of monitoring data from multiple small watersheds to identify drivers of agrochemical runoff from corn and sorghum agriculture

Paul Miller⁽¹⁾, millerp@waterborne-env.com; Malia Andrus⁽¹⁾; Chris Harbourt⁽¹⁾; Dazhi Mao⁽¹⁾; Jessica Prenger⁽¹⁾; Paul Hendley⁽²⁾; Robert Joseph⁽²⁾. (1) Geoinformation Management, Waterborne Environmental Inc., Champaign IL 61820 (2) Syngenta Crop Protection, LLC, Greensboro NC 27409

Over 150 site years of herbicide concentration data have been collected from second and third order streams draining from > 65 small, Midwest watersheds that represent corn and sorghum agriculture with a high potential for agrochemical runoff. To complement these monitoring data, very detailed assessments of watershed soils, slopes, and cropping have been developed using GIS tools. These data have been analyzed using a combination of statistical approaches including logistic regression, discriminant analysis, and principal components analysis, among other multivariate techniques, in order to identify key drivers of runoff that differentiate between sites with varied vulnerability characteristics. Automated analyses were conducted across many variables and, after simplification, a three factor model was found to successfully distinguish between classes of vulnerable sites. One key factor is the fraction of the watershed where cropped lands have shallow depths to restrictive soil layers co-occurring with slopes; this offers potential for field-scale application.

AGRO 94

Comparison of SWAT pesticide simulation approaches for ecological exposure assessments

Natalia Peranginangin⁽¹⁾,

natalia.peranginangin@syngenta.com; Michael F Winchell⁽²⁾; Raghavan Srinivasan⁽³⁾. (1) Syngenta Crop Protection, LLC, Greensboro NC 27419-8300 (2) Stone Environmental, Montpelier VT 05602 (3) Texas A&M University, College Station TX 77843

The Soil and Water Assessment Tool (SWAT) has proven to be an effective tool for evaluating pesticide exposure in flowing water bodies. To assess its potential for predicting ecological pesticide exposure for all headwater watersheds at national scale, a simpler parameterization strategy was considered while balancing computational efficiency and the appropriate scale and resolution of key input datasets. An approach for applying SWAT with minimal calibration was applied to 20 headwater watersheds across the Midwest corn belt. This calibration approach was applied to each of the watersheds using both medium resolution STATSGO soils data and high resolution SSURGO soils data. Subbasin size and land use heterogeneity were also varied in order to assess whether a simplified model structure could result in a level of model performance comparable to a more complex model. A comparison of pesticide simulation performance for these various model structures will be presented.

AGRO 95

Large-scale modeling of historical pesticide applications

Gerco Hoogeweg⁽¹⁾, hoogewegg@waterborne-env.com; Mark Cheplick⁽¹⁾; W. Martin Williams⁽¹⁾; Debra Denton⁽²⁾; Richard Breuer⁽³⁾. (1) Waterborne Environmental, Inc., Leesburg VA 20175 (2) Standards and TMDL Office, US Environmental Protection Agency, Sacramento CA 95814 (3) Environmental Water Quality and Estuarine Studies, California Department of Water Resources, Sacramento CA 95814

With increasingly faster computers and more detailed data, it becomes easier to model pesticide mass loadings into aquatic systems at a high-resolution for large geographical areas. A large-scale ecological risk assessment was recently completed to quantify spatial and temporal mass loadings of pesticides into tributaries to the Sacramento River, San Joaquin River, and Bay-Delta estuary for the purpose of guiding future risk assessments for sensitive and endangered species. Ten years of daily mass loadings were simulated for over nine million pesticide applications for 40 chemicals in a 164,000 km² area of California's Central Valley. Model input included historical pesticide-use data from the California Department of Pesticide Regulation's Pesticide Use and Registration (PUR) database, daily weather data from 19 stations in the California Irrigation Management Information System, detailed soils information (SSURGO) from the NRCS, and high resolution land use data from the Farmland Mapping and Monitoring Program (FMMP). Pesticide application sites represented in the simulations included fruit, vegetable, grain, nuts, rice, landscape maintenance, and structural applications. Environmental fate and transport models used for the analysis included the Pesticide Root Zone Model (PRZM), modified to simulate pesticide losses in irrigation tail water, and the rice water quality model (RICEWQ). This presentation details methods and results of the model simulations including discussions on those factors contributing to the highest contributions of mass loadings into aquatic systems.

AGRO 96

Importance of sediment analysis in monitoring current-use pesticides in streams

Michelle L Hladik, mhladik@usgs.gov; Kelly L Smalling; Kathryn M Kuivila. US Geological Survey, Sacramento CA 95819

Sediments are important media in aquatic ecosystems where contaminants occur leading to exposure of aquatic organisms, yet sediments are rarely analyzed for currentuse pesticides in monitoring programs. Data are presented from multiple studies in which both water and sediment (bed and/or suspended) phases were sampled. As expected, highly hydrophobic compounds (log $K_{oc} > 5$), such as pyrethroid insecticides, were detected primarily in sediments. Moderately hydrophobic compounds (log K_{oc} 2 to 4), such as azoxystrobin (fungicide), chlorpyrifos (insecticide), and trifluralin (herbicide), were also frequently detected in sediments. Typically, suspended sediments have a greater number of pesticides detected at higher concentrations than bed sediments. Since pesticides associated with sediments tend to be more persistent and have longer residence times in aquatic ecosystems, organism exposure can be different than for dissolved pesticides. It is critical to include analysis of sediments for a complete characterization of ecosystem exposure to pesticides in surface waters.

Sampling plans for water quality assessment

John W Green, John.W.Green@usa.dupont.com. Department of Engineering Technology, DuPont, Newark DE 19714

Sampling plans for monitoring chemical concentrations in rivers were investigated for two California streams of differing order to assess the relative merits of daily sampling versus less frequent sampling. The assessments were based on the ability to estimate time-weighted total and peak concentrations on a monthly or annual basis and to detect the presence of spikes in these concentrations. A secondary purpose was to determine the feasibility of predicting spikes in chemical concentrations from the river discharge rate. In these streams, some less frequent sampling plans were shown to provide almost the same utility as daily sampling for the first purpose and discharge rate was shown to have little correlation with chemical concentration.

AGRO 98

Continuous monitoring for pesticides in freshwater off-channel habitats using a lipid-free tubing passive-sampling device

Phillip Janney, janneypk@gmail.com; Jeffrey J Jenkins; Kim Anderson. Department of Environmental and Molecular Toxicology, Oregon State University, Corvallis OR 97331

Pesticide exposure to juvenile salmonids utilizing Pacific Northwest freshwater off-channel habitats during rearing and migration is of concern as a result of recent National Marine Fisheries Service Biological Opinions. We deployed a lipid-free tubing passive-sampling device (LFT) at 5 locations in the Pudding River basin, Willamette Valley, OR (HUC8: 17090009). This watershed is predominately agricultural and classified as habitat for salmonid species. LFT were deployed continuously in off-channel habitats, including backwaters, channel edge sloughs, and off-channel pools, at 3 - 4 week intervals from June 2010 to June 2011. Time-weighted average concentrations of freely dissolved pesticides were quantified by dual column gas chromatography with electron capture detection and confirmed with mass selective detection. The use of pesticide off-channel habitat monitoring results in assessing the risk to salmonids will be discussed.

AGRO 99

Exposure assessment for pronamide drinking water residues in California central coast lettuce production areas

Nick Poletika⁽¹⁾, npoletika@dow.com; Brian Bret⁽²⁾; Mike Winchell⁽³⁾. (1) Department of Field Exposure and Effects, Dow AgroSciences LLC, Indianapolis IN 46268 (2) Department of Regulatory and Government Affairs NAFTA, Dow AgroSciences LLC, Sacramento CA 95747 (3) Department of Applied Information Management, Stone Environmental, Inc., Montpelier VT 05602

Regulatory pesticide human exposure models are intentionally designed to be protective of individuals in populations. Consequently, they tend to be quite conservative in early assessment tiers, and predictions are generally refined with data in subsequent assessments. For drinking water obtained from surface water, pesticide exposure model concentration estimates for agricultural use generally are in the $\mu g \ L^{-1}$ to tens of $\mu g \ L^{-1}$ range, which can lead to concern if human health endpoints for a specific

pesticide are low values. Currently US EPA OPP accepts only targeted monitoring studies for refinement of model estimated concentrations. We present an alternative assessment method to targeted monitoring for a pesticide with a limited range of label crops and geographic regions of use that relies on proximity analysis of use sites and drinking water intakes. We also address national security issues related to sensitive intake location data and consider the general utility of the approach.

AGRO 100

Pesticides and pesticide degradates in source and finished water of community water systems supplied by rivers

Gregory Delzer, gcdelzer@usgs.gov; Joshua Valder. National Water Quality Assessment, US Geological Survey, Rapid City SD

In 2001, the US Geological Survey's National Water-Quality Assessment (NAWQA) Program began its second decade of intensive assessment activities. As part of this effort, a new assessment activity, termed Source Water-Quality Assessments (SWQAs), was implemented to focus on characterizing the quality of source water derived from rivers and aquifers used by large and very large community water systems (CWSs). The associated finished water was also studied. SWQAs complement existing drinking-water monitoring required by Federal, State, and local programs that focus primarily on post-treatment compliance monitoring. Through SWQAs, the NAWQA Program is increasing its emphasis on characterizing major sources of drinking water and continues to collaborate with other agencies and organizations involved with supplying and managing drinking water. This presentation will summarize findings for about 100 pesticides and pesticide degradates monitored in source water and the associated finished water of 21 CWSs supplied by rivers. Concentrations will be compared to human-health benchmarks and US Geological Survey Health-Based Screening Levels.

AGRO 101

Application of biological mass spectrometry and protein barcodes in agricultural and food chemistry

Jun Wang, wangjun2@hawaii.edu. Department of Molecular Biosciences and Bioengineering, University of Hawaii at Manoa, Honolulu HI 96822

Mass spectrometry (MS) has become an indispensible tool in proteomics. Proteomics involves identification and profiling of all proteins or as many as possible of proteins in a sample. In this presentation, two examples will be used to signify potential applications of matrix assisted laser desorption ionization tandem time of flight MS (MALDI MS) integrated with protein barcoding in agricultural and food chemistry. One is protein barcoding by MALDI MS to differentiate the geographical and floral origins of honey, which honey was used as a model food matrix. Another is MS barcoding of whole cell proteins for rapid and effective phenotypic identification of agricultural bacteria. The bacterial species that were studied include pesticidedegrading bacteria and nitrogen fixation bacteria. Several proteins were also selected as diagnostic markers. Integrative use of MS protein barcoding and diagnostic protein fragments provides a robust phenotypic approach for bacterial identification and classification.

Characterization of chitin synthase and chitinase gene families from the African malaria mosquito, *Anopheles gambiae*

Xin Zhang, xz65@k-state.edu. Department of Entomology, Kansas State University, Manhattan KS 66506

Chitin metabolism represents an attractive target site for combating insect pests as insect growth and development are strictly dependent on precisely toned chitin synthesis and degradation; this process is absent in humans and other vertebrates. However, current understanding of this process and the involved enzymes is rather limited in insects. Benzylphenolureas (BPUs) insecticides such as diflubenzuron inhibit chitin synthesis and have been widely used to control various agricultural and public health pests such as mosquito and fly larvae since the 1970's. However, the exact mechanisms of chitin synthesis inhibition are still elusive. In this study, the genes encoding two key enzymes involved in chitin biosynthesis and degradation, respectively, were identified and comprehensively characterized using reverse transcription PCR, real-time quantitative PCR, in situ hybridization, and immunohistochemichal analysis in African malaria mosquito, Anopheles gambiae. To explore the mechanisms of diflubenzuron, a non-radioactive method was adapted and optimized to examine the chitin synthase activity and its in vitro and in vivo inhibition by diflubenzuron, polyoxin D, and nikkomycin Z in mosquitoes. In addition, a chitosan/dsRNA nanoparticle-based RNA interference (RNAi) through larval feeding was developed to analyze the functions of each chitin synthase gene. This study suggested for the first time that RNAi in mosquito larvae is systemic. Furthermore, it demonstrated that the larvae fed on the nanoparticles assembled from AgCHS1 and AgCHS2 dsRNA increased larval susceptibilities to diflubenzuron and calcofluor white (CF, or dithiothreitol), respectively. These results suggest a great potential for using such a nanoparticle-based RNAi technology for highthroughput screening of gene functions and for developing novel strategies for pest management.

AGRO 103

Metolachlor fate in regionally adopted cropping systems of the SE United States

Paul M White, Jr⁽¹⁾⁽²⁾, paul.white@ars.usda.gov; Thomas L Potter⁽²⁾. (1) Sugarcane Research Unit, USDA-Agricultural Research Service, Houma LA 70360 (2) Southeast Watershed Research Unit, USDA-Agricultural Research Service, Houma LA 70360

Effective assessment of the risks of pesticide use and agronomic efficacy require data that accurately describes environmental fate under actual use conditions. This was demonstrated for the herbicide metolachlor in investigations focused on cropping systems in the southeast United States. Results showed that management practices like cover crops, co-application of fungicides, changes in herbicide formulation from liquid to granular, and gypsum may alter fate. During a field study in Southern Florida, we found metolachlor and ethane sulfonic acid levels were 16x and 2.4x lower in groundwater under cover crops. In combined field and laboratory studies in the Coastal Plain of Georgia, application of chlorothalonil and gypsum increased metolachlor DT50 by 2x and 1.5x, respectively. Granular metolachlor provided superior weed control but increases in soil persistence increase the potential for herbicide crop injury. Findings serve as a case-study and guide to investigations that are needed to make crop-specific management decisions.

AGRO 104

Degradation of *p*-nitrophenol by heterogeneous Fenton-like reactions on nano-magnetite: Process optimization using response surface methodology

Sheng-Peng Sun, ss969@cornell.edu; Ann T. Lemley. Graduate Field of Environmental Toxicology, Cornell University, Ithaca NY 14853

Heterogeneous Fenton-like reactions can effectively catalyze the oxidation of organic pollutants, including most agrochemicals at neutral pH conditions, which is beneficial for in situ remediation of polluted groundwater and soils. In the present study, degradation of the model compound pnitrophenol by heterogeneous Fenton-like reactions on nanomagnetite (Fe₃O₄) was investigated. A four factor central composite design coupled with response surface methodology was applied to evaluate and optimize the important variables. A significant quadratic model (P < 0.0001, $R^2 = 0.9442$) was obtained using analysis of variance (ANOVA), which was adequate to perform the process variables optimization. Optimum conditions for the degradation of p-Nitrophenol were determined to be 1.5 g L-1 Fe_3O_4 , 620 mM H_2O_2 , pH 7.0 and 25 - 45 mg L^{-1} pnitrophenol. Under the optimum conditions, more than 90% of p-nitrophenol was experimentally degraded after 10 h of reaction time which agreed well with the model predictions.

AGRO 105

CuO and ZnO nanoparticles affect production by a beneficial pseudomonad of metabolites important in plant performance

Christian Dimkpa, cdimkpa@usu.edu. Departments of Biological Engineering and Biology, Utah State University, Logan UT 84322

We are testing the effects of commercially available CuO and ZnO NPs on an environmental bacterium Pseudomonas chlororaphis O6 (PcO6) that increases plant growth and tolerance to stress. Secondary metabolites from this bacterium are important in interactions with other microbes (e.g., iron-chelating siderophores), plants (e.g., siderophores, auxins) and animals (e.g., antibiotics). At concentrations that did not affect long term culturability, CuO NPs reduced siderophore secretion into the media environment whereas ZnO NPs increased siderophore levels. Secretion of the plant growth-promoting auxin, indole acetic acid (IAA), by PcO6 also was differentially affected. Levels were enhanced by CuO NPs whereas ZnO NPs repressed. Thus, although the NPs may not cause lethal effects, they could modify production of metabolites involved in the interactions between plants and microbes. Concentration, shape, coatings and the ability to release metal ions are significant variables in determining the bioeffects of NPs.

Endangered Species Act: Interfacing with agricultural and natural ecosystems

Bernalyn McGaughey(1),

bmcgaughey@complianceservices.com; Lars W. J. Anderson⁽²⁾; Michael J Bodenchuck⁽³⁾. (1) CSI, Compliance Services International, Lakewood WA 98499 (2) Exotic and Invasive Weed Research, USDA-Agricultural Research Service, Davis CA 95616 (3) WS, Texas Wildlife Services, San Antonio TX 78201-1710

This presentation is based on a Council for Agricultural Science and Technology Commentary that explores the interaction between the regulatory policy of the Endangered Species Act, public perception, and science in relation to the interpretation of risk to endangered species from various stressors associated with agricultural practices. In the absence of definitive government policy, courts are establishing risk mitigation procedures that may adversely affect agricultural productivity and practices. The presentation will address several potential remedies, including (1) better communication, (2) clear policy and agency coordination, (3) recognition and consideration of long-term impacts, and (4) balanced and consistent implementation. The information in the commentary will be examined more closely by following some additional case examples not discussed in the publication.

AGRO 107

Insights from USDA on improving the ESA-pesticide assessment process

Sheryl H Kunickis, sheryl.kunickis@ars.usda.gov; Harold D Coble. Office of Pest Management Policy, US Department of Agriculture, Washington DC 20250

In response to litigation involving pesticides to protect endangered salmon, results from the current consultation process and resulting risk mitigation decisions threaten agricultural crop production in California and the Pacific Northwest. For example, it is estimated that as much as 34% of crop land will be removed because of the mandated ground and aerial buffers. Agricultural groups are frustrated as there is virtually no process to have input into the consultation process and have voiced their opinions that the data and models used do not accurately reflect agricultural practices (i.e., application rates, spray droplet sizes). USDA has a wealth of technical and programmatic resources founded on sound science that could add value to the consultation process. USDA is committed to working to ensure that agriculture is accurately reflected as we partner to protect endangered species and their habitat better - now and in the future.

AGRO 108

Growers, pesticides, and endangered species: Results of MCFA ESA workshop

Daniel A Botts, Dan.Botts@ffva.com. FFVA, Florida Fruit and Vegetable Association, Maitland FL 32794-8513

Results will be presented from the recent workshop on the role of grower-developed information in the risk assessment and risk mitigation consultation process involving the US Environmental Protection Agency, National Marine Fisheries Service, and US Fish and Wildlife Service. The workshop, sponsored by the Minor Crop Farmer Alliance, was designed to answer the following questions concerning pesticide use and potential pesticide exposure: (1) Is there grower

information that is valuable in the risk assessment and risk mitigation consultation process among the Agencies? (2) If grower information is useful, what information is most valuable, how should it be collected and entered into the process, and who screens the data for completeness and accuracy? (3) What is the appropriate entry point for growers in the evaluation process?

AGRO 109

Using litigation to push for programmatic reform of EPA's Endangered Species Protection Program

Collette L Adkins Giese,

cadkinsgiese@biologicaldiversity.org. Endangered Species, Center for Biological Diversity, Minneapolis MN 55449-5600

In January 2011, the Center for Biological Diversity and Pesticide Action Network sued the US Environmental Protection Agency for failing to consult with federal wildlife agencies over the impacts of several hundred pesticides known to be harmful to more than 200 federally threatened and endangered species across the country. Building upon previous litigation brought by the Center and other environmental groups, this national lawsuit is the most comprehensive legal action ever brought under the Endangered Species Act to protect imperiled wildlife from pesticides. In addition to discussing the national litigation, this presentation will evaluate the outcomes of previous litigation and offer suggestions for reform of EPA's Endangered Species Protection Program.

AGRO 110

Integrating FIFRA, ESA, and other legal requirements

David B Weinberg, DWeinberg@wileyrein.com. Legal, Wiley Rein LLP, Washington DC 20006

One of the greatest current challenges in pesticide regulation is the integration of FIFRA and Endangered Species Act requirements. FIFRA imposes on an expert agency deadlines to make informed decisions on product suitability, while ESA results in interminable reviews that ignore practical realities. The resulting confusion has created a framework of regulation by litigation with which no stakeholders are comfortable. This presentation will focus on up-to-themoment judicial interpretations of legal requirements and policy arena efforts to clarify and improve the evaluation process.

AGRO 111

Unintended consequences: A historical perspective on pesticides and endangered species with suggestions

Larry Turner, LTurner@ComplianceServices.com. CSI, Compliance Services International, Kelso WA 98626-8947

Since the US Environmental Protection Agency (EPA) was formed and the Endangered Species Act (ESA) was passed, the laws have seldom changed, but both EPA's risk assessment for pesticides and the responding Biological Opinions have become substantially more sophisticated over time. The early history of both of these and the development of an EPA implementation program is discussed. The nature of risk assessments used for threatened and endangered (T&E) species has paralleled those for other non-target species, but with the inclusion of more stringent criteria and site-specific considerations. The methods of consultations, responses to them, and proposed methods of implementing protections for T&E species have been subject to major influences based upon politics, resources, litigation, and

individual attitudes. Many actions of various participants have resulted in unforeseen, often unwelcome, circumstances; examples are presented. This presentation will include some suggestions for the future.

AGRO 112

Linking agricultural sustainability with healthy foods

James N Seiber, jnseiber@ucdavis.edu. Departments of Food Science and Technology and Environmental Toxicology, University of California-Davis, Davis CA 95616

The links between agriculture, food, and sustainability are receiving increasing attention. Decisions made in the agricultural field, processing plant, and wholesale and retail outlets may affect the food itself and its health beneficial and related qualities, as well as where and how it is best produced, processed, packaged, stored, and presented to the consumer. The value of the food, and increasingly the content of phytonutrients and nutraceuticals, are major factors in the success of a new food product, accompanying such well-understood qualities as taste, aroma, cost, and convenience. Carbon footprint, inputs of synthetic chemicals, fuel and energy requirements, and proximity to markets increasingly weigh in the decisions that affect the acceptability and sustainability of agricultural production leading to food products. Current strategies and trends, including the relative merits of organic versus conventionally-produced foods, will be discussed using examples from the recent literature.

AGRO 113

Studying sustainability from field to market

Terry Stone, terry-1.stone@syngenta.com; Brent Lackey; Rick Murdock; Jennifer Shaw. Sustainability Value Chain, Syngenta Crop Protection

Field to Market: The Keystone Alliance for Sustainable Agriculture brings together a diverse membership to address the agricultural challenge of the 21st century from farm to fork, while focusing on solutions that are grounded in science, focused on outcomes, and open to the full range of technology choices. Using publicly available data, the alliance has developed algorithms to create the online Fieldprint™ Calculator, a tool for corn, soybean, wheat, rice, and cotton that allows farmers to explore the environmental outcomes of their natural resource management decisions and compare those with state and national averages. This presentation will provide an overview of how the tool was developed as well as how it has been used by farmers in a pilot program. The program is designed to establish a farmer baseline and promote sustainable decisions through data analysis.

AGRO 114

Importance of herbicides for sustainable farming in the United States

Leonard Gianessi, Igianessi@croplifefoundation.org. Crop Protection Research Institute, CropLife Foundation, Washington DC 20005

Herbicides are sprayed on 220 million acres of US cropland annually. Their use has led to large decreases in the number of tillage trips for weed control. One-third of these acres are in no-till systems where herbicides substitute completely for tillage. This reduction in tillage has resulted in large decreases in soil erosion and sediment delivered to waterways. Soil moisture has been increased due to

reductions in tillage. Acres previously-fallowed have been brought into crop production due to increases in soil moisture which has resulted from the use of herbicides. Research into organic farming without the use of herbicides has substituted numerous tillage trips with associated increases in soil erosion and water use. Continued sustained soil and water conservation on US farms is dependent on the continued availability of effective herbicides. This presentation traces the history of weed control in the US, identifies the introduction of herbicides as a key milestone for sustaining soil resources, and explains the positive conservation impacts from the use of herbicides. Available data showing the impacts, on soil and water conservation, of not using herbicides are summarized.

AGRO 115

Plant biotechnology for sustainable agriculture: Research and development and an enabling policy framework

Denise Dewar, deb.carstoiu@croplife.org. Plant Biotechnology, CropLife International, Washington DC 20005

Farmers worldwide are increasingly faced with the challenge of judiciously using natural resources while feeding a growing population despite climate change and other extreme growing conditions. Sustainable agricultural practices are essential to ensuring the production of highquality foods while preserving natural resources for future generations. Innovations in plant biotechnology will enable more efficient use of water, nutrients, and maintain soil quality, and preserve natural lands. Science-based regulatory and policy frameworks, as well as capacitybuilding, are necessary to support continued agricultural research and development and the delivery of sustainable agricultural innovations to the marketplace. This session will review the sustainable agriculture product pipeline and the enabling policy environment needed to support best agricultural practices.

AGRO 116

Metabolism of [14C]dicamba in dicamba-tolerant cotton

Tracy L Whitehead, tracy.l.whitehead@monsanto.com; Mary J Mierkowski; Robert C Chott; Michael J Miller. Environmental Sciences Technology Center, Monsanto Company, St. Louis MO 63167

Dicamba (3,6-dichloro-2-methoxybenzoic acid) is a foliar or soil-applied herbicide used to control broadleaf weeds. A metabolism study was conducted with [14C]dicamba in dicamba-tolerant cotton to determine the nature of residues found in/on agricultural commodities of dicamba-tolerant cotton following treatment with radio-labeled dicamba. Small plots of dicamba-tolerant cotton were grown and treated with [14C]dicamba at two time points (preemergence and postemergence). Plants were then harvested as normal and metabolites were extracted, identified, and quantified using a combination of combustion, HPLC, LC-MS/MS, and GC-MS analyses. Metabolism of dicamba in dicamba-tolerant cotton proceeds by initial demethylation to form DCSA (3,6dichloro-2-hydroxybenzoic acid) by the action of the dicamba O-demethylase enzyme which is the product of the dicamba mono-oxygenase gene introduced to confer dicamba tolerance. DCSA is observed in cotton matrices in its free form as well as its 2-O-β-glucoside (DCSA glucoside). As a minor pathway, DCSA is converted by 5hydroxylation to DCGA (2,5-dichloro-3,6-dihydroxybenzoic acid) which is not observed in its free form but is present in cotton matrices as the 5-O- β -glucoside (DCGA glucoside).

Further metabolism of DCSA and DCGA proceeds via hydroxyl replacement of chlorine (apparently the chlorine in the 3 position), to give monochlorinated metabolites (observed as their glucosides). The minor metabolites 3,6dichloro-2-methoxybenzamide (dicamba amide) and 3,6dichloro-2-hydroxybenzamide (DCSA amide) were observed in preemergence treated matrices and are believed to be derived from soil metabolism of dicamba and subsequent uptake of the metabolites by the plants. Dicamba metabolites identified in the cotton metabolism study can be converted by acid hydrolysis primarily to the chemophores DCSA and DCGA. Thus, current residue enforcement methodology, which incorporates an acid hydrolysis step followed by methylation and analysis by GC, would be expected to be adequate for analysis of dicamba residues in dicamba-tolerant cotton in a manner similar to other crops utilizing dicamba for weed control.

AGRO 117

Sustainability standards: Biotech and organic coexistence

Thomas P Redick, tpr@geeclaw.com. Global Environmental Ethics Counsel, Clayton MO 63105

This presentation reviews sustainability standards/initiatives that address the coexistence of biotech crops and their organic or non-GMO counterparts. This would include two proposed American National Standards Institute standards (SCS-001 on sustainable agriculture and SCS-002 on lifecycle analysis), as well as the international "Global GAP" standard, the Roundtable on Responsible Soybeans and the Roundtable on Sustainable Biofuels. Biotech crops are routinely subjected to discriminatory treatment (e.g., a duty to prevent migration to organic crops) in standards that profess to be technology neutral toward biotech crops; only through direct intervention in such standard setting can these discriminatory precautionary approaches to biotech crops be modified. This presentation will discuss successful interventions and impending discrimination, particularly in biofuels standards, that may deny overseas market access and explains how standards create duties of care that can lead to negligence and nuisance liability for migration of biotech crops, further complicating biotech versus organic coexistence.

AGRO 118

Improved characterization of the temporal and spatial variability of potential surface water drinking water exposure by using environmental and historic monitoring databases

Paul Hendley⁽¹⁾, paul.hendley@syngenta.com; Wenlin Chen⁽¹⁾; Robert Joseph⁽¹⁾; Ron Williams⁽¹⁾; Chris Harbourt⁽²⁾. (1) Product Safety, Syngenta Crop Protection LLC, Greensboro NC 27409 (2) Waterborne Environmental Inc., Champaign IL 61820

The extensive atrazine surface water monitoring database totals over 300,000 samples including ~120,000 drinking water samples from high frequency seasonal monitoring programs covering more than 15 years and ~210 Community Water Systems (CWS). This wealth of frequent monitoring data sampled across a wide range of years and sites allows for robust conclusions to be drawn with very high statistical certainty regarding the highest centiles of potential atrazine exposures. To complement the monitoring data, site-specific details have also been accumulated on CWS watersheds, source waters, and water handling procedures. This information has been used to understand better the expected temporal concentration patterns at an

individual CWS. We will outline how these and related data (e.g., daily flow and chemical monitoring data from Heidelberg University) have been used to examine approaches for optimizing sampling strategies for assessing potential drinking water concentrations in surface water.

AGRO 119

Time series model for estimating pesticide exceedance probabilities for streams

Aldo Vecchia, avecchia@usgs.gov; Karen Ryberg. North Dakota Water Science Center, US Geological Survey, Bismarck ND 58503

A statistical time series model for detecting trends in pesticide concentration data from rivers and streams is extended for use in estimating *n*-day concentration exceedance probabilities for time frames of daily (n = 1) and longer. The model represents concentration data in terms of trend, seasonal variability, flow-related variability, systemic variability (true short-term variability), and noise (random perturbations related to laboratory or sampling irregularities). The trend can be empirically based and/or depend on data related to change in pesticide application amounts. Seasonal variability depends on application timing and rate, while the flow-related variability depends on orthogonal functions of daily streamflow representing different time scales. Separating systemic variability from noise and correctly identifying serial correlation in the systemic variability are particularly important considerations for estimating exceedance probabilities for different time scales. An R-based procedure for fitting the time series model is illustrated using concentration and flow data from the US Geological Survey National Water-Quality Assessment Program.

AGRO 120

Investigating sampling designs for pesticide surface water monitoring using available daily or near-daily measurements

Wenlin Chen⁽¹⁾, wenlin.chen@syngenta.com; Paul Mosquin⁽²⁾; Robert L Sielken⁽³⁾; Paul Hendley⁽¹⁾; Ron Williams⁽¹⁾; Sunmao Chen⁽¹⁾; Robert Joseph⁽¹⁾; Andrew Merritt⁽¹⁾. (1) Product Safety, Syngenta Crop Protection, LLC, Greensboro NC 27409 (2) Statistics and Epidemiology, RTI International, Research Triangle Park NC 27709 (3) Statistics, Sielken & Associates Consulting, Inc., Bryan TX 77802

High frequency sampling (e.g., daily) for water quality monitoring at multiple sites requires an intensive effort and is operationally challenging. We will present a statistical simulation method using two available data sets with daily or near-daily measurements during the pesticide application season (April 1 - July 31) to investigate various sampling frequency options. The two daily or near-daily surface water data sets were from the Ohio watershed monitoring program (Heidelberg University) and Syngenta's atrazine ecological monitoring program. Scenarios with different sampling frequencies are simulated and the results are compared to the measured data for each year and site. Performance of each scenario is quantified by metrics comparing the simulated samples to the true values from measurement. This work demonstrates how lower frequency monitoring data can be used to estimate potential maximum shorter duration concentrations. These evaluations also confirm that cost-effective sampling regimes can be designed to address water quality management needs.

Estimation of upper percentiles of chlorpyrifos surface water concentration from yearly monitoring program data

Paul L. Mosquin⁽¹⁾, mosquin@rti.org; G. Gordon Brown⁽¹⁾; Roy W. Whitmore⁽¹⁾; Nick Poletika⁽²⁾. (1) Statistics and Epidemiology, RTI International, Research Triangle Park NC 27709 (2) Field Exposure and Effects, Dow AgroSciences LLC, Indianapolis IN 46268

This talk presents a finite population method to estimate annual 95th, 99th, and 99.9th centiles of surface water chlorpyrifos concentrations and associated confidence intervals using historical surface-water pesticide-monitoring programs with a large number of measurements. The method provides reliable estimates, accounting for infrequent sample collection, measurements below reporting limits, and the strong seasonality present in these datasets. Data from three monitoring programs are considered: the USGS National Water Quality Assessment Program (NAWQA), the Heidelberg University National Center for Water Quality Research (NCWQR) monitoring data, and the Washington State Department of Agriculture/Department of Ecology surface water monitoring program. Precision of estimates and necessary sample sizes will be discussed. Results for temporal trends will be provided including a comparison of estimates before and after chlorpyrifos was withdrawn from residential use in 2001.

AGRO 122

Combining long-term herbicide monitoring with identification of vulnerable areas in restricitve layer watersheds

Robert N. Lerch, bob.lerch@ars.usda.gov; Claire Baffaut; E. John Sadler; Newell R. Kitchen; Kenneth A. Sudduth. Cropping Systems and Water Quality Research Unit, USDA-Agricultural Research Service, Columbia MO 65211

Long-term monitoring of herbicide concentrations and loads has been conducted at Goodwater Creek Experimental Watershed (GCEW) located in northeastern Missouri, a watershed dominated by soils with a naturally-formed smectitic claypan. From 1992 to 2006, trends in herbicide concentration and load were only observed for compounds in which major changes in usage had occurred. For example, atrazine use increased 25% from 1992 to 2006 and no trends were observed in load or concentration. Atrazine loads did, however, vary greatly over the 15 year period analyzed, ranging from 1 to 14% of applied. A newlydeveloped, cumulative vulnerabiliy index explained 63% of the variation in annual atrazine loads for GCEW, and it explained 85% of the variation in unit area loads when extended to the entire Salt River basin. Efforts developed to identify vulnerable areas within these watersheds have shown that the top soil depth over the claypan and slope are critical risk factors for transport by surface runoff.

AGRO 123

Application of high resolution elevation data (LiDAR) to assess natural and anthropogenic agricultural features affecting the transport of pesticides at multiple spatial scales

Joshua J Amos⁽¹⁾, amosj@waterborne-env.com; Christopher Holmes⁽¹⁾; JiSu Bang⁽²⁾; Paul Hendley⁽²⁾; Lucy Fish⁽³⁾. (1) Spatial Technologies Group, Waterborne Environmental, Inc., Leesburg VA 20175 (2) Environmental Safety, Syngenta Crop Protection, LLC, Greensboro NC 27419 (3) Environmental Safety, Syngenta Crop Protection, LLC, Braknell Berkshire RG42 6EY, United Kingdom

LiDAR (Light Detecting and Ranging) data, covering a 155 square kilometer region in Nebraska, was inspected for its utility in assessing natural and managed agricultural features at the field and watershed scales. This approach was used to assess qualitatively the landscape features affecting potential runoff at a sub-field scale. Quantitative metrics describing the topography, hydrology, and natural vegetation were calculated from the LiDAR data and summarized for all fields in the study area. Integrating high resolution aerial imagery with the LiDAR data enabled the identification of engineered features such as terracing, overhead irrigation, and intakes for tile drainage systems. Natural processes identified in the data include concentrated and diffuse flow patterns towards the edge of a field; in-field depressions with the potential for surface water storage; and vegetation diversity of riparian areas characterized by canopy height and density. Processing was conducted using publically available LiDAR and Geographic Information System (GIS) data and typical GIS software and functions. This study is intended as an initial examination into the utility of LiDAR to assess field runoff vulnerability and assist stewardship.

AGRO 124

Updates to percent crop area methods: Extending drinking water assessments to tropical climates and refinements to the regional values

Nathan Snyder⁽¹⁾, snydern@waterborne-env.com; Aldos Barefoot⁽²⁾. (1) Engineering, Waterborne Environmental Inc., Leesburg VA 20175 (2) Environmental Safety Assessment, Dupont Crop Protection, Newark DE

US EPA drinking water risk assessments utilize a percent crop area (PCA) factor derived from major crops to adjust the index reservoir modeling result and to estimate the concentration expected in surface water. Examples of improvements to the current regional PCA values used will be presented to include the use of modern watershed and cropping information for refined regional default PCAs for minor crops developed and for crop distributions within smaller watersheds. PCA factors for Hawaii and Puerto Rico will also be presented. Regional PCAs are an interim step in moving from national PCAs to PCAs developed from actual drinking watersheds. In the time since the development of regional PCAs, updates to watersheds and land cover data have become available at much higher resolution, and it is now possible to improve drinking water estimates using cropping data distributed through PCA adjusted EECs (Estimated Environmental Concentration) in actual drinking watersheds.

Development of a modeling system to estimate pesticide runoff from urban areas in California

W. Martin Williams⁽¹⁾, williamsm@waterborne-env.com; Kelly Moran⁽²⁾; Yuzhou Luo⁽³⁾; Debra L. Denton⁽⁴⁾; Richard S. Breuer⁽⁵⁾; J. Mark Cheplick⁽¹⁾; Gerco Hoogeweg⁽¹⁾. (1) Waterborne Environmental, Inc., Leesburg VA 20175 (2) TDC Environmental, San Mateo CA 94403 (3) Department of Pesticide Regulation, California Environmental Protection Agency, Sacramento CA 95812 (4) Standards and TMDL Office, US Environmental Protection Agency, Sacramento CA 95814 (5) Environmental Water Quality and Estuarine Studies, California Department of Water Resources, Sacramento CA 95814

Detections of pyrethroids and other insecticides in aquatic systems around urban areas in California have raised concerns about pesticide runoff from outdoor applications in urban and residential settings. Modeling pesticide transport from urban areas is an uncertain endeavor due to a lack of detailed data and established modeling procedures. A modeling system was developed to estimate the runoff of five widely-used pyrethroids across a 164,000 km² study area in California. County-level, use data were spatially distributed across the study area using detailed land use data. Homeowner and professional applicator surveys were used to allocate pyrethroid applications to buildings, lawns, and other impermeable and permeable surfaces. Washoff studies were used to develop model input parameter values for hard surface applications. Pyrethroid runoff corresponding to rainfall and to irrigation events were simulated to provide a better understanding of the spatial and temporal distribution of pyrethroid mass loadings to aquatic systems in the study area.

AGRO 126

Applying advances in chemistry to benefit developing world agriculture

Deborah Delmer⁽¹⁾, ddelmer@gmail.com, One Shields Avenue, Davis California 95616 . (1) College of Biological Sciences, University of California-Davis, Davis California

According to the IFAD Rural Poverty Report of 2011, 70% of the world's 1.4 billion extremely poor live in rural areas. This fact naturally places a high priority on enhancing the productivity and economic viability of small-holder agriculture in the developing world. Constraints to such agriculture are numerous and include lack of access to improved varieties of crops and livestock, high disease pressure coupled with low use of pesticides, poor soil fertility coupled with rising costs of fertilizer, poor water management, weak infrastructure, poorly organized output markets, and lack of strong pro-agriculture policies. Coupled with rising food and energy costs and increasingly erratic weather patterns, the challenges are great. Since many of these problems might be ameliorated with better application of existing technologies, one might ask how cutting-edge advances in science, and, in particular, in the various branches of chemistry, are also relevant. This lecture will highlight how new advances in the various branches of chemistry such as low-temperature catalysis, nanotechnology, new approaches to energy production, chemical genomics, biochemistry and molecular genetics have the potential to make significant contributions to the advancement of global agriculture.

AGRO 127

Method for the analysis of atrazine, simazine, metolachlor, and atrazine metabolites in water samples collected by polar organic chemical integrative sampler

Julie Eble⁽¹⁾, julie.eble@criticalpathservices.com; T.J. Mayer⁽²⁾; Michael F Pennell⁽¹⁾; Karen M L'Empeurer⁽¹⁾; Ganesh S Moorthy⁽¹⁾; Spencer Drummond⁽¹⁾; Sidney J Hill⁽¹⁾. (1) Critical Path Services, LLC, Garnet Valley PA 19060 (2) Syngenta United States

A method was developed for the recovery and analysis of residues of atrazine, simazine, s-metolachlor, and the atrazine metabolites, deethylatrazine (DEA), deisopropylatrazine (DIA), and 2-chloro-4,6-diamino-striazine (DACT), continuously collected from stream water using POCIS samplers. After shipping, individual POCIS units were disassembled, the sorbent removed and the analytes extracted from the sorbent with acetonitrile. The solvent in the resulting extracts was exchanged for acetonitrile/water (5:95) to facilitate analysis by LC-MS/MS using reversed-phase chromatography. The LOQ (limit of quantitation) for atrazine, simazine, s-metolachlor, and the atrazine metabolites DEA (G30033) and DIA (G28279) was 0.5 ng in the POCIS (0.1 ppb as injected); the LOQ for DACT (G28273) was 5 ng in the POCIS (1 ppb as injected). Method specifics including recovery data will be presented. The strengths and weaknesses of the approach and possible options for future work will also be discussed.

AGRO 128

LC-MS/MS analytical method for the determination of PREVICUR residues in poultry matrices and eggs

Tony Nguyen, tony.nguyen1@bayer.com; Sean Moore. R&D, Bayer CropScience, Stilwell KS 66085

An analytical method was developed for the determination of PREVICUR (Propyl [3-(dimethylamino)propyl]carbamate; propamocarb) residues in poultry tissues and eggs. PREVICUR is a systemic fungicide and seed treatment product manufactured by Bayer CropScience for specific control of *Phycomycetous* disease in turf, ornamentals, vegetables, seeds, golf courses, and tobacco. The analytical method involved extraction with acetonitrile (ACN) and diluting with the initial extract. PREVICUR residues in the diluted extract were then quantitated by LC/ESI-MS using a Thermo Finnigan Quantum Ultra AM triple quadrupole mass spectrometer. The limit of quantitation (LOQ) was 0.01 ppm for all the matrices, with Limit of Detection (LOD) values ranging from 0.005 ppm to 1.0 ppm . Recovery at the LOQ for the various matrices all ranged from 95 to 109%.

AGRO 129

Application of capillary electrophoresis to identification of pesticide photolysis products

Randy Weintraub,

randy.weintraub@symbioticresearch.net; Dan Safapour. Environmental Fate, Symbiotic Research, Mount Olive NJ

Photolysis is a potential significant route of pesticide transformation in the environment. Evaluating the photodegradation products often presents an analytical challenge to the environmental fate scientist. Unchanged pesticide and photodegradates often encompass a board range of polarities and frequently include highly polar compounds. Attempts to resolve all these analytes in a single chromatographic run can be time-consuming and still remain

incomplete. Highly polar analytes often remain ambiguous or and difficult to evaluate whether individual photodegradates qualify as 'significant' by exceeding 10% of total residues. Capillary electrophoresis (CE) offers a versatile alternative to high performance liquid chromatography (HPLC) to tackle these challenges in pesticide photolysis studies. We present CE coupled with mass spectrometry in studying aqueous photolysis of imidacloprid and pendimethalin, and compare results to HPLC and published literature.

AGRO 130

Analysis of bee relevant matrices for imidacloprid, imidacloprid olefin, and 5-hydroxy imidacloprid by modified QuEChERS extraction and analysis by LC/MS/MS with stable, isotopically-labeled internal standard

Jaime Brungardt, jaime.brungardt@bayer.com; Bill Leimkuehler. Environmental Research, Bayer CropScience, Stilwell KS 66085

The analytical method measures residues of imidacloprid and its metabolites, imidacloprid-olefin, and 5-hydroxy imidacloprid, in bee relevant matrices. Nectar is prepared directly by dilution with HPLC mobile phase containing a stable, isotopically-labeled internal standard. Other bee related matrices, such as pollen, blooms, and whole honey bees are extracted using QuEChERS methodology (i.e., hydration, salting-out, and extraction with acetonitrile and a one-step clean-up with dispersive SPE using Bondesil-PSA). The extracts are analyzed by high performance liquid chromatography/tandem mass spectrometry (LC/MS/MS). The method limit of quantitation (LOQ) is 1 ppb in nectar and 2 ppb in other bee relevant matrices.

AGRO 131

Quantitative determination of thiamine in corn (*Zea mays*) grain by high performance liquid chromatography-tandem mass spectrometry

Fred A Claussen, fclaussen@eplbas.com. Agricultural Chemistry, EPL Bio Analytical Services, Niantic IL 62551

A procedure for the determination of thiamine (vitamin B1) in corn (Zea mays) grain utilizing high performance liquid chromatography with tandem mass spectrometry detection (HPLC-MS/MS) was validated. New HPLC columns containing a pentalflurophenylpropyl (PFPP) stationary phase provide an improved means of analyzing polar molecules by HPLC. Water soluble vitamins such as thiamine have been particularly troublesome due to silanol interactions which result in peak tailing. When coupled with tandem mass spectrometry detection, the PFPP column becomes even more powerful due to sensitivity and selectivity advantages. The reported method provides a rapid, sensitive and selective technique for the determination of thiamine in corn grain to support nutrient composition studies with biotech seed. These studies are required by regulatory agencies to determine if any unintended changes in the nutritional profile of biotech seeds occur. The assay precision was 5%. Spiking recovery values ranged from 78-106%. The method limit of quantitation (LOQ) was 0.5 ppm.

AGRO 132

Extraction of microbial secondary metabolites from fermentation broths using polymeric resins

Gary Yuen, gyuen@marronebio.com; Ratnakar N Asolkar; Vu Bui; Huazhang Huang; Marja E Koivunen; Pamela G Marrone. Department of Chemistry, Marrone Bio Innovations, Davis CA 95618

Microbial secondary metabolites produced in fermentation are viable sources for new biopesticides with novel modes of action. Concentration and isolation of bioactive compounds require efficient extraction of metabolites in the microbial whole cell broth. Conventionally, liquid-liquid extraction using organic solvents has been the method of choice. We explored the idea of extracting natural product compounds using polymeric adsorbents with variable surface area and pore envelope size: Amberlite XAD4, XAD16 and XAD7HP. For extraction efficiency experiments, three natural product compounds with different molecular weights and logP values were used: gibberellic acid (GA3), thaxtomin A, and emodin. Amberlite XAD4 was most efficient in binding highly water soluble compounds such as GA3. Both aromatic XAD16 and acrylic XAD7HP extracted hydrophobic compounds (thaxtomin and emodin) more efficiently than the aromatic resin, XAD4. Based on extraction efficiencies, an optimal resin mixture for fermentation broths was designed and tested against the common ethyl-acetate liquid-liquid extraction.

AGRO 133

New pesticidal compounds from Burkholderia sp

Ratnakar N Asolkar, rasolkar@marronebio.com; Marja E Koivunen; Ana Lucia Cordova-Kreylos; Huazhang Huang; Lisa Chanbusarakum; Pamela G Marrone. Marrone Bio Innovations, Davis CA 95618

Natural products from microbial sources have been successfully used for the development of new biopesticides for crop protection. Interesting chemical structures and novel modes of action make these secondary metabolites very attractive due to improved efficacy, environmental and non-target safety, and resistance management. As part of a search for new leads for biopesticides, microbes isolated from various sources are screened for activities against various pests such as insects, plant pathogens, nematodes and weeds. A novel bacterium Burkholderia sp. Isolated from a soil sample has shown potent insecticidal, fungicidal, nematicidal and herbicidal activities. Bioassay-quided isolation of the active fermentation broth resulted in the discovery of active metabolites belonging in three different structural classes. New compounds named templazole A and B and templamide A and B show good pesticidal activity. Studies are underway to identify remaining bioactive secondary metabolites, to optimize fermentation medium, and to enhance pesticidal efficacy via formulation development.

Using microbes for synthesizing agrochemical metabolites

Mark J Schocken, SchockenConsult@aol.com. Department of Consulting Services, Schocken Consulting, LLC, Sudbury MA 01776

Using common microbes to synthesize potential metabolites of agrochemicals in sufficient quantities can serve as an important alternative to conventional chemical synthesis for preparing reference standards or to predict metabolic/degradation pathways in animals, plants and soils. Certain microbial species have been shown to produce metabolites of agrochemicals remarkably similiar to those produced by mammals, birds, fish, soil and, to some extent, plants. This similarity in metabolite profile is largely explained by the presence of cytochrome P-450monooxygenases in these organisms. This poster reviews results of previously published microbial transformations of the fungicide cyprodinil, the herbicide clomazone and other pesticides and compares microbial metabolites to metabolites/degradates formed in animal, plant and soil metabolism studies to demonstrate the utility of the approach.

AGRO 135

Discovery of spiroindolines: A new class of insecticides with a novel mode of action

Peter Maienfisch⁽¹⁾, peter.maienfisch@syngenta.com; Jerome Cassayre⁽¹⁾; Richard S Roberts⁽¹⁾; Paul A Worthington⁽¹⁾; Dave J Hughes⁽¹⁾; Louis-Pierre Molleyres⁽¹⁾; Fredrik Cederbaum⁽¹⁾; Elke Hillesheim⁽¹⁾; Ann Sluder⁽²⁾; Fergus Earley⁽¹⁾; Sheetal Shah⁽¹⁾. (1) Syngenta Crop Protection AG, Basel CH-4002, Switzerland (2) Cambria Biosciences LLC, Woburn MA 01801

Substituted spiro[indoline-3,4'-piperidine] compounds (spiroindolines) are a recently discovered class of insecticides which act at the vesicular acetylcholine transporter (VAChT). Our initial optimization program resulted in the discovery of SYN876, a new exploratory insecticide for the control of lepidopteran pests. This presentation will describe the discovery, optimization, synthesis, biology, mode of action and some structure-activity relationships of these novel spiroindoline compounds.

AGRO 136

Effect of halogen and trifluoromethyl substituents on the biological activity of spiroindolines

Peter Maienfisch, peter.maienfisch@syngenta.com; Jerome Cassayre; Louis-Pierre Molleyres; Richard S Roberts; Dave J Hughes; Elke Hillesheim. Syngenta Crop Protection AG, Basel Basel CH-4002, Switzerland

Spiroindolines are a recently discovered class of insecticides active against a wide range of lepidopteran pests. As part of our optimization program we investigated the effect of halogen and trifluoromethyl substituents on the spiroindoline core (R1), the cinnamyl moiety (R2) and the pyridyl group (R3). This presentation will report the synthetic methodology applied to the preparation of our target compounds as well as the biological activity and structure-activity relationships of halogenated and trifluoromethyl substituted spiroindolines.

AGRO 137

Synthesis and biological activity of spiroindoline *N*-oxides

Peter Maienfisch, peter.maienfisch@syngenta.com; Richard S Roberts; Jerome Cassayre; Louis-Pierre Molleyres; Tammo Winkler; Elke Hillesheim. Syngenta Crop Protection AG, Basel CH-4332, Switzerland

Syngenta researchers have recently discovered a new class of exploratory insecticides active against a wide range of lepidopteran pests – the spiroindolines. In order to alter the physico-chemical properties of the lead compound SYN876, such as lipophilicity, basicity and photostability, we designed and synthesized the spiroindolines-*N*-oxides. This presentation will report the synthesis, insecticidal activity, properties and structure-activity trends of this novel spiroindoline subclass.

AGRO 138

Effect of bedding material on air quality of bedded manure packs in livestock facilities

Mindy J. Spiehs⁽¹⁾, mindy.spiehs@ars.usda.gov; Tami M. Brown-Brandl⁽¹⁾; Daniel N. Miller⁽²⁾; David B. Parker⁽¹⁾. US Meat Animal Research Center, USDA-Agricultural Research Service, Clay Center NE 68933 (2) Agroecosystems Management Research Unit, USDA-Agricultural Research Service, Lincoln NE 68583

Bedding materials may affect air quality in livestock facilities. The objective of this study was to compare headspace concentrations of odorous volatile organic compounds (VOCs), total reduce sulfur (TRS), CO₂, CH₄, and N₂O when corn stover, bean stover, wheat straw, switch grass, pine wood chips, pine wood shavings, ground corn cobs, and paper were used as bedding in lab-scale bedded manure packs. Ground corn cobs and paper produced higher VOCs, CO₂, and CH₄ concentrations than other bedding materials. Wood shavings also produced high concentrations of CO₂ but had significantly lower VOC concentrations than other bedding materials. Corn stover had the highest TRS concentration. Nitrous oxide was similar across all bedding treatments. Results of this study indicate that ground corn cobs or paper may increase odor and greenhouse gas production when used in deep-bedded livestock facilities.

AGRO 139

Flow characteristics of a dynamic flux chamber

Bryan Woodbury, bryan.woodbury@ars.usda.gov; David Parker; Roger Eigenberg; Mindy Spiehs. US Meat Animal Research Center, USDA-Agricultural Research Service, Clay Center NE 68933

Gases are emitted from accumulated manure on the feedlot surface. Research has shown these emissions are not uniform across the pen. Considerable research has gone into measuring feedlot emissions using a variety of modeling methods. However, these methods do not allow for assessing spatial variability across the pen surface. Flux chamber can measure spatial variability; however, the internal flow characteristics of these chambers have not been documented. Understanding the chamber flow characteristics will improve the application of this technology for determining emissions from feedlot surfaces. A series of tracer studies have been conducted at flow rates of 1, 5 and 10 L min⁻¹ to determine tracer break-through curves. Moment analysis of the tracer gas break-through-curve will be done to evaluate internal flow characteristics.

Volatile organic compounds in pesticide formulations: Methods to estimate ozone formation potential

Laura L McConnell⁽¹⁾, laura.mcconnell@ars.usda.gov; Mazyar Zeinali⁽²⁾; Cathleen J Hapeman⁽¹⁾; Anh Nguyen⁽¹⁾; Walter F Schmidt⁽¹⁾; Cody J Howard⁽¹⁾. (1) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, Beltsville MD 20705 (2) nEnvironmental, LLC, Columbia MD

The environmental fate and toxicity of active ingredients in pesticide formulations has been investigated for many decades, but relatively little research has been conducted on the fate of pesticide co-formulants or inerts. Some coformulants are volatile organic compounds (VOCs) and can contribute to ground-level ozone pollution. Effective product assessment methods are required to reduce emissions of the most reactive VOCs. Six emulsifiable concentrate pesticide products were characterized for percent VOC by thermogravimetric analysis (TGA) and gas chromatographymass spectrometry (GC-MS). TGA estimates exceeded GC-MS by 10 - 50% in all but one product, indicating that for some products a fraction of active ingredient is released during TGA or that VOC contribution was underestimated by GC-MS. VOC profiles were examined using TGA-Fourier transform infrared (FTIR) evolved gas analysis and were compared to GC-MS results. An ozone formation potential (OFP) for each product was calculated using the chemical composition from GC-MS and published maximum incremental reactivity (MIR) values. OFP values ranged from 0.1 to 3.1 g ozone/g product. A 24-h VOC emission simulation was developed for each product assuming a constant emission rate calculated from an equation relating maximum flux rate to vapor pressure. Results indicate 100% VOC loss for some products within a few hours, while other products containing less volatile components will remain in the field for several days after application. An alternate method to calculate a product OFP was investigated utilizing the fraction of the total mass of each chemical emitted at the end of the 24-h simulation.

AGRO 141

Atmospheric contributions of endosulfan to South Florida ecosystems

Cathleen J Hapeman⁽¹⁾, cathleen.hapeman@ars.usda.gov; Laura L McConnell⁽¹⁾; Thomas Potter⁽²⁾; Bruce Schaffer⁽³⁾; Richard Curry⁽⁴⁾. (1) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, Beltsville MD 20705 (2) Southeast Watershed Research Laboratory, USDA-Agricultural Research Service, Tifton GA 31793 (3) Tropical Research and Education Center, University of Florida, Homestead FL 33031 (4) Biscayne National Park, National Park Service, Homestead FL 33033

The environmental health of the unique and fragile ecosystems of South Florida has been declining. Initially, nutrient inputs from agricultural activities and urban encroachment have been implicated in contributing to the loss of organism diversity; however, the frequent prophylactic application of pesticides is being examined as another possible challenge to these sensitive ecosystems. Pesticide release to the atmosphere is enhanced in this region due to the calcareous soils, low-water holding capacity, frequent rainfall and irrigation, high humidity and temperatures, and a transmissive aquifer system. Endosulfan has previously been identified as presenting a major hazard potential to aquatic organisms in this region. Air and rain samples were collected over five-year period and results suggest that the atmospheric contributions of

endosulfan may be much greater than previously realized. These data will be useful for regulators, extension specialists, and decision-makers in modifying agricultural management practices to protect sensitive ecosystems.

AGRO 142

Standardization of flux chambers and wind tunnels for area source emission measurements at animal feeding operations

David B Parker⁽¹⁾, david.parker@ars.usda.gov; Bryan L Woodbury⁽¹⁾; Steven L Trabue⁽²⁾; Lingshuang Cai⁽¹⁾; Mindy J Spiehs⁽¹⁾; Roger A Eigenberg⁽¹⁾; Tami M Brown-Brandf⁽¹⁾; Marty B Rhoades⁽³⁾; Edward A Caraway⁽³⁾. (1) US Meat Animal Research Center, USDA-Agricultural Research Service, Clay Center NE 68933 (2) National Laboratory for Agriculture and the Environment, USDA-Agricultural Research Service, Ames IA 50011 (3) Department of Agricultural Sciences, West Texas A&M University, Canyon TX 79016

Researchers and practitioners have used many varied designs of wind tunnels and flux chambers to measure the flux of volatile organic compounds, odor, and ammonia from area sources at animal feeding operations. The measured fluxes are used to estimate emission factors or compare treatments. We show that flux of these gas-film limited compounds varies greatly among the types and configurations of measurement devices, leading to highly varied flux estimations of unknown accuracy or comparability. A method was developed for standardizing and comparing flux measurements among the various devices. The method is based on mass-balance-measured evaporative flux at standard temperature. We demonstrate the method using the USEPA flux chamber and two wind tunnels. The method can be adapted to any design of flux chamber or wind tunnel using standard equipment at low

AGRO 143

Modeling pesticides and their chemical transformation products

Rong Li⁽¹⁾⁽²⁾, rongli@ucar.edu. (1) Atmospheric Chemistry Division, National Center for Atmospheric Research (NCAR), Boulder CO 80301 (2) Department of Mechanical Engineering, University of Colorado, Boulder CO 80301

Pesticides have adverse health effects, yet their transformation products may be more toxic and persistent than their parent compounds. To our knowledge, there have been no studies that investigated the regional distribution and behaviour of chemical transformation products of pesticides in the environment. Using a multi-media model that we developed, we modeled toxaphene, an insecticide, and its chemical transformation products in North America. The model can simulate complex atmospheric interactions among many species including pesticides, their reaction products, particulate matter, and ozone. Results show that atmospheric concentrations of the transformation products have strong spatial and temporal variability and can reach the levels that are higher than those of the parent pesticide. While analytical standards are typically lacking for pesticide chemical transformation products, and the life cycle impact assessments typically focus only on the effects of the parent compound, it may be necessary to consider transformation products in chemical risk assessments.

Monitoring of endocrine disrupting chemicals (EDCs)suspected pesticide residues in orchard soils in Korea

Jae Yun Lee⁽¹⁾, qufvv@naver.com; Hyun Ho Noh⁽¹⁾; Kyung Won Kang⁽¹⁾; Kwang Hun Lee⁽¹⁾; Hyo Kyoung Park⁽¹⁾; Song Lim Choi⁽¹⁾; Eun Young Lee⁽²⁾; Kee Sung Kyung⁽¹⁾. (1) Chungbuk National University, Republic of Korea (2) Dongbu Hannong Co., Ltd., Republic of Korea

Seventeen pesticides which were suspected as endocrine disrupting chemicals (EDCs) classified by World Wildlife Fund (WWF) have been using in agricultural field in Korea. This experiment carried out to survey the residual characteristics of the EDCs-suspected pesticides in orchard soils. Forty samples were collected from orchard soils in Korea and pesticide residues in the soil were analyzed with a GLC and an HPLC by multiresidue analysis method, followed by confirmation of the suspected peaks as pesticide by mass spectrometry. Two pesticides such as endosulfan and fenvalerate were detected from 12 samples, representing detection rate was 30%. Concentration of EDCs-suspected pesticides detected from the orchard soils ranged from 0.041 to 0.219 mg/kg in case of endosulfan (sum of endosulfan and endosulfan sulfate).

AGRO 145

Search for neuraminidase inhibitors from Okinawan plants

Shinkichi Tawata⁽¹⁾, b986097@agr.u-ryukyu.ac.jp; Atul Upadhyay⁽²⁾; Jamnian Chompoo⁽²⁾; Tadahirio Makise⁽³⁾. (1) Faculty of Agriculture, University of Ryukyus, Nishihara-cho Okinawa, Japan (2) Department of Biochemistry and Applied Bioscience, Kagoshima University, Kagoshima, Japan (3) Plant Sciences, Makise Clinic, Nagagusuku Okinawa, Japan

With the ever present threat of a pandemic derived from influenza viruses and the emergence of resistant to synthetic drugs, the importance of the search for novel compounds from plant-based source intensifies. In this regard, we investigated the neuraminidase (NA) inhibitory compounds in two Okinawan plants, Alpinia zerumbet (alpinia) and Leuceana leucocephala (leuceana). We isolated 5,6dehydrokawain, dihydro-5,6-dehydrokawain (DDK), and labdadiene from the rhizomes of alpinia. These compounds showed mixed type inhibition with IC₅₀ ranging from 24.6 to 36.6 mM. It was also found that DDK was a slow, timedependent reversible inhibitor of NA with probably methoxy group as its functionally active site. We also isolated a nonprotein amino acid, mimosine from leuceana and examined its NA inhibitory activities. We found that mimosine showed competitive inhibition with an IC₅₀ of 9.8 mM and Km value of 0.0012 min⁻¹. Since our study revealed that Okinawan plants contain different kinds of NA inhibiting compounds, we continue identifying active compounds from different Okinawan plants and synthesizing more potent compounds analogs.

AGRO 146

Time-course residual characteristics of cyflufenamid and fluquinconazole in squash

Kwang Hun Lee⁽¹⁾, 00984800@hanmail.net; Hyun Ho Noh⁽¹⁾; Kyung Won Kang⁽¹⁾; Jae Yun Lee⁽¹⁾; Hyo Kyoung Park⁽¹⁾; Song Lim Choi⁽¹⁾; Sang Soon Yun⁽²⁾; Seok Won Shim⁽²⁾; Myung Soo Anh⁽²⁾; Kwang III Kim⁽²⁾; Chung Woo Jin⁽²⁾; Jae Choel Ryu⁽²⁾; Sang Kyun Oh⁽²⁾; Kee Sung Kyung⁽¹⁾. (1) Chungbuk National University, Republic of Korea (2) National Agricultural Products Quality Management Service, Republic of Korea

This study was carried out to elucidate the time-course residual pattern of the commonly used fungicides, cyflufenamid and fluquinconazole in squash. The pesticides were sprayed onto the squash at recommended and double doses at the 10 days before the harvest and then sampling was done at 0, 1, 2, 3, 5, 7 and 10 days after spraying under greenhoues conditions. The amounts of pesticides residues in the crop were analyzed with HPLC-DAD and GC-ECD. Limites of detection (LODs) were 0.01 mg/kg for cyflufenamid and 0.001 mg/kg for fluquinconazole. Mean of the recoveries were from 85.63 to 93.66% in case of cyflufenamid and from 92.00 to 102.85% in case of fluquinconazole, respectively. Biological half-lives of cyflufenamid and fluquinconazoleethyl were 1.7 and 1.3 days at the recommended dose and 2.5 and 1.5 days at the double dose, respectively. Initial amount of test pesticides at the recommended and double doses exceeded their MRLs, but residue concentrations of pre-arranged harvest were less than their MRLs. The estimated daily intakes (EDIs) of the pesticides in the crop harvested at 10 days after spraying were less than 1.6% of their acceptable daily intakes (ADIs), representing that risk of the pesticides would be very low.

AGRO 147

Establishment of pre-harvest residue Ilmits (PHRL) of fungicide myclobutanil and dimethomorph in Korean melon under greenhouse condition

Ji-Hwan Kim, jekim@knu.ac.kr; Young-Hwan Jeon; Hyoyoung Kim; Jung-In Hwang; Ji-Woon Ahn; Jang-Eok Kim. Department of Applied Biosciences, College of Agriculture and Life Sciences, Kyungpook National University, #1370 Sangyuk-dong, Buk-gu, Deagu Deagu Metropolitan City 702-701, Republic of Korea

Pre-Harvest Residue Limits (PHRL) of myclobutanil and dimethomorph during cultivation of Korean melon were established by utilizing the dissipation curve and biological half-life. Initial concentrations of myclobutanil in Korean melon were 0.14 mg/kg and 0.23 mg/kg at recommended and double dose rate, respectively, of which those were below KFDA MRL 1.0 mg/kg. The equations of biological halflife were determined by $C_t = 0.1204e^{-0.136x}$ (half life: 5.1 days) and $C_t = 0.2073e^{-0.11x}$ (half life: 6.3 days) at recommended and double dose rate, respectively. In case of dimethomorph, initial concentrations were 0.17 mg/kg and 0.27 mg/kg, below MRL 0.5 mg/kg, and biological half-life equations were $C_t = 0.1235e^{-0.157x}$ (half life: 4.4 days) and C_t = $0.2604e^{-0.051x}$ (half life: 13.6 days). Therefore, the PHRLs of myclobutanil were recommended as 2.97 and 1.72 mg/kg for 10 and 5 days before harvest, respectively, and in case of dimethomorph was recommended as 0.99 and 0.70 mg/kg, respectively.

Residual characteristics and estimated dietary intake of emamectin benzoate in leaf mustard

Sang Soon Yun⁽¹⁾, yss0520@naqs.go.kr; Yun Jeong Kim⁽¹⁾; Seok Won Shim⁽¹⁾; Kwang III Kim⁽¹⁾; Chung Woo Jin⁽¹⁾; Sang Kyun Oh⁽¹⁾; Jae Choel Ryu⁽¹⁾; Sang Youn Park⁽¹⁾; Hyun Ho Noh⁽²⁾; Kee Sung Kyung⁽²⁾. (1) National Agricultural Products Quality Management Service, Republic of Korea (2) Chungbuk National University, Republic of Korea

This study was carried out to investigate the residue patterns and estimate the dietary intakes of the commonly used insecticides, emamectin benzoate in leaf mustard under greenhouse conditions. The pesticide was sprayed onto the leaf mustard at recommended and double doses at the 7 days before the harvest and then sampling was done at 0, 1, 2, 3, 4, 5, 6 and 7 days after spraying. The analytical samples were prepared by Quick, Easy, Cheap, Effective, Rugged and Safe (QuEChERS) method and the pesticide residue was determined by LC-MS/MS. Limites of detection (LODs) of emamectin benzoate was 0.002 mg kg-1 and its recovery ranged from 105.7 to 107.3%. Biological half-lives of emamectin benzoate were 0.8 days at the recommended dose and 1.0 days ate the double dose. The estimated daily intakes (EDIs) of the pesticide in the crop harvested at 4 days after spraying was less than 0.4% of its acceptable daily intakes (ADIs), representing that risk of the pesticide would be low.

AGRO 149

Monitoring of pesticide residues in leafy vegetables collected from wholesale and traditional markets in Korea

Kee Sung Kyung⁽¹⁾, kskyung@cbnu.ac.kr, Seongbong-ro 410, Cheongju Chungcheongbuk-do, Republic of Korea; Hyun Ho Noh⁽¹⁾; Kyung Won Kang⁽¹⁾; Kwang Hun Lee⁽¹⁾; Jae Yun Lee⁽¹⁾; Hyo Kyoung Park⁽¹⁾; Song Lim Choi⁽¹⁾; Eun Young Lee⁽²⁾. (1) Chungbuk National University, Republic of Korea (2) Dongbu Hannong Co., Ltd., Republic of Korea

In order to monitor residue pattern and to assess dietary intake of pesticides in the leaf vegetables on the markets in Korea, twenty-three leafy vegetables, such as chard, perilla leaves, welsh onion, water dropwort, broccoli, lettuce leaves, red lettuce leaves, celery, spinach, shinsuncho, Korean cabbage, kale, wrap kale, crown daisy, marsh mallow, cabbage, lettuce head, Chinese cabbage, radish leaves, red chard, Chinese vegetable, chicory, leek, were collected from markets on July and August in 2010. A total of 637 samples were analyzed by multi-residue analysis method using a GLC-ECD/NPD and an HPLC-DAD/FLD and confirmed with a GC-MSD for suspected peak of pesticides in leafy vegetables. Six pesticides, such as alachlor, diazinon, dicofol, dithiopyr, chlorfenapyr and metolachlor, were detected from 8 samples. Detection frequency of the pesticides was 1.3% but amount of all of pesticides detected were below their maximum residue limit (MRL). No difference in residual patterns of pesticides observed between the wholesale and traditional markets. The estimated daily intakes (EDIs) of the pesticides detected were less than 15.7% of their acceptable daily intakes (ADIs).

AGRO 150

Multiresidue analysis method for unregistered oragnophosphorus pesticides in Korea for imported agricultural products

Young-Hwan Jeon⁽¹⁾, jekim@knu.ac.kr; Hyo-Young Kim⁽¹⁾; Jeong-In Hwang⁽¹⁾; Jung-Ah Do⁽²⁾; Moo-Hyeog Im⁽²⁾; Joong-Keun Lee⁽³⁾; Young-Deuk Lee⁽⁴⁾; Jang-Eok Kim⁽¹⁾. (1) Department of Applied Biosciences, Kyungpook National University, Daegu Daegu Metropolitan City 702-701, Republic of Korea (2) National Institute of Food and Drug Safety Evaluation, Osong 363-951, Republic of Korea (3) Korea Health Industry Development Institute, Osong 363-951, Republic of Korea (4) Division of Life and Environmental Science, Daegu University, Daegu 712-714, Republic of Korea

Organophosphorus pesticides are still widely used around the world. The official analytical method of 17 organophosphorus pesticides which were unregistered for use in Korea needs to be check the residue amounts of them for imported agri-food. Brown rice and orange used as representative samples are extracted with acetonitrile in the presence of sodium chloride to induce liquid phase separation. The acetonitrile phase is subjected to further clean-up with SPE florisil cartridge using 20% acetone/nhexane. The recovery rates of 17 pesticides in fortified matrix with levels of 0.04 and 0.4 mg/kg were between 80.1% and 108%, respectively. The limit of quantification for all pesticides by GC-FPD was 0.04 mg/kg. The characteristics of this method were confirmed with selectedion monitoring program on GC-MS, the retention times and monitoring ions. This method can surely be used as an official method for routine analysis of unregistered organophosphorus pesticides in Korea for imported agrifood.

AGRO 151

Estimation of the dietary intake of flusilazole and hexaconazole in squash at different sampling stage before harvest

Hyun ho Noh⁽¹⁾, pavar@hanmail.net; Kwang hun Lee⁽¹⁾; Jae Yun Lee⁽¹⁾; Kyung Won Kang⁽¹⁾; Song Lim Choi⁽¹⁾; Hyo Kyuong Park⁽¹⁾; Sang Soon Yun⁽²⁾; Chung Woo Jin⁽²⁾; Sang Kyun Oh⁽²⁾; Kee Sung Kyung⁽¹⁾. (1) Chungbuk National University, Republic of Korea (2) National Agricultural Products Quality Management Service, Republic of Korea

In order to estimate the dietary intake of the fungicide flusilazole and hexaconazole in squash at different stage before harvest, the pesticides were sprayed onto the squash at recommended and double doses 10 days before harvest and then sampling was done at the prearranged day after spraying. And then, their residues were analyzed with a GC-NPD. Detection limits of the pesticides were 0.005 mg·kg-1 for flusilazole and 0.004 mg·kg-1 for hexaconazole and mean recoveries of flusilazole and hexaconazole were from 91.52 to 102.02% and from 99.70 to 105.28%, respectively. Amount of flusilazole and hexaconazole on the application day of sprayed pesticides in squash were 0.095 and 0.040 mg kg-1 for recommended dose and 0.147 and 0.061 mg·kg-1 for doubled dose, respectively. Residue level of the harvest day of 10 day after spraying in squash was less than the LOQ of both flusilazole and hexaconazole. Half-life of flusilazole in squash were 1.9 days at the recommended dose and 2.2 days at the doubled dose. And also that of hexaconazole in squash were 1.2 days at the recommended dose and 1.5 days at the doubled dose. The estimated dietary intakes of the test pesticides by intake of the crop

harvested 10 days after spraying was estimated less than 2.1% of their ADIs.

AGRO 152

Regulatory improvements to the Endangered Species Act consultation process for pesticide registrations

Ya-Wei Li, yli@defenders.org; Jason Rylander; Caroline Kennedy. Endangered Species, Defenders of Wildlife, Washington DC 20036

This presentation will first summarize what we believe are the most important parameters and goals of section 7(a)(2) pesticide consultations. This includes the need for US Environmental Protection Agency (US EPA) to complete consultations with US Fish and Wildlife Service (USFWS) before registering any new pesticides. Our presentation will then discuss regulatory and policy recommendations that would enable US EPA and USFWS to complete hundreds of nationwide consultations more efficiently and effectively. This discussion will underscore how US EPA's current ecological risk assessment must become more effective at addressing the impacts of pesticide use on imperiled species.

AGRO 153

Application of the Endangered Species Act's best scientific data available standard

Patrick J. Donnelly⁽¹⁾, pdonnelly@crowell.com; L. Michael Bogert⁽¹⁾; Lorenz R. Rhomberg⁽²⁾. (1) Crowell & Moring LLP, Washington DC 20004 (2) Gradient Corporation, Cambridge MA 02138

The ESA requires federal agencies to use the "best scientific...data available" as the basis for decisions. Critics of the ESA scientific assessments often assert that federal agencies fail to provide a clear rationale for the choice of information used or excluded when making decisions, nor are limitations of data used to support decisions identified or explained fully. Currently, there are no federal rules or guidelines that explicitly describe what constitutes the "best scientific data available" or that ensure consistency in the application of this standard. However, as the available body of scientific data relating to listed species will rarely, if ever, be definitive, the problem lies more in the way scientific data are applied to decisions. We propose an approach, Hypothesis-Based Weight of Evidence, as a means to improve transparency and accountability and to communicate the uncertainties from the data effectively, giving proper consideration to contrary data and alternative, scientifically-plausible interpretations.

AGRO 154

Producing food and fiber where endangered species live

Heather Hansen, heather@wafriends.org. WFFF, Washington Friends of Farms and Forests, Olympia WA 98501

Nearly two-thirds of Washington State is covered by the "reasonable and prudent alternatives" in the first Biological Opinion resulting from the Washington Toxics Coalition lawsuit regarding protection of Pacific salmonids. This includes the land that produces over 92% of the nation's raspberries and over 50% of its apples along with a quarter of the vegetables for processing. From the standpoint of agriculture, these recommendations are neither reasonable nor prudent. Congress formally recognized the need to include agricultural producers in the development of

endangered species-related restrictions on pesticides when it included Section 1010 in the 1988 Amendments to the Endangered Species Act. The conference report reads in part, "Federal agencies shall implement the Endangered Species Act in a way that protects endangered and threatened species while minimizing, where possible, impacts on production of agricultural food and fiber commodities." Thus, regulators should take into account the science-based practices already implemented by growers to minimize the impact of pesticides on the environment when new, ESA-related restrictions are proposed.

AGRO 155

Endangered species pesticide protection programs in North Dakota: Past, present, and future

Jessica Johnson, jnjohnson@nd.gov. Endangered Species Protection Program, North Dakota Department of Agriculture, Bismarck ND 58505-0020

The North Dakota Department of Agriculture has been committed to protecting endangered species from pesticides for the past two decades. The first program began in the nineties, and that program gave way to a program that would fit in with EPA's new endangered species protection plan and mandatory bulletins. In early 2008, the Department submitted a new state-initiated endangered species protection plan to EPA for approval. Under the plan, the Department commits to supply EPA with data and recommendations as the Agency develops and implements measures to better mitigate the risk of pesticides to listed species in North Dakota. Data to be supplied by the state include state-specific pesticide use information, distribution and biology information on listed species, cropping data, information on the overlap between potential pesticide use and listed species habitat, data from environmental monitoring studies, and soil type information. The hope is to develop measures that are not only protective of listed species, but also reasonable, to ensure public acceptance of the program and buy-in for pesticide-use restrictions specifically intended to protect listed species. At present the department is working on filling in data gaps, specifically real world monitoring data of environmental exposure. For the past four years, the department has conducted statewide surface water monitoring for over 180 pesticides. The monitoring includes sites chosen for their proximity to suspected spawning areas of the endangered pallid sturgeon.

AGRO 156

California's pesticide use reporting system

Larry Wilhoit, lwilhoit@cdpr.ca.gov. Department of Pesticide Regulation, Sacramento CA 95812

California regulations require that all agricultural pesticide use and some non-agricultural uses be reported to the Department of Pesticide Regulation. The data are stored in the Pesticide Use Reporting (PUR) database for all years from 1990 to the present, averaging 2.5 million records a year. These data include the amount and pesticide applied, date and location of each application, crop treated, area treated, acres planted, application method, grower identification code, and field identification code. The PUR database is used by many different individuals and organizations for a wide range of purposes, including the evaluation of exposures of endangered species to pesticides, estimation of human dietary risk, epidemiological studies correlating pesticide use with human illnesses, and evaluation of pest management programs. The data are extensively checked for errors, especially before data are

made available to the public. Some errors, for example the consequence of misplaced decimal points, result in considerably overstated use, and even one error can significantly affect analyses database users may conduct.

AGRO 157

Role of state pesticide agencies in the endangered species assessment process: Examples from Florida

Max Feken, max.feken@freshfromflorida.com. Bureau of Pesticides, Florida Department of Agriculture, Tallahassee FL 32399

US EPA is currently relying on state pesticide agencies to perform preliminary endangered species assessments for pesticide registrations including emergency exemptions (FIFRA Section 18) or Special Local Need (Section 24c) registrations. Considering the disparity of resources available at the state level, EPA is instructing the states "to provide as much information as possible regarding the proposed use relative to potential implications for endangered and threatened species." The Florida Department of Agriculture and Consumer Services utilizes various data sources to determine proximity of endangered species to crop/land use associated with a particular pesticide. Florida has access to extensive spatial data on land use and endangered species habitat from other state agencies, but in comparison to western states like California and Washington, Florida's pesticide use data is meager. Examples are provided of data sources that can be used by states with similar pesticide data constraints.

AGRO 158

Bioenergy buffers: Creating sustainable agricultural landscapes

David Gustafson, david.i.gustafson@monsanto.com. Environmental Sciences Technology Center, Monsanto Company, St. Louis MO

US agriculture is being challenged to meet growing global demand, while also minimizing any negative environmental impacts associated with crop production. One idea to help meet these challenges is to create more sustainable agricultural landscapes through the implementation of "Bioenergy Buffers." The basic concept is to plant perennial bioenergy crops (e.g., Miscanthus, switchgrass) around all sides of conventional row crop fields. This would provide multiple ecosystem services: reduced runoff of sediment, nutrients, and crop chemicals; direct and indirect GHG sequestration and emission avoidance; a more diversified source of bioenergy feed stocks; potential habitat for beneficial wildlife; inter-connected corridors for migration; protection of endangered species; and barriers to crop chemical drift. Implementation of Bioenergy Buffers will require modification of certain conservation incentive programs to allow harvest in such areas. Work has begun to quantify the sustainability benefits of these systems and to evaluate practical agronomic aspects associated with their implementation.

AGRO 159

Ecosystem services framework for agricultural key performance indicators

Suzanne Ozment, suzanne.ozment@wri.org. Business & Ecosystems, World Resources Institute, Washington DC

Agricultural systems can provide critical benefits to society beyond food, such as flood mitigation, maintenance of air

quality, habitat, and clean water. These ecosystem services, in turn, support agricultural productivity. Unfortunately, there is insufficient information available to industry about how agricultural systems provide ecosystem services and few support tools for farmers to optimize ecosystem services in ways that enhance long-term viability. While sustainability programs have successfully developed key performance indicators (KPIs) to benchmark the direct environmental impacts of agriculture (like water and energy use), we have generally struggled to develop KPIs for ecosystem services. This presentation will introduce an ecosystem services framework for agricultural KPIs which will provide guidance to identify, measure, and value ecosystem services on a farm over time. The conceptual framework will draw on lessons learned from several payments for ecosystem services programs and will be applicable to food, beverage, and agriculture supply chain management initiatives.

AGRO 160

Measuring sustainability in the agri-food sector: Use and development of Eco-Efficiency Analysis

Martijn Gipmans⁽¹⁾, martijn.gipmans@basf.com, Germany; Peter Saling⁽²⁾; Dirk Voeste⁽³⁾. (1) Plant Biotechnology, BASF Plant Science Company GmbH, Limburgerhof, Germany (2) Sustainability Evaluation, BASF SE, Ludwigshafen 67056, Germany (3) Sustainability Evaluation, BASF SE, Limburgerhof 67117, Germany

Sustainability initiatives have been ongoing for over 15 years in the chemical industry. As a result the sustainability evaluation tools, Eco-Efficiency and SEEBALANCE® analysis, were developed that are comparative methods utilizing a Life Cycle Assessment approach with the whole life cycle of a product being considered. Such tools can assist strategic decision-making and facilitate the identification of product and process improvements. We will discuss the development and use of Eco-Efficiency Analysis, the potential to apply this tool on agricultural production processes, such as soybean or corn cultivation, and measuring sustainability in the agrifood sector.

AGRO 161

From isoprene to Taxol®: Modular architecture in terpenoid biosynthesis

Mustafa Koksal, mkoksal@sas.upenn.edu. Department of Chemistry, University of Pennsylvania, Philadelphia PA

Biosynthetic mechanisms are the finest examples of "green" and sustainable production of important chemicals such as those derived from terpenoids. Terpenoid synthases (TSs) catalyze the most complex reactions in biology and are involved in important steps of biosynthetic routes that produce common plant natural products, many of which have significant commercial value. In our recent studies, we have determined the structures of isoprene synthase, which produces the raw material for rubber; taxadiene synthase, which produces the precursor of blockbuster cancer drug Taxol®; and ent-copalyl diphosphate synthase, which synthesizes the precursor of important plant hormones (gibberellins). These structures provide significant information about TS catalysis and suggest structural and evolutionary linkage among all known TSs. Our structural knowledge of TSs could provide additional diversity in natural products through engineering catalytic properties of

Sustainability initiatives in agriculture: The role of science

Patricia J Rice⁽¹⁾, patricia.rice@basf.com; Pamela Rice⁽²⁾; Jeanette Van Emon⁽³⁾; Ellen Arthur⁽⁴⁾. (1) Crop Protection, BASF Corporation, Research Triangle Park NC 27709 (2) USDA-Agricultural Research Service, St. Paul MN United States (3) NERL, US Environmental Protection Agency, Las Vegas Nevada (4) Bayer CropScience

A sustainable society is one that can meet its needs while preserving natural resources for future generations. Key components of this goal are production of a robust food supply while protecting human health and the environment, conserving precious resources, and balancing economic viability. Rapid world-wide population growth will continue to challenge twenty-first century agriculture. Ensuring adequate food, fiber, and fuel for a growing population will require increased crop yields on less cultivated land, strain limited natural resources, and increase the need for continued advancement in more sustainable solutions through sound science. This presentation will discuss current sustainability initiatives, the role of science, available tools, and research needs.

AGRO 163

Regulating pesticide products used in the home: Comparison of biomonitoring data and exposures estimated with regulatory models

Jason E Johnston, jjohnston@exponent.com; Xiaoyu Bi. Chemical Regulation and Food Safety, Exponent, Washington DC 20036

A key element in regulating pesticides is the prediction of potential exposures that may be associated with the use of proposed products. For residential use products, the US EPA uses standard operating procedures (SOPs) to estimate exposures in support of registration decisions. In 2009, US EPA presented proposed revised SOPs at a public meeting of the Science Advisory Panel. In recent years, pesticide registrants have been developing data to better understand exposure associated with their products. One such study, in which biomonitoring exposure data was collected from individuals who use spot-on products on their pets, found exposures ranging over four orders of magnitude. The purpose of this analysis is to compare measured exposures from that study with those predicted according to the current and proposed SOPs for spot-on products. The analysis identifies factors in the SOPs which might be refined to provide more representative exposure estimates.

AGRO 164

Monitoring knockdown resistance in the human head louse populations using three molecular tools

Kyong Sup Yoon⁽¹⁾, kyoon@vasci.umass.edu; John M Clark⁽¹⁾; Si Hyeock Lee⁽²⁾; Gamal E Aboelghar⁽³⁾; Deok Ho Kwon⁽²⁾; Domenic J Previte⁽⁴⁾; Bryan C Poole⁽¹⁾. (1) Department of Veterinary and Animal Sciences, University of Massachusetts, Amherst MA 01003 (2) Department of Agricultural Biotechnology, Seoul National University, Seoul 151-742, Republic of Korea (3) Department of Pesticides, Menoufiya University, Shibin El Kom Menoufiya Governorate, Egypt (4) Molecular and Cellular Biology Program, University of Massachusetts, Amherst MA 01003

Knockdown resistance (*kdr*), mainly conferred by three point mutations (M815I, T917I, and L920F) in the para-

orthologous, voltage-sensitive, sodium-channel gene, is a major attribute of permethrin-resistant head lice. Using a tier system of three molecular resistance detection protocols, kdr frequencies of field populations have been efficiently worldwide. Quantitative sequencing (QS) suitable for a primary resistance monitoring tool to screen a large number of louse populations can detect kdr alleles as low as 7.4%. For more precise determination of *kdr* allele frequencies, the real-time PASA (rtPASA) has been used to monitor frequencies below the QS detection limit at levels as low as 1.13%. The serial invasive signal amplification reaction (SISAR), developed for determining both kdr allele frequency and allelic zygosity of individual lice, has uncovered eight different kdr diplotypes in Egyptian lice. The QS, rtPASA, and SISAR have facilitated large-scale routine monitoring of kdr in field-collected head louse populations.

AGRO 165

Resistance-breaking acetylcholinesterase inhibitors for the malaria mosquito, *Anopheles gambiae*

Paul R Carlier⁽¹⁾, pcarlier@vt.edu; Qiao-Hong Chen⁽¹⁾; FNU Astha⁽¹⁾; James M. Mutunga⁽²⁾; Dawn M. Wong⁽¹⁾; Jianyong Li⁽³⁾; Polo C.-H. Lam⁽⁴⁾; Maxim M. Totrov⁽⁴⁾; Jeffrey R. Bloomquist⁽⁵⁾. (1) Department of Chemistry, Virginia Tech, Blacksburg VA 24061 (2) Department of Entomology, Virginia Tech, Blacksburg VA 24061 (3) Department of Biochemistry, Virginia Tech, Blacksburg VA 24061 (4) Molsoft LLC, San Diego CA 92121 (5) Emerging Pathogens Institute, Department of Entomology and Nematology, University of Florida, Gainesville FL 32610

Growing pyrethroid resistance threatens malaria control in sub-Saharan Africa. To address this problem, we seek to develop acetylcholinesterase (AChE) inhibitors that are safe to humans and possess low cross-resistance to An. gambiae carrying the G119S AChE resistance mutation. Reasoning that the G119S mutation reduces the volume of the AChE active site, we explored carbamate inhibitors that replace the typical 6-membered aromatic ring with a smaller core. We will disclose a series of pyrazole-based carbamates that show good contact toxicity to AKRON strain An. gambiae, which carries both the G119S AChE mutation and the L1014F kdr mutation of the voltage-gated, sodium-ion channel. Kinetic studies of the inhibition of WT and G119S An. gambiae AChE demonstrate that greater potency against the G119S enzyme accompanies their observed higher toxicity relative to standard carbamate insecticides. We will also disclose structural features that confer good An. gambiae/human AChE inhibition selectivity.

AGRO 166

Sarmentine as a bioherbicide

Huazhang Huang, hhuang@marronebio.com; Christy M Morgan; Ratnakar N Asolkar; Marja E Koivunen; Pamela G Marrone. Department of Chemistry, Marrone Bio Innovations, Davis CA 95618

Sarmentine, a known compound isolated from the fruits of *Piper sarmentosum* and *P. nigrum* has various, previously-reported, biological functions, such as antiplatelet aggregation, antiplasmodial, antimycobacterial, and antituberculosis activity. A novel function (i.e., phytotoxicity) was discovered using bioassay-guided purification of the crude extract of *P. longum* fruit. Phytotoxicity was examined with weed and crop seedlings. Results indicated that sarmentine is a contact herbicide with broad-spectrum activity. A series of sarmentine analogs were synthesized to study the structure-activity relationship (SAR) of sarmentine analogs. Results suggested that phytotoxicity required

certain functionalities, i.e., the analogs of the acid moiety of sarmentine were active, but the amine and its analogs were inactive. The ester analogs and amide analogs with a primary amine of sarmentine were also inactive. This study suggests that sarmentine is a promising lead molecule for synthetic herbicides. Plant extracts containing sarmentine can also be used as effective contact bioherbicides.

AGRO 167

Mp708 a maize ($Zea\ mays$) line resistant to herbivory constitutively releases (E)- β -caryophyllene

Ashli E Brown⁽¹⁾, abrown@bch.msstate.edu; Whitney E Crown Smith⁽¹⁾⁽²⁾; Renuka Shivaji⁽¹⁾; William P Williams⁽³⁾; Dawn S Luthe⁽⁴⁾; G. V. Sandoya⁽⁴⁾; Chad Smith⁽⁵⁾. (1) Department of Biochemistry, Molecular Biology, Entomology, and Plant Pathology, Mississippi State University, Mississippi State MS 39762 (2) College of Veterinary Medicine, Mississippi State University, Mississippi State MS 39762 (3) Corn Host Plant Resistance Research Unit, USDA-Agricultural Research Service, Mississippi State MS 39762 (4) Department of Crop and Soil Sciences, Pennsylvania State University, University Park PA 16823 (5) Department of Plant and Soil Sciences, Mississippi State University, Mississippi State MS 39762

Maize an important US agricultural crop is often destroyed by insect feeding. Maize generates a variety of responses to pest attack from activation of wound-response pathways, such as jasmonic acid (JA) biosynthesis, to the release of volatile compounds. Mp708 is an inbred-line resistant to feeding by fall armyworm (FAW). The underlying resistance mechanisms are not completely understood. Mp708 has been shown to express JA and other octadecanoid compounds constitutively prior to infestation. Tx601, a genotype susceptible to FAW, activates JA pathway only in response to feeding, suggesting that Mp708 is primed for attack. Analysis of the volatiles released by the resistant and susceptible lines was conducted using SPME-GC/MS. We have demonstrated the presence of (E)-β-caryophyllene, which is commonly associated with resistance, is released constitutively in Mp708. FAW larvae showed a preference for Tx601 over Mp708 whorl tissue. Identifying volatiles correlated with resistance could lead to the integration of these traits into commercial varieties.

AGRO 168

Persistence and transferability of pyrethroid insecticides on urban concrete surfaces

Weiying Jiang⁽¹⁾, wjian001@ucr.edu; Darren Haver⁽²⁾; Andrew Soeprono⁽³⁾; Michael Rust⁽³⁾; Jay Gan⁽¹⁾. (1) Department of Environmental Sciences, University of California-Riverside, Riverside CA 92521 (2) University of California South Coast Research and Extension Center, Irvine CA 92618 (3) Department of Entomology, University of California-Riverside, Riverside CA 92521

Urban insecticide use is of great environmental concern because of pesticide runoff and contamination to urban watersheds. However, in contrast to the intensive urban use, insecticide persistence and transport in urban environments, especially on hardscapes, is poorly understood. In this study, we investigated pyrethroid persistence and runoff potential on concrete, and evaluated formulation effects on pesticide transferability from concrete to water. Significantly higher levels of permethrin and bifenthrin were found in runoff for ready-to-use (RTU) solid formulations than liquid formulations, which may be attributed to facilitated transport by granules. Lower runoff potential for RTU liquid and professional formulations was likely caused by strong

retention of pyrethroids in concrete porous matrix. Pyrethroid degradation on concrete was observed, as indicated by increased *cis/trans*-permethrin ratio and appearance of polar permethrin degradate in the runoff. Prolonged pyrethroid persistence on concrete and sustained runoff indicate the importance to mitigate long-term pesticide runoff from urban hardscapes.

AGRO 169

Sulfentrazone aquatic field dissipation study in Canada

Audrey W Chen⁽¹⁾, audrey.chen@fmc.com; Don Martens⁽²⁾; Meselu Abetew⁽³⁾. (1) Global Regulatory Sciences, FMC Corporation, Ewing NJ 08628 (2) AgQuest, La Salle MB ROG 0A2, Canada (3) ALS Laboratory Group, Edmonton AB T6E 5C1, Canada

An aquatic dissipation study for sulfentrazone herbicide was conducted in a small-scale pond near Elm Creek, Manitoba, Canada in 2009. One control and three replicate treated limnocorrals representing normal viable aquatic community were established in the pond. Sulfentrazone was added to surface water at typical application timing, simulating a runoff or aerial drift event. NaBr was also applied to limnocorrals as an indicator of system integrity. There were a total of 12 sampling events during the study conduct (June to November). Water from surface and subsurface and sediment samples were collected and analyzed for sulfentrazone and its major aquatic metabolite (methyl triazole). The half-life and DT₅₀ were 29.2 and 27.0 days, respectively, in the aquatic system; the study was terminated after the 5-month sampling event. The study design and analytical and dissipation data will be presented. Comparisons of the actual half-life and the theoretical values used in the modeling in estimating the concentrations in surface water will be discussed.

AGRO 170

Spatial distribution of iodide concentrations in California groundwater

Timothy L Negley⁽¹⁾, timothy.negley@arcadis-us.com; Andrew C Newcombe⁽¹⁾; Virginia B Houck⁽¹⁾; Carolyn B Meyer⁽¹⁾; Craig Nordmark⁽²⁾; John Troiano⁽²⁾. (1) Risk Assessment and Ecological Sciences, ARCADIS US, Inc., Syracuse NY (2) California Department of Pesticide Regulation, Sacramento CA

The spatial distribution and sources of existing iodide concentrations in groundwater of the United States are not well documented. Moreover, a health effects level has not been established for iodide in drinking water. Therefore, it is unclear if, and to what degree, anthropogenic sources may substantially contribute to existing iodide concentrations in groundwater and the potential for human health effects. A detailed literature review and evaluation of publicly available databases was undertaken to quantify iodide groundwater concentrations in the State of California. Data mined from public sources were assessed to quantify iodide variability in groundwater and were statistically analyzed using General Linear Modeling (GLM) to characterize better the key environmental factors responsible for iodide variability in groundwater. Results indicated that sodium concentrations accounted for a large amount of the iodide variability observed in groundwater. Results also suggest that iodide variability may be largely driven by current or historic marine influences.

Rice cultivation, pesticide load and water contamination

Tanu Jindal⁽¹⁾, tjindal@amity.edu. Safety and Management, Amity Institute for Environmental Toxicology, New Delhi Uttar Pradesh, India

Rice is cultivated throughout the world under submerged conditions. The high water requirements and the heavy pesticide load used in rice paddies have resulted in contamination of associated surface water. A study was undertaken to analyse the contamination by pesticides in surface and groundwater samples in a rice growing area. A survey for pesticide use and rice variety grown by farmers was conducted in association with the monitoring study. Eight tube wells from rice fields in Greater Noida, India were selected for study. Samples of river and tube wells were taken before, mid and end of cropping season and also post harvest. Among the various pesticides analyzed, 41% samples were found contaminated with organochlorine pesticides and 27% samples were contaminated with organophosphate pesticides above MRL values. Concentration of organochlorine pesticides ranged from 0.017 to 0.917 µg/l, and organophosphate pesticides ranged from 0.141 to 1.926 µg/l. Average value of contamination is 42% to 85% in organochlorine pesticides and organophosphate pesticides respectively.

AGRO 172

Endangered species assessments conducted under FIFRA: Fomesafen registration review case study

Daniel Campbell, dan.campbell@syngenta.com; Monty Dixon; Steven Wall; Jay Overmyer. Departments of Regulatory Affairs and Product Safety, Syngenta Crop Protection, LLC, Greensboro North Carolina 27419

The Endangered Species Act of 1973 requires federal agencies to assess potential impacts to federally-listed threatened or endangered species and their habitats for any activity permitted, funded, or conducted by that agency. The Environmental Protection Agency is updating these assessments as part of their Registration Review program. This program involves review of pesticides on a 15-year cycle and uses a three phase process that is designed to include public involvement through comment periods. The herbicide fomesafen, the active ingredient in Syngenta's Reflex®, Flexstar®, Flexstar® GT and Prefix® products, is one of the first active ingredients to be considered under Registration Review. The status of the fomesafen review will be presented as a case study including suggested improvements in the process and methods.

AGRO 173

Fomesafen endangered species assessment: Novel approaches for assessment refinement

Jay Overmyer, jay.overmyer@syngenta.com; JiSu Bang; Richard Brain; Kevin Henry; Jeff Perine; Steven Wall. Syngenta Crop Protecton, LLC, Greensboro NC 27419

Fomesafen is one of the first active ingredients in EPA's new Registration Review program undergoing a national-level ecological risk and effects assessment for federally-listed endangered and threatened species. After review of EPA's initial draft assessment, several areas were identified where additional data or modeling could be used to refine the assessment. These areas included soil residue, aquatic metabolism, efficacy, plant recovery and taxonomic

sensitivity data, as well as geo-spatial data for identifying the proximity of endangered species to areas of potential fomesafen use. Methods for assessing and determining the potential for direct and indirect effects to non-target organisms were also explored, along with refinements to exposure models including T-REX, TerrPlant, AgDRIFT®, and AGDISP. This presentation will discuss available data and techniques that are important in refining a national-level endangered species assessment for fomesafen.

AGRO 174

FIFRA Registration Review and the Endangered Species Act: Clomazone case study

Ashlea Frank⁽¹⁾, afrank@complianceservices.com; Bernalyn McGaughey⁽¹⁾; Gary Mitchell⁽²⁾; John Cummings⁽³⁾; Stephen Longacre⁽³⁾. (1) CSI, Compliance Services International, Lakewood WA 98499 (2) Agricultural Products, FMC Corporation, Ewing NJ 08628 (3) Agricultural Products, FMC Corporation, Philadelphia PA 19103

Clomazone, a herbicide registered by FMC Corporation, was selected to be one of the products serving as the first or "pilot" assessment of endangered species with regard to EPA's compliance to the Endangered Species Act when undertaking Registration Review. This presentation will examine EPA's approach to the assessment and the registrant's approach to providing supportive data to EPA's assessment. Additionally, comments on FIFRA-ESA compliance and EPA's species assessment that were submitted during the public comment period will be examined. The clomazone assessment continues to be considered as a pilot assessment for developing a process for consultation between EPA and the Services. Consequently, this presentation will also examine the status of this process.

AGRO 175

Invasive weed and endangered species interactions: Can herbicides facilitate a positive outcome?

K. George Beck, george.beck@colostate.edu; Scott Nissen; James Sebastian. Department of Bioagricultural Sciences and Pest Management, Colorado State University, Fort Collins CO 80523-1179

Invasive weeds are aggressive and displace native plant communities, especially forbs and shrubs. Previous research showed that quinclorac and imazapic were successfully used to control an invasive weed and not affect survival or fecundity of an endangered species. Experiments conducted at high elevation sites in western Colorado with aminopyralid applied mid- or late-summer or fall at 53 and 126 g ai ha⁻¹ decreased native forb abundance only 21 to 44% at the latter two timings. Results from another Colorado experiment showed that aminopyralid successfully decreased abundance of Russian knapweed (Acroptilon repens) and allowed 11 of 16 seeded forbs, shrubs, and grasses to establish to aid site recovery. These data show that herbicides can be used to decrease invasive weed abundance while providing native plant communities with an opportunity to recover over time. Thus, buffer zones need not be universally applied and such decisions should be based upon sound science.

Cranberry insect pest management and Karner Blue butterfly protection: A Wisconsin case study

Kenneth D Racke⁽¹⁾, kracke@dow.com; Lori G Bowman⁽²⁾; Cathy Carnes⁽³⁾. (1) Regulatory Sciences and Government Affairs, Dow AgroScience, Indianapolis IN 46268 (2) Agrichemical Management, Wisconsin Department of Agriculture, Trade and Consumer Protection, Madison WI 53708 (3) Green Bay Wisconsin Field Office, US Fish and Wildlife Service, New Franken WI 54229

Cranberry production in Wisconsin occurs in portions of the state containing stands of wild lupine, a host for the endangered Karner blue butterfly (Lycaeides melissa samuelis). Growers manage several Lepidoptera pests and their tools include insecticide sprays. During 2005, the insecticide Intrepid™ 2F (AI: methoxyfenozide) was approved by US EPA for use in managing Lepidoptera pests of cranberries. EPA's assessment concerns for potential spray drift impacts on Karner blue populations resulted in adoption of labeling restrictions for a 1-mile no-spray buffer around sandy habitat supporting wild lupine. This buffer rendered the product essentially unusable by cranberry growers. At their request, during 2007 a formal ESA consultation process was initiated with the US Fish and Wildlife Service (USFWS). The outcome of a cooperative process involving growers, local USFWS office, state regulatory officials, EPA, and the registrant was identification of an alternate set of mitigation measures compatible with agricultural practices. These measures were incorporated into the very first active EPA Endangered Species Protection Program (ESPP) county bulletins. This case study highlights important lessons concerning successful integration of ESA considerations and agricultural interests.

AGRO 177

Adaptive management of aquatic plants in the Sacramento-San Joaquin Delta in compliance with the Endangered Species Act: Applying lessons learned for strategic planning

Lars W.J. Anderson, Iwanderson@ucdavis.edu. Exotic and Invasive Weed Research, USDA-Agricultural Research Service, Davis CA 95616

Over the past 25 years, several state, federal, and local agencies have succeeded in reducing negative impacts from water hyacinth (Eichhornia crassipes (Mart.) Solms) and Brazilian waterweed (Egeria densa Planch) in the Sacramento-San Joaquin Delta. The Delta is relied upon by over 25 million Californians for potable water as well as for agricultural, recreational, and industrial uses. The Delta harbors several species listed as threatened and endangered; thus, Section 7 consultations with NOAA-Fisheries (NMFS) and the US Fish and Wildlife Service (USFWS) were part of the management planning and strategies. Success came from several related approaches that included: (1) use of Best Management Practices (BMP's); (2) compliance with US EPA National Pollutant Discharge Elimination System (NPDES); (3) engaging regulatory personnel with on-the-water experiences to familiarize them with the problem and the environment; (4) informal discussions of risk-benefits issues; (5) collaborative planning to fill data gaps; (6) public outreach; and (7) refining and adapting monitoring and control methods throughout the project period.

AGRO 178

Vertebrate pesticides and the ESA

Michael J. Bodenchuk,

michael.j.bodenchuk@aphis.usda.gov. Texas Wildlife Services, USDA-Animal and Plant Health Inspection Service, San Antonio TX 78249

Use of vertebrate pesticides is the most cost-effective method for removing pest wildlife, but conflicts may arise with the Endangered Species Act (ESA). Procedural components can become especially problematic when government programs hold the registration for or utilize pesticide products. Multiple consultations with differing opinion language complicate effective pesticide use and raise questions concerning the actual risks and analyses used in the process. This paper discusses pesticide use for prairie dogs and covotes as examples of ESA implementation and notes successful and not-so-successful implementation of restrictions. These examples will show effective processes as well as those that need improvement. Many of the improvements do not require ESA revision, but rather a commitment to utilize consistent language and interpretations.

AGRO 179

Ten-years of pesticide volatilization monitoring

John H. Prueger⁽¹⁾, john.prueger@ars.usda.gov; Tim J. Gish⁽²⁾; Lynn G. McKee⁽²⁾; William P. Kustas⁽²⁾; Joseph G. Alfieri⁽²⁾; Jerry L. Hatfield⁽¹⁾; Laura L. McConnell⁽²⁾; Cathleen J. Hapeman⁽²⁾; Cody J. Howard⁽²⁾. (1) National Laboratory for Agriculture and the Environment, USDA-Agricultural Research Service, Ames IA 50010 (2) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, Beltsville MD 20705

Pesticides are an integral component of modern agricultural production systems. Offsite movement and transport of pesticides pose a critical concern with respect to humans, animals, plants air and water quality. We introduce and present the results from a long-term volatilization study spanning over a decade. This 10-year study was conducted to improve our understanding of how local meteorology and antecedent soil conditions influence year to year variability in watershed-scale herbicide volatilization. The study was conducted at a 21-ha watershed site located at the Beltsville Agricultural Research Center. Site location, herbicide formulations, and agricultural management practices remained unchanged throughout the duration of the study. Metolachlor and atrazine were co-applied as a surface broadcast spray. A flux gradient technique was used to compute volatilization fluxes for the first 5 days after application using herbicide concentration profiles and turbulent fluxes of heat and water vapor as measured from eddy covariance measurements. Results demonstrate that volatilization losses for these two herbicides were high even though both have relatively low vapor pressures. Cumulative volatilization losses after 5 days ranged from 5 to 63% of that applied for metolachlor and about 2 to 12% for atrazine. This research confirms that herbicide volatilization is an extremely important process that will need to be better understood if environmental impacts are to be determined and improved management strategies developed.

NEW INVESTIGATOR AWARD. Pesticide emission model: Evaluation of performance in predicting pesticide emissions from the Chesapeake Bay region

Cody J. Howard⁽¹⁾, cody.howard@ars.usda.gov; John H. Prueger⁽²⁾; Tim J. Gish⁽¹⁾; Cathleen J. Hapeman⁽¹⁾; Laura L. McConnell⁽¹⁾; Lynn G. McKee⁽¹⁾. (1) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, Beltsville MD 20705 (2) National Laboratory for Agriculture and the Environment, USDA-Agricultural Research Service, Ames IA 50011

The ecosystem health decrease in the Chesapeake Bay region has been well documented with reports demonstrating eutrophication, increased toxicity, and a decrease in biodiversity. One area that has come under recent scrutiny is the use of the pesticides on the Delmarva Peninsula and other highly rural areas surrounding the region. Current and legacy pesticides have been shown to represent a pollution source and have been measured at significant concentrations in air, rain, and soil samples in this region. Unfortunately, as pesticide emissions are not currently regulated by the states in the region, detailed pesticide emissions inventories for use in regional air quality models (i.e., Community Multiscale Air Quality or CMAQ) are not easily obtained. In the current study, a detailed analysis of the use of the Pesticide Emissions Model (PEM), previously used to determine atrazine deposition to the Great Lakes, to develop emissions inventories is demonstrated. The PEM model utilizes meteorological data, pesticide properties, and use data to generate emissions data which can then be fed directly into air quality models to determine the fate and transport of those pesticides.

AGRO 181

Reducing near-field agricultural fumigant emissions through efficacious changes in regional application practices

Vincent R Hebert⁽¹⁾, vhebert@tricity.wsu.edu; Dennis Johnson⁽²⁾; Philip Hamm⁽³⁾; Don Horneck⁽³⁾. (1) Department of Entomology, Washington State University-Tri Cities, Richland WA 99354 (2) Department of Plant Pathology, Washington State University, Pullman WA 99164 (3) Department of Botany and Plant Pathology, Oregon State University, Hermiston Agricultural & Extension Center, Hermiston OR

Regional field-scale pre-plant potato metam sodium surface and soil incorporated fumigation demonstrations were conducted in southeastern Washington State from 2008 to 2010. These combined fumigant flux/efficacy demonstrations were developed to compare traditional center pivot and low drift chemigation to soil-incorporated, shank-application methods. Demonstrations were performed during the cooler fall period when commercial soil fumigations were occurring. Soil-incorporated, shank injection appreciably reduced methyl isothiocyanate (MITC) emissions compared to surface fumigant applications. However, a consistent trend towards higher production yields was observed for surface fumigations. Incremental adjustments in soil-incorporation depth could increase product efficacy while retaining the benefit of reduced field-edge buffers and lowering MITC bystander inhalation exposure. These demonstrations provide agricultural producers, crop consultants, and registrants with regional flux and potato efficacy information to make informed management decisions, especially where field applications can occur in proximity to residential communities and difficult to evaluate locations.

AGRO 182

Predicting transport, fate, and pest control after fumigating soil with methyl iodide

Lifang Luo, luo_lf@hotmail.com; Scott Yates. US Salinity Laboratory, USDA-Agricultural Research Service, Riverside CA 92507

Protecting soil, water and air from pesticide contamination requires a fundamental understanding of the synergies of the fate, transport and pest-control processes. Pest management systems are needed that protect crop yields while minimizing harmful environmental and public health effects. A study was conducted to determine the feasibility of predicting pesticide distribution in soil, pest control, and volatile emissions after methyl iodide (MeI) fumigation. The objectives were to: 1) measure volatilization, degradation, distribution, and pest survival in a 2-D soil chamber, and 2) develop and test a 2-D mathematical model to predict fumigant behavior and control of three classes of plant pests: nematodes, fundi and weeds. After 24 h fumigation, 28.9% of MeI volatilized and 6.8% remained in soil. Predictions and measurements showed that fungi [Fusarium oxysporum] were not suppressed, >90% of citrus nematodes [Tylenchulus semipenetrans] were killed; and that weed seeds [Echinochloa crus-galli] were controlled within 20-cm of the injection point. This study demonstrates that models could be used to develop best management practices that minimize emissions while protecting crops from pests.

AGRO 183

Assessment of pesticide drift and deposition downwind of ground spray applications: A case study examining the impact of droplet size, boom height, and wind speed

Richard J Londergan⁽¹⁾, richard.londergan@arcadis-us.com; A C Newcombe⁽¹⁾; Thomas M Wolf⁽²⁾. (1) ARCADIS US Inc., Chelmsford MA 01824 (2) Environment Team, Agriculture and Agri-Food Canada, Saskatoon SK S7N OX2, Canada

Pesticide airborne drift and deposition downwind from ground spraying applications were investigated using ground spray drift experimental datasets compiled by Agriculture and Agri-Food Canada. The primary study objective was to develop a series of empirical curves characterizing spray deposition versus downwind distance as a function of spray application parameters and meteorology. Using measurements from 29 field experiments, best-fit curves were developed to predict deposition versus distance for ground spray applications as a function of spray quality (droplet size), boom (release) height, and wind speed. The dataset characterized deposition for spray quality ranging from fine to very coarse drop-size distributions, at two release heights, for wind speeds between 3 and 12 m/s, and for distances extending to 120 m downwind of the spray swath. A series of curves for deposition versus travel time were developed for data subsets based on spray quality and release height. Deposition declined more rapidly with travel time as droplet size and release height increased.

Volatile organic compound emissions from agriculture in Central Valley, California

Carsten Warneke⁽¹⁾⁽²⁾, Carsten.Warneke@noaa.gov; Joost A de Gouw⁽¹⁾⁽²⁾; John B Nowak⁽¹⁾⁽²⁾; Jeff Peischl⁽¹⁾⁽²⁾. (1) CIRES, University of Colorado, Boulder CO 80305 (2) CSD, NOAA Earth System Research Laboratory, Boulder CO 80305

Seven research flights were conducted in the Central Valley of California to investigate the emissions from rice fields in the Sacramento Valley and from cattle farms in the San Joaquin Valley during the CalNex aircraft mission in 2010. Volatile organic compounds (VOCs) were measured downwind together with other gas and erosol species including methane and ammonia. Methanol is used to colorcode the flight tracks of the aircraft in Figure 1 and the data are used to determine VOC emissions from those sources.

AGRO 185

Speciation of VOCs from complex sources: Validation of reactivity-weighted emissions

Peter G Green, pggreen@ucdavis.edu. Department of Civil & Environmental Engineering, University of California-Davis, Davis CA 95616

Agencies in regions with severe air quality challenges, such as California's San Joaquin Valley (SJV), have raised concerns about volatile organic compounds (VOCs) emitted from complex sources which are suspected to contribute to persistent high levels of ground-level ozone formation. Agricultural and composting sources are prime examples of sources involving complex biology and chemistry that have recently come under scrutiny. The goal of our series of studies is to characterize the mixture of VOCs with a sufficient variety of techniques in order to assess their ozone formation potential (OFP). By matching short-term OFP in the field (with a mobile ozone chamber) to photochemical model calculations, we can assert that our speciation of VOCs is relatively complete with respect to ozone formation. This approach has been applied to orchards receiving solvent-based pesticide spraying, livestock and poultry (with their fresh waste), animal feeds, green waste compost, and biosolid co-composting.

AGRO 186

Mass balance evaluation of alcohol emission from cattle feed

Sasha D Hafner⁽¹⁾, sasha.hafner@ars.usda.gov; Felipe Montes⁽²⁾; C. Alan Rotz⁽²⁾; Cody Howard⁽¹⁾. (1) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, Beltsville MD 20705 (2) Pasture Systems and Watershed Management Research Unit, USDA-Agricultural Research Service, University Park PA 16802

Silage on dairy farms has been recognized as an important source of volatile organic compounds (VOCs) to the atmosphere, and therefore a contributor to tropospheric ozone. Considering reactivity and likely emission rates, ethanol, 1-propanol, and acetaldehyde probably make up the largest contribution to ozone formation. Accurate estimates of emission rates of these compounds are not available. Previous studies have measured VOC emission rates using flux chambers, which underestimate rates in the field, or wind tunnels, which may provide more accurate estimates. In this work, we describe a mass balance approach for estimating VOC emission from cattle feed and

measurements of ethanol, 1-propanol, methanol, and acetaldehyde emission from corn silage on a dairy farm in Maryland, USA. We anticipate that our approach will provide more accurate estimates of emission rates and the effect of temperature and air flow on emission from silage under farm conditions.

AGRO 187

Comparison of flux chamber devices for ammonia emission measurement

Michael L. Hile, mlh144@psu.edu, 230 Agricultural Engineering Building, University Park Pennsylvania 16802; Eileen F. Wheeler; Robin C. Brandt; Patrick A. Topper. Department of Agricultural and Biological Engineering, Penn State University, University Park PA 16802

Dairy manure ammonia emissions from a mechanicallyventilated test room were compared to emissions measured using four flux chamber designs. Aerial ammonia concentration and whole-room air flow rates were used to establish benchmark whole-room ammonia emission rates. Flux chamber systems that employed little or no internal air mixing underestimated whole-room ammonia emissions by 11 to 70%. The flux chamber equipped with an internal mixing fan but no control over air movement uniformity exhibited ammonia emission rates that were 153 to 308% of the whole-room ammonia flux. Ammonia emission rates from the flux chamber utilizing a variable-speed recirculating fan with horizontally-directed air movement averaged 102% of whole-room ammonia emission rates using an average air velocity of 0.52 m/s. Controlling air movement/velocity over the enclosed surface improved the accuracy of ammonia emission rate measurements compared to flux systems that rely on low velocity or no chamber mixing.

AGRO 188

Chiral chemistry and toxicity assessments for pyrethroid pesticides

Robert W. Gerlach, Robert.Gerlach@gdit.com. QSAR & PBPK Modeling, General Dynamics Information Technology, Henderson NV 89074

Pyrethroids compose, by amount, the largest class of pesticides currently used in the United States. Their use in commercial, industrial, agricultural, and domestic settings makes study of their toxicity of general concern. These concerns extend from single exposure episodes to one pyrethroid to chronic exposure to several pyrethroids. The toxicological fate of pyrethroids in humans is modeled by identifying exposure routes and levels, following the distribution and metabolism within the body, and examining the elimination paths. Complex PBPK/PD models can be formulated which track exposure, absorption, distribution, reaction, and elimination over time. Traditionally, these PBPK/PD models track a particular pesticide, along with various metabolites and biomarkers. However, pyrethroids typically contain one or more chiral centers, resulting in numerous stereoisomers in many commercial products. Each stereoisomer differs in effectiveness for its intended use and also in its toxicity. This paper discusses the development of chiral analytical techniques in parallel to the advances in commercial chiral production methods to assess the current status of related PBPK parameters for toxicity models.

Direct chiral separation of pyrethroid isomers by HPLC with chiral stationary phases

Masahiko Okamoto, okamotom@sc.sumitomo-chem.co.jp. Organic Synthesis Research Laboratory, Sumitomo Chemical Co., Konohana-ku Osaka, Japan

The direct chiral separation of pyrethroids: allethrin, phenothrin, resmethrin, furamethrin, tetramethrin, etc., was performed by HPLC with a variety of chiral stationary phases. During this process, the reversal of enantiomer elution order was observed. Several examples of such unusual behavior will be presented.

AGRO 190

Biotransformation and enzymatic reactions of pyrethroid insecticides in mammals

Hideo Kaneko, kaneko@sc.sumitomo-chem.co.jp. Environmental Health Science Laboratory, Sumitomo Chemical Co., Ltd, Osaka 554-8558, Japan

Synthetic pyrethroids, a major insecticide group, are used worldwide to control agricultural and household pests. Biotransformation of pyrethroids in mammals including humans usually proceeds in two steps: Phase 1 reactions, oxidation and cleavage of the ester bond, and Phase 2 reactions, formation of hydrophilic and lipophilic conjugates. Oxidation reactions are mediated by several CYP (P-450) isoforms and the ester bond is mainly cleaved by carboxylesterase (CES) in animals and humans. CYPs and CESs involved in the metabolism of pyrethroids depend on chemical structures. Major isoforms of CYPs and CESs may be determined on their intrinsic activity and abundance. However, it is noteworthy that there may be actually no poor metabolizers for pyrethroids in humans, because several CYP isoforms and carboxylesterase(s) are known to be involved in their biotransformation. In addition, species, age, and sex differences for biotransformation of pyrethroids will be discussed.

AGRO 191

Prediction and use of environmentally- and physiologically-relevant properties of pesticides

Robert D Clark, bob@simulations-plus.com; Michael B. Bolger; Jason Boyd. Life Sciences, Simulations Plus, Inc., Lancaster NY 93534

The role of quantitative structure-activity relationships (QSARs) in agrochemistry was once limited to predicting activity against target pests or safety in crop species. Today it has expanded to include quantitiative structure-property relationships (QSPRs) relevant to movement through the environment as well as to QSARs for toxic effects on species other than targeted pests and crops. Creating broadly applicable global QSAR and QSPR models requires careful collection and curation of data from the open literature as well as application of advanced modeling and analysis tools, particularly when the predicted properties are going to be used to address regulatory concerns or to estimate human exposure by computational simulation. Many such models have been developed over the years for ADMET Predictor (TM); we will describe the results of applying them to typical pesticides as well as to how the predicted properties can be used effectively in carrying out pharmacokinetic simulations using GastroPlus(TM).

AGRO 192

Characterization of potential age-related differences in pyrethroid pharmacokinetics

James V Bruckner⁽¹⁾, bruckner@rx.uga.edu; T G Osimitz⁽²⁾; S. Anand⁽³⁾; D. Minnema⁽⁴⁾; W. Schmitt⁽⁵⁾. (1) Pharmaceutical and Biomedical Sciences, University of Georgia, Athens GA 30602 (2) Science Strategies, LLC, Charlottesville VA 22902 (3) Stine-Haskell Research Center, DuPont Crop Protections, Newark DE 19714 (4) Syngenta Crop Protection, Inc, Greensboro NC 27419 (5) Bayer Crop Science AG., Alfred-Nobel-Str. 50 D - 40789 Monheim am Rhein, Germany

There is a new initiative by the Council for the Advancement of Pyrethroid Human Risk Assessment (CAPHRA) to develop physiologically-based pharmacokinetic (PBPK) models to assess potential susceptibility of infants and children to pyrethroids. Comprehensive studies of selected pyrethroids will be conducted in our laboratory on maturing rats, and the findings used to develop/refine PBTK models. In situ, in vitro, and in vivo experiments will be performed to assess the age-dependency and influence of the following physiological processes on pyrethroids' PK: human and rat plasma protein binding; rat gastrointestinal (GI) absorption; rat blood-brain barrier (BBB) permeability; and human GI and BBB transport. The human colon adenocarcinoma cell line, Caco-2, is being used to measure time- and concentration-dependence of pyrethroid uptake. Cells grown on Transwell® inserts provide discrete apical and basolateral chambers which allow measurement of permeability constants and efflux ratios for ¹⁴C-labeled pyrethroids. The human brain microvascular endothelial cell line, hCMEC/D3, will be utilized as a model system to assess BBB transport. These experiments are designed to provide rate constants and other input parameters for rat and human PBPK models for selected pyrethroids.

AGRO 193

Fifteen steps to percutaneous penetration-man to animal: Why important?

Howard I Maibach, MaibachH@Derm.ucsf.edu. School of Medicine, Department of Dermatology, University of California-San Francisco, San Francisco CA 94143-0989

During WWII, Trager developed the *in vitro* percutaneous model. Shortly thereafter, Blank and Scheuplein provided the fundamental data that form the basis of most current QSAR models. Subsequent experimental data, and new *in vivol vitro* models provide insights, suggesting that flux is not a single one step diffusion, but instead a complex series of at least 15 identificable steps, most of which can be quantified. The clinical relevancies of these insights will be presented.

AGRO 194

On the estimation and use of dermal permeability coefficients

John C Kissel⁽¹⁾, jkissel@u.washington.edu; Annette L Bunge⁽²⁾. (1) Department of Environmental and Occupational Health Sciences, University of Washington, Seattle WA 98195 (2) Chemical Engineering, Colorado School of Mines, Golden CO 80401

Dermal absorption can be conceptualized as thermodynamically-driven diffusion through a membrane. This permits mathematical representation of the process using Fick's law. The permeability coefficient is conventionally estimated as the ratio of flux to driving force expressed as a concentration gradient at steady state. The resulting coefficient is vehicle specific. Theoretically such a permeability coefficient should be roughly constant (with allowance for damage, moisture content, interpersonal variation in skin characteristics, etc.) for a given compound, vehicle, temperature, and skin location. In practice, many authors violate the standard assumptions required for estimation of permeability coefficients and then report values that are actually non-transferable fitting constants. Frequently-encountered estimation errors include misspecification of the driving force and evaluation of nonsteady state results using the steady state form of Fick's law. Lack of adherence to theoretically-defensible practice has produced unnecessary confusion in the peer-reviewed literature.

AGRO 195

Percutaneous absorption of pesticide formulations

William G Reifenrath, wgr@stratacor-inc.com. Research and Development, Stratacor, Inc., Richmond CA 94804

To study differences between in vitro and in vivo percutaneous absorption of pesticide formulations, we examined the role of the dermis as an artificial in vitro barrier and the role of the solvent or vehicle on percutaneous penetration and skin retention. Radiolabeled compounds with varying partition coefficients (paraoxon, benzoic acid, parathion, and DDT in alcohol or acetone formulation) were studied in the pig, both in vitro and in vivo, as a function of time. If in vitro dermal residues are taken into account, there was good agreement between in vitro and in vivo percutaneous absorption, for a range of compounds including lindane, malathion, permethrin, and piperonyl butoxide. The kinetics of in vitro permeation of the solvents themselves were also studied. The relatively high K_p values for solvents explains their ability to facilitate permeation into the viable layers of skin. Solvents combined with surfactants (e.g., emulsions) can further increase percutaneous absorption of pyrethroids.

AGRO 196

Pesticide aquatic exposure scenarios and modeling for juvenile Pacific salmonid floodplain habitat

Nick Poletika⁽¹⁾, npoletika@dow.com; Zhenxu Tang⁽²⁾; Scott Jackson⁽³⁾. (1) Department of Field Exposure and Effects, Dow AgroSciences LLC, Indianapolis IN 46268 (2) Department of Environmental Research, Bayer CropScience, Stilwell KS 66085 (3) Department of Stewardship and Strategy, BASF Corporation, Research Triangle Park NC 27709

Aquatic exposure modeling for pesticides is often used in regulatory decision-making to estimate exposure to endangered and/or threatened species. For pesticides applied near juvenile Pacific salmonid habitat, exposure modeling generally employs a highly conservative scenario consisting of a narrow, shallow static water body immediately adjacent to and downwind of a treated site. These habitat types are infrequently present in floodplains with commercial agriculture and developed areas due to the construction of control structures such as dams and levees. A more typical scenario can be defined by habitat types such as side channels, alcoves, and backwater pools. We present modeling results for a side channel using the PRZM/AGRO modeling system. Sensitivity analysis for important habitat parameters is discussed, and applications for evaluating combined reductions in spray drift and runoff off-site transport are suggested. We also relate water concentration

estimates for an insecticide to standard short-term toxicity data in the context of risk assessment.

AGRO 197

Spatial and temporal distributions of salmon and their prey: Implications for estimating their exposure to agricultural pesticides

Steve Cramer⁽¹⁾, stevec@fishsciences.net; Mark Teply⁽²⁾; Larry Dominguez⁽²⁾. (1) Cramer Fish Sciences, Gresham OR 97030 (2) Cramer Fish Sciences, Lacey WA 98503

Migratory organisms present a challenge when predicting exposure to pesticides given their uneven distribution in time and space. We will present the biological and ecological foundation for describing the spatial and temporal patterns of juvenile salmon and their prey. We will describe several distinct migration patterns employed by juvenile spring Chinook salmon that can account for meaningful differences between use in natal and non-natal streams. These stream types can be highly correlated with agricultural lands. We also describe habitat preferences that can account for meaningful differences between use in backwater, offchannel habitat types - expected to yield higher pesticide concentrations – and those in main channels. We also describe the distribution of prey taxa that can account for meaningful differences in potential indirect effects. These distributions are the basis for a quantitative framework, described in a companion presentation, for estimating exposure of salmon to pesticides.

AGRO 198

Modeling the exposure of salmon to agricultural pesticides

Mark Teply⁽¹⁾, markt@fishsciences.net; Steve Cramer⁽²⁾; Nick Poletika⁽³⁾. (1) Cramer Fish Sciences, Lacey WA 98503 (2) Cramer Fish Sciences, Gresham OR 97030 (3) Dow AgroSciences, Indianapolis IN 46268

Migratory organisms present a challenge when predicting exposure to pesticides given their uneven distribution in time and space. We will present a spatially and temporally explicit framework for estimating the co-occurrence of juvenile salmon and agricultural pesticides in the Willamette Basin, Oregon. This framework incorporates information about patterns of juvenile salmon distribution, described in a companion presentation, which when considered along with information about patterns of pesticide concentrations can provide the basis for estimating potential exposure through direct contact. This framework also incorporates information about the spatial and temporal distribution of the salmon prey base, which when considered along with information about sensitivity of prey taxa to pesticides can provide the basis for estimating potential indirect effects. In both instances, we demonstrate that by using information about the distribution of juvenile salmon and their prey, the framework yields a better understanding of the proportion of organisms potentially impacted by agricultural pesticides.

Modeling risk to aquatic species subject to realistic, dynamic exposures using a generalized form of Haber's Law

Richard Reiss⁽¹⁾, rreiss@exponent.com; Ken Bogen⁽²⁾. (1) Exponent, Alexandria VA 22310 (2) Exponent, Oakland CA 94607

The Endangered Species Act requires assessing potential pesticide risks to salmonid-habitat aquatic species, including salmonids and their prey in the Pacific Northwest. Where agricultural spray drift dominates exposures to flowing water, realistic risk models must account for the discrepancy between constant levels of exposure over 48 to 96 hours that typically are used in aquatic toxicity tests and nonlinear patterns of rapid pesticide dispersion that occur in flowing water. This discrepancy is addressed by applying the analytic solution of a dynamic, generalized version of Haber's Law conditioned on expected rates of exponential concentration decline, which can be estimated from a widely-used, stream-dispersion model. We applied this approach to specific organophosphate pesticides to illustrate the range of substantial magnitudes by which standard regulatory methods now overestimate risk to aquatic species.

AGRO 200

Risks of pesticide mixtures to salmon in the Pacific Northwest

Dwayne R. J. Moore⁽¹⁾, dmoore@intrinsikscience.com; R. Scott Teed⁽²⁾. (1) IES, Intrinsik Environmental Sciences (US), Inc., New Gloucester ME 04260 (2) IES, Intrinsik Environmental Sciences, Inc., Ottawa ON K2C 2B5, Canada

The National Marine Fisheries Service released "Biological Opinions" concluding that carbamate and organophosphate (OPs) pesticides jeopardize salmon populations in the Pacific Northwest. The opinions relied on highly conservative assumptions. We conducted a study to estimate the risks of carbamates and OPs to salmonids. Washington State has conducted a multi-year monitoring study in salmonidbearing streams. We used data on the effects of carbamates and OPs to brain AChE activity in juvenile coho salmon to estimate toxicity of water samples in Washington State. Estimated brain AChE inhibition for pesticide mixtures rarely exceeded 20% (<0.5% of samples). This level of inhibition would not cause sub-lethal or lethal effects to salmonids. Similar results were found using NAWQA data from the Pacific Northwest. Laboratory studies with a pesticide mixture typical of urban streams in Washington State showed no effects on coho salmon. Therefore, carbamate and OPs pose little risk to salmonids in the Pacific Northwest.

AGRO 201

Application of a GIS-based approach to quantifying pesticide-use site proximity to salmonid habitat

Michael F Winchell⁽¹⁾; JiSu Bang⁽²⁾; Barbara Patterson⁽¹⁾; Katie A Budreski⁽¹⁾; Richard A Brian⁽²⁾; Steven B Wall⁽²⁾. (1) Stone Environmental, Inc., Montpelier VT (2) Syngenta Crop Protection LLC, Greensboro NC

Characterizing and quantifying the proximity of potential pesticide-use sites to endangered species habitats are integral components of pesticide exposure risk assessments. One region of interest has been the salmonid evolutionarily significant units (ESUs) and distinct population segments (DPSs) in the Pacific Northwest and California. The

availability of spatial datasets that classify stream and river segments by salmonid habitat type, combined with high resolution crop datasets, has allowed for refined estimates of potential use areas within these regions. The automated GIS procedures were applied to the 28 endangered or threatened ESUs/DPSs to characterize proximity and magnitude of potential use areas to the salmon habitats within different ESUs, for different crop uses, and the different types of habitats. The results demonstrated that the GIS-based approaches used in this study could produce refined, best available quantification of potential pesticide-use areas in relation to the salmon habitats in the 28 ESUs/DPSs.

AGRO 202

Assessment of the potential risks of dimethoate to aquatic endangered species using the joint probability distribution analysis

Qingli Ma⁽¹⁾, qma@exponent.com; Richard Reiss⁽¹⁾; Clifford Habig⁽¹⁾; Paul Whatling⁽²⁾. (1) Health and Environmental Sciences, Exponent, Inc., Washington DC 20036 (2) Regulatory, Cheminova, Inc., Arlington VA 22209

The joint probability distribution analysis (JPDA) utilizes the full exposure distribution and the dose-response curve to determine the probability of an adverse effect occurring and the magnitude of the effect. It accounts for uncertainty from variations in exposure concentrations and species sensitivities and can better address the probability of risks of pesticides than the standard, regulatory risk quotient (RQ) method. In this application, the concern is for effects of dimethoate on salmonid prey which have differing sensitivity. Thus, accounting for variability in response is important. While the RQ method showed potential risks to aquatic invertebrates, JPDA showed no risks, despite using an exposure model that likely significantly overestimates water concentrations. This paper demonstrates the application of the JPDA methodology to refine an ecological risk assessment and develop more accurate risk estimates.

AGRO 203

Thermal reconstitution from sorbent tube odorant collections: Progress toward a robust, integrated strategy for capture, transport, archiving, and deferred "'re-play" of environmental odor events

Donald Wright⁽¹⁾, don.wright@plumechasers.com; Fred Kuhrt⁽²⁾; David Eaton⁽³⁾; Jacek Koziel⁽⁴⁾. (1) Don Wright & Associates, LLC (2) Microanalytics (a MOCON Company) (3) Epsilon Corp (4) Iowa State University

This submission reports on the authors' progress-to-date toward the optimization of a more robust and flexible environmental odor sampling strategy. In this approach, odor sampling is carried out utilizing sorbent tubes for preconcentration of the VOC odorants from a measured volume of air. Sample reconstitution is affected, in-laboratory, by thermal desorption into a purge gas stream and making up with humidified air to the final volume required to achieve a composition and odor 'match' to the originally-sampled environment. This integrated approach potentially carries a number of significant advantages: (a) superior odorant recovery performance for sorbent tubes across a wide volatility range; (b) long-term cold-storage stability with respect to adsorbed volatiles; and (c) minimization of storage time in the unstable vapor form. Odor event 're-play' can be directed to the appropriate targeted forum, including odor analysts, sensory panelists, and seated jurors in civil litigation actions.

Optical fiber ammonia sensors for air quality monitoring

Shiquan Tao, stao@wtamu.edu; Yu Huang; Lucas Wieck. Mathematics, Chemistry, and Physics, West Texas A&M University, Canyon TX 79016

Ammonia is a major air pollutant emitted from agricultural practices, such as animal feeding and fertilizer application. Sensor technologies with capability of continuous real-time monitoring of ammonia concentration in air are needed in order to study the contribution of ammonia emission from agricultural activities to the health of local residents, agricultural workers, as well as animals. We have developed fiber optic ammonia sensors using different sensing reagents and polymers for immobilizing the reagents. Reversible fiber optic sensors with detection limit down to low ppby level have been developed. The response time of these sensors ranged from seconds to tens of minutes depending on transducer design. Potential interferences from moisture and carbon dioxide were examined. A strategy for developing fiber optic sensor network for continuous, real-time monitoring of ammonia spatial distribution will be discussed based on these test results.

AGRO 205

Comparison of VOC emissions from conventional and alternative biofuel crops

Martin Graus⁽¹⁾⁽²⁾, martin.graus@noaa.gov; Allyson Eller⁽¹⁾⁽³⁾; Ray Fall⁽¹⁾⁽⁴⁾; Bin Yuan⁽⁵⁾; Yaling Qian⁽⁶⁾; Philip Westra⁽⁷⁾; Joost de Gouw⁽¹⁾⁽²⁾; Carsten Warneke⁽¹⁾⁽²⁾. (1) Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder CO 80309 (2) Chemical Sciences Division, National Oceanic and Atmospheric Administration, Boulder CO 80309 (3) Department of Ecology and Evolutionary Biology, University of Colorado, Boulder CO 80309 (4) Department of Chemistry and Biochemistry, University of Colorado, Boulder CO 80309 (5) College of Environmental Sciences and Engineering, Peking University, Beijing, China (6) Department of Horticulture and Landscape Architecture, Colorado State University, Fort Collins CO 80523 (7) Department of Bioagricultural Sciences and Pest Management, Colorado State University, Fort Collins CO 80523

Plants emit substantial amounts of volatile organic compounds (VOCs) into the atmosphere where they can contribute to ozone and aerosol formation. Composition and emission rates of those biogenic VOCs vary strongly between plant species and are governed by phenological, physiological, and environmental factors. Fuel ethanol production in the US utilizes cornstarch as main feedstock. Cellulosic ethanol fermentation is in transition from smallscale trials to industrial production and will take advantage of abundant cellulose sources (e.g., switchgrass or tree species). Leaf level emission factors of VOCs from corn and switchgrass were measured in the field and will be presented along with whole plant VOC emission rates measured from greenhouse grown plants. The corn and switchgrass emissions will be compared with those from tree species which have been studied much more extensively in the literature. The goal of this research is to determine plant species with low emissions to minimize air quality impacts.

AGRO 206

Weather-based conditional sampling of ammonia near livestock operations using passive samplers

Jay M Ham, jay.ham@colostate.edu; Christina Williams; Joshua Stratton; Thomas Borch. Department of Soil and Crop Sciences, Colorado State University, Fort Collins CO 80523

Passive samplers can be used to measure spatial variations of ammonia near livestock operations, but results are often confounded by changing weather conditions during extended deployment periods (e.g., 1 to 2 weeks). A new type of conditional sampler was developed that only exposes the passive samplers when a user-defined set of wind and weather conditions are met. The NH₃ samplers where housed in air-tight boxes that could be opened and closed with a motorized actuator controlled by a datalogger. Samplers were deployed on portable tripods equipped with an anemometer, wind vane, thermometer, and humidity sensor. Multiple sampling tripods were deployed near cattle feedlots and dairies and programmed to only expose the passive samplers when the upwind source area represented a specific zone of the operation. This methodology allows improved mapping of high NH₃ emission zones and more accurate measurements of downwind concentration aradients.

AGRO 207

Emissions from swine barns: Effects of slurry age

Kristoffer E.N. Jonassen, krj@lf.dk. Department of Housing and Environment, Pig Research Centre, Danish Agriculture & Food Council, Copenhagen DK-1609, Denmark

The emission of odor and ammonia from finisher units increases with the size of the finishers and the age of the slurry in the pits underneath the floor. This study has focused on the age of the slurry and how often the pits have to be drained to obtain the lowest emissions. The study was carried out in six identical experimental sections during one batch of finishers. The only difference between the sections was the age of the slurry in the pits. Odor, hydrogen sulfide, and ammonia were measured for nine weeks. The emissions were lowest in the first week after draining of the pits, and then the emissions increased until they reached a constant level within two weeks after draining. Greenhouse gasses were measured for two weeks in the last part of the production period.

AGRO 208

Characterization of VOCs and odorants on PM from animal feeding operations

Steven L. Trabue⁽¹⁾, steven.trabue@ars.usda.gov; Ronaldo Maghirang⁽²⁾; David Parker⁽³⁾; Laura L McConnell⁽⁴⁾. (1) National Laboratory for Agriculture and the Environment, USDA-Agricultural Research Service, Ames IA 50011 (2) Department of Biological and Agricultural Engineering, Kansas State University, Manhattan KS 66506 (3) US Meat Animal Research Center, USDA-Agricultural Research Service, Clay Center NE 68933 (4) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, Beltsville MD 20705

Little is know about the emissions of PM from animal feeding operations, yet PM is thought to be a prime transport mechanism for both odors and biological material. In this study, TSP, PM_{10} and $PM_{2.5}$ from several different animal feeding operations (AFOs) were analyzed for VOC profiles at

control, source and downwind locations (50 - 400 m). Sample were analyzed by thermal desorption GC-MS (TD-GC/MS) technique. The VOC compounds associated with PM from AFO were oxygenated and dominated by n-alkanoic acids with C_{16} and C_{18} as the most abundant compounds. The VOC profile for each PM size fraction were similar for each production/animal facility.

AGRO 209

Interaction of urea hydrolysis, CO₂ emission, and pH on ammonia emission from dairy barn floors

Felipe Montes, felipemontesus@yahoo.com; Sasha D. Hafner; C. Alan Rotz. Pasture System and Watershed Management Research Unit, USDA-Agricultural Research Service, University Park PA 16802

Our group has developed a mathematical model of CO_2 and NH_3 emission from dairy manure that includes interactions between these emissions and manure pH. This model has been used to simulate emission dynamics for manure (a mixture of urine, bedding, and feces) with completely hydrolyzed urea, which does not include the urea hydrolysis process occurring in urine layers on barn floors. We use a Lambert omega function methodology to update urea degradation kinetic parameters and extend our model to simulate NH_3 emission dynamics from urine layers. Model predictions show that ammonia volatilization from urine layers is controlled by urea hydrolysis and the effects of its products (NH_3 and CO_2) on pH, resulting in ammonia volatilization dynamics that are very different than those for manure.

AGRO 210

Monthly, seasonal, and annual methane emissions from a beef cattle feedyard

Richard W Todd, richard.todd@ars.usda.gov; N. Andy Cole. Conservation and Production Research Laboratory, USDA-Agricultural Research Service, Bushland TX 79012

Gaseous emissions from animal feeding operations are of increasing interest as concerns about global warming and subsequent climate disruption increase. Confined animals directly emit about two-thirds of greenhouse gases from US animal agriculture, mostly as methane from enteric fermentation: half of those emissions are from beef cattle. Our objective was to quantify multi-year, whole-farm methane emissions from a commercial beef cattle feedyard. During 2009 and 2010, we monitored two source areas at the feedyard, cattle pens, and retention pond, which included enteric, manure and runoff water methane emissions. Methane concentration over source areas and background was measured using open path laser spectroscopy. An inverse dispersion model was used to quantify emissions. Methane flux densities and per capita emission rates are reported and integrated for monthly, seasonal, and annual periods. Results are compared to estimates from US EPA inventory methods.

AGRO 211

DairyGEM: A software tool for whole farm assessment of emission mitigation strategies

C. Alan Rotz, al.rotz@ars.usda.gov; Felipe Montes; Sasha D. Hafner. Pasture Systems and Watershed Management Research Unit, USDA-Agricultural Research Service, University Park PA 16802

Accurate assessment of the impact of management on agricultural emissions requires consideration of many farm components and their interactions. A comprehensive assessment is needed because changes made to reduce one emission type or source may increase another. A new software tool was developed that uses process-level simulation to predict ammonia, hydrogen sulfide, and greenhouse gas emissions from dairy production systems. A partial Life Cycle Assessment is included to determine the farm gate carbon footprint. This educational tool, called the Dairy Gas Emission Model or DairyGEM, can be used to study the effects of management changes on all of the major farm emission sources from feed production to the return of manure back to the land. Education received through these comprehensive evaluations will lead to the development of more sustainable dairy production systems. More information and the DairyGEM software are available on the Internet at

http://www.ars.usda.gov/Main/docs.htm?docid=21345.

AGRO 212

Human metabolic interactions of pesticides: Induction and cytotoxicity

Andrew D Wallace, andrew_wallace@ncsu.edu; Ernest Hodgson. Department of Environmental and Molecular Toxicology, North Carolina State University, Raleigh NC 27695

Studies by our group have indicated potential for interactions based on cytochrome(s) P450 (CYPs) induction and cytotoxicity. For example fipronil is a potent inducer at low doses but cytotoxic at higher doses in human hepatocytes. Chlorpyrifos is bioactivated by CYPs to the toxic chlorpyrifos-oxon (CPO) and the non-toxic trichloropyridinol (TCP). Epidemiological studies raise concerns that human diseases are linked to CPS exposure. We showed variation in liver CPS metabolism and metabolite production. To investigate variation in humans from CPS exposure, hepatocytes were treated with CPS, RNA prepared, and microarray analysis performed (Affymetrix Gene Chip Human Genome Arrays) to identify regulated genes and pathways regulated in different individuals. A number of genes were differentially expressed including genes regulating detoxication enzymes, retinol metabolism, and actin cytoskeletonal regulation. Our findings suggest that exposure to CPS leads to gene expression changes that are largely common across individuals, but also indicate unique attributes.

Human metabolic interactions of pesticides: Inhibition

Ernest Hodgson, ernest_hodgson@ncsu.edu; Andrew D Wallace. Department of Environmental and Molecular Toxicology, North Carolina State University, Raleigh NC 27695

Agrochemicals regulation utilizes single chemical hazard determination in surrogate animals that show little variation. Relevance to real world situations is questionable, because dose and species extrapolations require uncertainty factors and agrochemicals are typically used as mixtures. Human studies provide information on population variation, subgroups at increased risk, and interactions among agrochemicals and endogenous metabolites. How components in agrochemical mixtures affect each others toxicokinetics is largely unknown. Metabolism and interactions of agrochemicals have been investigated using human liver microsomes and CYP isoforms. Chlorpyrifos, carbaryl, carbofuran, and fipronil are metabolized by liver microsomes, CYP2B6 and CYP3A4 being the important CYPs. Permethrin is hydrolyzed by esterase(s) present in human liver microsomes and cytosol. Phosphorothioates are potent inhibitors of CYP metabolism of steroid hormones as well as some diesel fuel components and other pesticides, including carbaryl and fipronil. Fipronil also inhibits testosterone metabolism. Expression of CYP2B6 with age and variation in chlorpyrifos metabolism is discussed.

AGRO 214

In vitro and in vivo experimental data for pyrethroid pharmacokinetic models: The case of bifenthrin

Michael F Hughes⁽¹⁾, hughes.michaelf@epa.gov; James M Starr⁽²⁾; Edward J Scollon⁽³⁾; Michael J DeVito⁽⁴⁾. (1) Office of Research and Development, National Health and Environmental Effects Research Laboratory, US Environmental Protection Agency, Research Triangle Park NC 27711 (2) Office of Research and Development, National Exposure Research Laboratory, US Environmental Protection Agency, Research Triangle Park NC 27711 (3) Office of Pesticide Programs, Health Effects Division, US Environmental Protection Agency, Washington DC 20460 (4) National Institute of Environmental Health Sciences, National Toxicology Program, NIH, Research Triangle Park NC 27709

Pyrethroids are a class of neurotoxic synthetic pesticides. Exposure to pyrethroids has increased due to declining use of other classes of pesticides. Our studies are focused on generating in vitro and in vivo data for the development of pharmacokinetic models for pyrethroids. Using bifenthrin as a model compound, the rat and human hepatic intrinsic clearance are 224 and 20 mL/min/kg bw, respectively. Oxidative in vitro metabolism of bifenthrin predominates over hydrolysis. Peak bifenthrin blood and brain concentrations in the rat after oral administration of 0.3 and 3 mg/kg occur at 1 and 4 - 6 hr, respectively. The momentary bifenthrin brain concentration correlates with the neurotoxic effect in the rat independent of time. This type of data can be used for development of animal pharmacokinetic models with extrapolation to human models leading to decreased uncertainties in the risk assessment of the pyrethroids. (This abstract does not necessarily represent US EPA or NIH policy.)

AGRO 215

Paraoxonase 1 (PON1) status in risk assessment for organophosphate exposure and pharmacokinetics

Clement E Furlong⁽¹⁾, clem@uw.edu; Toby B Cole⁽¹⁾; Gail P Jarvik⁽¹⁾; Wan-Fen Li⁽²⁾; Allan E Rettie⁽³⁾; Rebecca J Richter⁽¹⁾; Kenneth E Thummel⁽⁴⁾. (1) Department of Medicine, Division of Medical Genetics, and Department of Genome Sciences, University of Washington, Seattle WA 98195-7720 (2) Department of Medicine, Division of Medical Genetics, University of Washington, Seattle WA 98195-7720 (3) Department of Medicinal Chemistry, University of Washington, Seattle WA 98195-7720 (4) Department of Pharmaceutics, University of Washington, Seattle WA 98195-7610

Paraoxonase 1 (PON1), an HDL-associated multifunctional enzyme, is important in protecting against exposures to chlorpyrifos/chlorpyrifos oxon, diazinon/diazoxon, and vascular disease; and in the case of certain drugs, PON1 bioactivates some while inactivating others. Two coding region polymorphisms have been described (L55M and Q192R), one of which (Q192R) affects the catalytic efficiency of substrate hydrolysis. In addition to the coding region polymorphisms, single nucleotide polymorphisms (SNPs) in the PON1 promoter region influence expression of PON1. The term PON1 status includes determination of both the functional Q192R polymorphism for an individual as well as their plasma activity level and is determined by a twosubstrate assay protocol, measurements of which are crucial for determining risk of pesticide exposure or disease and rates of drug metabolism. Epidemiological studies that examine only PON1 single nucleotide polymorphisms are inadequate for determination of risk or rates of metabolism. (Supported by NIH Grants ES009883, ES09601, ES04696, ES07033, HL67406, HL074366.)

AGRO 216

Carboxylesterases: Dual roles in lipid and pesticide metabolism

Matthew K. Ross, mross@cvm.msstate.edu. Center for Environmental Health Sciences, Mississippi State University, Mississippi State MS 39762

Carboxylesterases (CES, EC 3.1.1.1) are members of a superfamily of serine hydrolases that hydrolyze ester, amide, and carbamate bonds. Several different CES genes exist in mammalian species with evidence of multiple gene duplication events occurring throughout evolutionary history. Five CES genes are reported in the Human Genome Organization database, although CES1 and CES2 are the two best characterized human genes. An emerging picture of the CES family suggests that these enzymes have roles in the metabolism of both xenobiotic and endobiotic compounds. Pesticides, such as the pyrethroids and organophosphates, are important xenobiotic substrates that are metabolized by CES, whereas cholesteryl esters, triacylglycerols, 2arachidonoylglycerol, and prostaglandin glyceryl esters are endobiotics that are substrates for CES. Functional studies using selective chemical inhibitors, siRNA, and gene knockout models are providing valuable insights into the physiological functions of CES, and suggest that CES may be a novel target for the treatment of diseases such as diabetes and atherosclerosis. This presentation will examine the known physiological functions of CES and the interactions between pesticides and lipids that occur at the level of the CES enzymes, including the kinetic rate constants that describe the metabolism of these compounds.

Behavioral changes in young and adult rats: Indications of cholinesterase inhibition

Virginia C Moser⁽¹⁾, moser.ginger@epa.gov; Pamela M Phillips⁽¹⁾; Katherine L McDaniel⁽¹⁾; David W Herr⁽¹⁾. (1) Toxicity Assessment Division, US Environmental Protection Agency, Research Triangle Park NC 27711

Inhibition of acetylcholinesterase has long been accepted as the basis for neurotoxicity produced by organophosphorus (OP) and N-methyl carbamate chemicals. Functional or behavioral alterations result from acute exposure to these chemicals. We have conducted behavioral evaluations and concurrent cholinesterase inhibition for many OPs and carbamates in both adult and preweanling rats. In many cases, a within-subject design allows direct correlations, and in one case (carbaryl), tissue levels are also available to complete the linkages from dosimetry to effect. Overall, we have shown that there are several patterns of behavior: enzyme correlations and that these are chemicalspecific. Furthermore, these correlations are distinctly different between adult and young animals. These data can be modeled to inform PBPK/PD predictions of OP and carbamate neurotoxicity. (This is an abstract of a proposed presentation and does not reflect US EPA policy.)

AGRO 218

Comparison of esterase sensitivity, metabolic efficiency, and toxicity levels of two organophosphorus insecticides, parathion, and chlorpyrifos

Janice E. Chambers⁽¹⁾, chambers@cvm.msstate.edu; Howard W. Chambers⁽²⁾. (1) Center for Environmental Health Sciences, Mississippi State University, Mississippi State MS 39762 (2) Department of Entomology and Plant Pathology, Mississippi State University, Mississippi State MS 39762

Phosphorothionates, weak anticholinesterases, are bioactivated by P450 to potent oxon metabolites by desulfuration. P450-mediated detoxication, dearylation, can also occur, and is more effective against chlorpyrifos than parathion. The oxons can persistently inhibit serine esterases, including nervous system acetylcholinesterase (the target enzyme), and protective β-esterases such as carboxylesterases. Chlorpyrifos-oxon (CPO) is a more potent inhibitor of serine esterases than is paraoxon (PO). The oxons can be hydrolyzed by paraoxonase (PON) which is more efficient with CPO than PO. Despite greater potency of CPO as an anticholinesterase, chlorpyrifos is 10 - 20 fold less acutely toxic than parathion because of greater detoxication of chlorpyrifos. However, using a sensitive indirect assay for CPO hydrolysis with human serum, overall level of PON activity as monitored at high oxon concentrations does not influence the amount of CPO that is hydrolyzed at low more toxicologically relevant concentrations, presumably because PON is not saturated. (Support: NIH ES00190, ES04394, ES15107)

AGRO 219

Advancements in Endangered Species Act effects determination for pesticide registration actions

Edward W Odenkirchen, odenkirchen.edward@epa.gov. Office of Pesticide Programs, US Environmental Protection Agency, Washington DC 20460

Pesticide registration activities by the US Environmental Protection Agency under the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) must also consider the potential for adverse effects to federally-listed threatened and endangered species (listed species) in accordance with provisions in Section 7 of the Endangered Species Act (ESA). Many of the registration decisions undertaken by the Agency include large geographical areas with the potential for pesticide use to be in proximity to a variety of listed species. The number and geographical scope of these regulatory actions and the high degree of biological activity associated with pesticidal chemicals to one or more taxa have lead to a recognized need to develop rapid, geographically-specific, and biologically-relevant risk assessment methods to account for the potential dispersal of pesticides across the landscape and the potential to impact listed species directly and indirectly. This presentation will present a number of technical challenges and the progress made to address these challenges as the agency moves toward a nationwide approach to meeting ESA responsibilities for FIFRA actions.

AGRO 220

Using GIS to assess pesticide exposure to threatened or endangered species for ecological risk assessment

James Cowles, jim.cowles@agr.wa.gov. Washington Department of Agriculture, Olympia WA 98504-2560

With the listing of salmon for protection under the Endangered Species Act, the Washington State Department of Agriculture (WSDA) determined that the traditional environmental data sets for pesticide registration decisions were insufficient to accurately determine potential exposure and subsequent effects of pesticides on salmonids and other listed species in Washington State. WSDA has implemented a program to spatially determine the location and use of pesticides in relationship to salmonid habitat and monitor pesticide residues in salmon-bearing streams in Washington State. Data elements developed include a geographic information system (GIS) incorporating the location of commodities grown in Washington, the estimation of state specific pesticide use and collection of water quality data. Examples and limitations of these data sets for assessing exposure to salmonids and terrestrial species are presented.

Development of a spatial-temporal co-occurrence index to evaluate pesticide risks to threatened and endangered species

Gerco Hoogeweg⁽¹⁾, hoogewegg@waterborne-env.com; Debra Denton⁽²⁾; Richard S. Breuer⁽³⁾; Gregg Hancock⁽¹⁾; Patti TenBrook⁽²⁾. (1) Waterborne Environmental, Inc., Leesburg VA 20175 (2) US Environmental Protection Agency, Region 9, San Francisco CA 94105 (3) Environmental Water Quality and Estuarine Studies, California Department of Water Resources, Sacramento CA 95814

Increasingly, the spatial and temporal co-occurrence of pesticide mass loadings and threatened and endangered species is discussed as part of agrochemical product registration and regulation in the United States. However, methodologies have not been developed to address this issue in a transparent and standardized manner. An index method was developed to evaluate the spatial and temporal co-occurrence of pesticides and species, and then applied in a large ecosystem assessment project in California. The cooccurrence index combines monthly species abundance with statistical distributions of pesticide exposure events exceeding toxicity benchmarks for 40 widely-used pesticides. The frequency of co-occurrence was determined for 12 aquatic and semi-aquatic species. The application of the methodology is presented for three species, including the delta smelt, the Central Valley fall-run Chinook salmon, and the California red-legged frog.

AGRO 222

Access to NatureServe's best available data on the locations of endangered species

Shara Howie⁽¹⁾, shara_howie@natureserve.org; Kat Maybury⁽²⁾; Leslie Honey⁽²⁾. (1) Conservation Services, NatureServe, Boulder CO 80303 (2) Conservation Services, NatureServe, Arlington VA 22209

NatureServe is the exclusive source of a fully aggregated dataset of the known locations of threatened, endangered, and other at-risk species throughout the US. We and our member natural heritage programs also have extensive expertise in creating models to predict additional species locations. We will discuss these best available data and how they can be accessed and used to determine the potential risk that pesticide exposure may pose to these species. In particular, we will discuss access to precise locality data, and we will demonstrate a new application that enables screening of an area for the known or predicted presence of threatened and endangered (T&E) species. These tools represent new portals to this information and offer potential solutions for predicting, minimizing, and avoiding conflicts with pesticide use.

AGRO 223

DriftWatch.org: Pesticide sensitive crops and habitats registry implementation results

Leighanne Hahn⁽¹⁾, HahnL@purdue.edu; Larry Theller⁽²⁾; Adam Reimer⁽³⁾; Bernie Engel⁽²⁾. (1) Water Quality/Endangered Species Program, Office of Indiana State Chemist, West Lafayette IN 47907-2063 (2) Agricultural and Biological Engineering, Purdue University, West Lafayette IN 47907-2093 (3) Forestry and Natural Resources, Purdue University, West Lafayette IN 47907-2061

The Driftwatch.org Pesticide Sensitive Crop and Habitats Registry was developed through a collaboration of producers of pesticide sensitive specialty crops, stewards of at-risk habitat (including pollinators), and pesticide applicator communities. The DriftWatch Registry assists producers in mapping their field(s) and identifying their specialty crop type on the publicly accessible website www.driftwatch.org. A second registry enables automated pesticide applicator notifications. Pesticide applicators can view sensitive fields and contact information in the area of their scheduled applications. Nearby habitats of endangered species are displayed, as are other themed data such as watersheds with public drinking water intakes. The goal of the developers of the registry is to facilitate effective communication between the specialty crop grower, pesticide applicator, and stewards of surrounding at risk habitat. This presentation will share recent survey outcomes measuring attitudes, motivations ,and behaviors of pesticide applicators towards natural resource concerns and the use of the DriftWatch.org website.

AGRO 224

Use of risk-based spray drift buffers for protection of non-target areas

Scott H. Jackson⁽¹⁾, scott.jackson@basf.com, 26 Davis Drive, PO Box 13528, Research Triangle Park NC 27709; Mark Ledson⁽²⁾. (1) Regulatory Stewardship and Strategy, BASF Corporation, Research Triangle Park NC 27709 (2) Application Technology, Syngenta Crop Protection, Greensboro NC 27409

Regulatory authorities have started a shift in spray drift label language from protecting threatened and endangered species and habitat to protecting non-target areas including grasslands, forested areas, shelter belts, woodlots, hedgerows, riparian areas, and shrub lands. We outline a process for using spray drift models to determine buffer distances using non-target species study NOEC, EC₂₅ or EC₅₀ endpoints. The conservatively protective nature of this approach is explored, as well as its current use in regulatory practices. Use of the presented method provides adequate protections for former, current, or future habitat. Use of risk-based buffers should be included as part of an accepted toolbox of fixes for non-target species exposure concerns.

AGRO 225

Development of a website (www.Pre-Serve.org) to help protect threatened and endangered plants near crop production

Katherine H Carr, katherine.h.carr@monsanto.com; Joy L Honegger; Spencer R Mortensen; David I Gustafson. Regulatory, Monsanto Company, Saint Louis MO 63141

In 2008, Monsanto Company began its Glyphosate Endangered Species Initiative to help protect threatened and endangered (T&E) species from potential effects of the application of glyphosate herbicides to crops, including those containing Roundup Ready® technology. Monsanto developed a user-friendly website (www.Pre-Serve.org) to provide growers with information regarding areas where T&E plants may be present near land used for crop production. The user follows a 4-step process to locate the application site using a map-based interface, and then determines if specific application instructions must be followed. These instructions provide the user with a site map, a habitat description, and detailed application instructions. Within defined areas, the instructions specify a rate limit for ground applications; for aerial applications, if the described habitat is downwind from the application site, a drift buffer is specified with its size based on spray-droplet size category and application rate.

Comparing two micrometeorological techniques for estimating trace gas emissions from distributed sources

Kyoung S Ro⁽¹⁾, kyoung.ro@ars.usda.gov; Melvin H Johnson⁽¹⁾; Patrick G Hunt⁽¹⁾; Thomas Flesch⁽²⁾. (1) Coastal Plains Soil, Water, and Plant Research Center, USDA-Agricultural Research Service, Florence SC 29501 (2) Department of Earth and Atmospheric Science, University of Alberta, Edmonton, Canada

Measuring trace gas emission from distributed sources such as treatment lagoons, treatment wetlands, land spread of manure, and feedlots requires micrometeorological methods. In this study, we tested the accuracy of two relatively new micrometeorological techniques, vertical radial plume mapping (VRPM) and backward Lagrangian stochastic (bLs) techniques. These techniques were combined with a path integrated optical remote sensing (PI-ORS) system consisting of a tunable diode absorption spectrometer mounted on an automatic positioning device. Integrated VRPM software (Arcadis Inc., NC) controls the automatic positioning device to direct the laser beams to various retroreflectors on the ground and the tower. WindTrax software (Thunder Beach Scientific, Nanaimo, Canada) interfaces concentration and wind sensor data with the bLs dispersion model. Three different distributed emission sources were simulated; 3.1 m and 27 m squares of perforated PVC pipe networks and soaker hoses stretching out to make a star-shaped circular emission source with diameter of 40 m. Known rates of the CH₄ gas were released during the validation studies. The actual masses of CH₄ gas released were measured with a floor scale periodically. For single source emissions, the VRPM method measured CH₄ emission rate at $Q_{VRPM}/Q = 1.38 \pm 0.28$; the bLs method measured emission rate at $Q_{bLs}/Q = 0.98 \pm 0.24$. The accuracy of the bLs technique improved with number of path integrated concentration (PIC) data. For double emission sources, the accuracy of the VRPM method decreased significantly ($Q_{VRPM}/Q = 1.76 \pm 0.28$). The accuracy of bLs method decreased slightly for the double emission sources $(Q_{bLs}/Q = 0.93 \pm 0.23)$. The impact of number PICs and footprint on accuracy of these two techniques will also be discussed.

AGRO 227

Source apportionment and tracing of agricultural and fossil fuel reactive N emissions using stable isotopic composition

Joseph D Felix⁽¹⁾, jdf47@pitt.edu; Emily M Elliott⁽¹⁾; Ronaldo Maghirang⁽²⁾; John Briggs⁽²⁾; Laura McConnell⁽³⁾; Timothy Gish⁽³⁾; Meredith Hastings⁽⁴⁾; David Gay⁽⁵⁾. (1) Department of Geology and Planetary Science, University of Pittsburgh, Pittsburgh PA (2) Kansas State University (3) Beltsville Agricultural Research Center, USDA-Agricultural Research Service (4) Brown University (5) NADP

Reactive nitrogen emissions (NO_x and NH₃) are significant contributors to global water and air quality degradation. Agricultural operations and fossil fuel combustion are significant sources of reactive N; however source partitioning remains a challenge. The stable isotopic composition (δ^{15} N) of reactive N may be a valuable tool for characterizing source, transport, and fate of reactive N emissions, but limited studies have been conducted characterizing δ^{15} N of reactive N sources. Here, we report progress on a comprehensive inventory of δ^{15} N of reactive N from various agricultural and fossil fuel sources. The ability of δ^{15} N to trace reactive N emission across varying spatial scales was

assessed using three approaches: 1) establishing local transects radiating from reactive N emission sources; 2) deploying NH_3 samplers at 9 US monitoring sites in conjunction with AMoN; and 3) reconstructing the regional influence of agricultural emissions to nitrate deposition recorded in an ice core from Summit, Greenland.

AGRO 228

Measurements of isocyanic acid (HNCO) from agricultural burning

James M Roberts⁽¹⁾, James.M.Roberts@noaa.gov; Trevor C. VandenBoer⁽²⁾; Steven B. Brown⁽¹⁾; William P. Dube⁽³⁾; Nicholas Wagner⁽³⁾; Cora Young⁽³⁾; Charles A. Brock⁽¹⁾; Ann Middlebrook⁽¹⁾; Roya Bahreini⁽³⁾; Patrick R. Veres⁽⁴⁾; Anthony K. Cochran⁽⁵⁾; Carsten Warneke⁽³⁾; Martin Graus⁽³⁾; Joost A. de Gouw⁽³⁾; Ian R. Burling⁽⁶⁾; Robert J. Yokelson⁽⁶⁾. (1) Chemical Sciences Division, NOAA/ESRL, Boulder CO 80305 (2) Department of Chemistry, University of Toronto, Toronto ON M5A 2N4, Canada (3) CIRES, University of Colorado, Boulder CO 80309 (4) Atmospheric Chemistry, Max Planck Institute for Chemistry, Mainz 55020, Germany (5) NOAA/ISET, North Carolina A&T, Greensboro NC 27411 (6) Department of Chemistry, University of Montana, Missoula MT 59812

Agricultural burning is a common management practice that may have increased importance if carbon-positive practices such as biochar are encouraged. The emissions from burning have impacts on air quality that need to be considered. Our recent laboratory test burns and field measurements have shown that HNCO is produced in biomass fires at significant concentrations, up to 600 parts-per-billion by volume (ppbv). In addition, solubility measurements, reactivity considerations, and the biochemistry of carbamylated proteins imply that HNCO could be a significant cause of smoke-related health effects. As a consequence, these emissions need to be integrated into agricultural burning policies and practices.

AGRO 229

Residual carbaryl in treated pine bark and the presence of carbaryl in wood smoke

Chris Peterson⁽¹⁾, cjpeterson@fs.fed.us; Sheryl Costello⁽²⁾. (1) Insects, Diseases, and Invasive Plants Unit, USDA Forest Service, Starkville MS 39759 (2) Forest Health Protection, USDA Forest Service, Golden CO 80401

This in-progress study measures the dissipation of carbaryl on the bark of ponderosa and lodgepole pines treated for the prevention of mountain pine beetle, Dendroctonus ponderosae, infestation and the presence of the compound in wood smoke. The concentration of carbaryl was lower in ponderosa pine bark, probably because of a dilution effect caused by the thickness and porosity of ponderosa pine bark relative to lodgepole pine bark. There was no significant dissipation of carbaryl from application in June 2010 to February 2011 on either species. Dissipation between the October and February sampling dates was not expected to be high due to the low temperatures and because precipitation during this time was in the form of snow instead of rain. Carbaryl was readily detected in wood smoke from both tree species when measured by pulling the smoke from burning bark samples through a filter.

Detailed modeling of ozone formation from animal feed emissions in the San Joaquin Valley

Cody J. Howard⁽¹⁾, cody.howard@ars.usda.gov; Jianlin Hu⁽²⁾; Peter G. Green⁽²⁾; Michael J. Kleeman⁽²⁾. (1) Beltsville Agricultural Research Center, USDA-Agricultural Research Service, Beltsville MD 20705 (2) Civil and Environmental Engineering, University of California at Davis, Davis CA 95616

The San Joaquin Valley (SJV) in California currently experiences some of the highest surface ozone (O₃) concentrations in the United States even though it has a population density that is an order of magnitude lower than many urban areas with similar ozone problems. Previous studies have used approximate calculations to show that animal feed emissions (silage) may form up to 25 tons/day of ozone in the SJV making silage among the top sources of volatile organic compounds (VOCs) that contribute to ozone formation in the region. In the present study, detailed air quality model calculations are used to rigorously evaluate surface-level ozone concentrations from animal feed emissions and to compare this source to other leading VOC sources. The air quality model tracks emissions, transport, chemical reaction, and deposition of all species involved in the ozone formation process. Calculations are applied during a typical stagnation event in July 2005 using a horizontal grid resolution of 4 km to cover all of central California. Comparisons are made between (1) base case emissions (including mobile sources and animal feed) vs. no feed emissions, (2) base case emissions vs. no mobile source emissions, and (3) base case emissions vs. no mobile source VOC emissions (leaving mobile source NO_x emissions unchanged). The results demonstrate the effect of animal feed VOC emissions on actual ozone concentrations in the SJV while at the same time evaluating the efficacy of VOC vs. NO_x controls in the SJV.

AGRO 231

Airborne observations of ammonia emissions from agricultural sources and their implications for ammonium nitrate formation in California

John B Nowak⁽¹⁾⁽²⁾, john.nowak@noaa.gov, 325 Broadway, R/CSD-7, Boulder CO 80305; J Andrew Neuman⁽¹⁾⁽²⁾; Roya Bahreini⁽¹⁾⁽²⁾; Ann Middlebrook⁽²⁾; Charles A Brock⁽²⁾; Gregory J Frost⁽¹⁾⁽²⁾; John S Holloway⁽¹⁾⁽²⁾; Stuart A McKeen⁽¹⁾⁽²⁾; Jeff Peischl⁽¹⁾⁽²⁾; Ilana B Pollack⁽¹⁾⁽²⁾; James M Roberts⁽²⁾; Thomas B Ryerson⁽²⁾; Michael Trainer⁽²⁾; David D Parrish⁽²⁾. (1) Cooperative Institute for Research in Environmental Sciences, University of Colorado at Boulder, Boulder CO 80309 (2) Earth System Research Laboratory, NOAA, Boulder CO 80309

Ammonia (NH₃) is the dominant gas-phase base in the troposphere. As a consequence, NH₃ abundance influences aerosol formation and composition. Anthropogenic emissions of NH₃ and NO_x (NO + NO₂), which in sunlight can be oxidized to form nitric acid (HNO₃), can react to form ammonium nitrate aerosol. Two major NH₃ sources from agricultural activity are animal waste and crop fertilization. Agricultural activity (i.e., dairy farms), and urban centers (i.e., Fresno, Los Angeles (LA)) are sources of ammonium nitrate gas-phase precursors in both the Central Valley and the LA Basin of California. Airborne measurements of NH₃, HNO₃, particle composition, and particle size distribution made aboard the NOAA WP-3D aircraft as part of CalNex 2010 were used to quantify NH₃ emissions from agricultural sources, to describe the vertical structure and transport of NH₃ from these sources, to examine their impact on

ammonium nitrate formation, and to contrast the Central Valley with the LA Basin.

AGRO 232

Comparative study of observed and CMAQ modeled coarse particulate matter

Rong Li⁽¹⁾⁽²⁾, rongli@ucar.edu; Christine Wiedinmyer⁽¹⁾; Michael P. Hannigan⁽²⁾; Kirk R. Baker⁽³⁾. (1) Atmospheric Chemistry Division, National Center for Atmospheric Research (NCAR), Boulder CO 80301 (2) Department of Mechanical Engineering, University of Colorado, Boulder CO 80301 (3) Office of Air Quality, Planning, and Standards (OAQPS), US Environmental Protection Agency, Research Triangle Park NC 27711

Coarse particulate matter (PM_{10-2.5}) has been linked to mortality and morbidity. However, few studies have quantified its emissions from different sources, determined the ambient chemical composition, and/or temporal and spatial variability. Additionally, accurate PM_{10-2.5} modeling tools are needed by the scientific community and regulatory agencies for mitigation strategy development and health effect assessments. We evaluated PM_{10-2.5} by comparing measurements from US EPA's Air Quality System and other sources to output from an annual simulation (2005) from the CMAQ (Community Multiscale Air Quality) regional chemical transport model. Preliminary results show that the model significantly underestimates observed PM_{10-2.5} concentrations. Differences are also found in diurnal and seasonal cycles between modeled and observed concentrations. We also evaluated the chemical composition of the observed and modeled PM_{10-2.5}. CMAQ does not include organic materials in $PM_{10-2.5}$; however, speciation measurements show that organics constitute a significant component. This study has identified some important gaps for our model development.

AGRO 233

Characterization of pyrethroid insecticide interactions with cloned human Na⁺ channels in high-throughput patch clamp

Glenn E Kirsch, gkirsch@chantest.com; Yuri A Kuryshev. Research, ChanTest Corporation, Cleveland OH 44128

Automated patch clamp enables high-throughput assessment of ion channel interactions with drugs and toxicants under conditions that preserve channel function. We have optimized an automated assay for assessing pyrethroid insecticide activity in a panel of 8 voltage-gated, human Na⁺ channels stably expressed in CHO cells. A single point, 50 µM, screen identified 10 of 11 pyrethroids as Na⁺ channel gating modifiers (slowing of channel inactivation and/or induction of persistent Na+ current). The most sensitive channels included isoforms expressed in CNS (hNav1.2), PNS (hNav1.8/ β_3), and cardiac (hNav1.5) tissues. Bioallethrin and esfenvalerate were found to increase $hNav1.8/\beta_3$ current in a concentration-dependent manner with EC₅₀ values of 7.2 and 6.8 μM, respectively. Thus, an automated assay can provide sensitive, functional screening to detect potential Na+ channel toxicity. The method should facilitate large-scale screening for early-stage toxicity testing, determination of structure-activity relationships, and development of in vitro databases to support models for toxicity prediction.

Pyrethroid actions on sodium channels: Isoform and species selectivity

David M. Soderlund, dms6@cornell.edu. Department of Entomology, Cornell University, Geneva NY 14456

The insecticidal activity of pyrethroids results from their disruption of the gating of nerve membrane sodium channels. Assessing the action of pyrethroids on sodium channels in mammals is complicated by the existence of a family of channel proteins, each of which exhibits unique developmental and anatomical distribution patterns, functional properties, and pharmacology. Using the Xenopus oocyte expression system to characterize the action of pyrethroids on mammalian sodium channels of defined structure, we have found substantial variation in pyrethroid sensitivity among rat sodium channel isoforms. We also employed this system in initial experiments to compare orthologous rat and human isoforms and have discovered an unexpected species difference in the sensitivity of Na_v1.3 sodium channels, the principal isoform expressed in the developing brain. Isoform and species differences in channel sensitivity are important factors to consider in the development of quantitative models of pyrethroid action and their use in human risk assessment.

AGRO 235

Pyrethroid effects on sodium flux, calcium flux, and network activity assessed in cortical neurons

Timothy J Shafer⁽¹⁾, shafer.tim@epa.gov, MD B105-03, RTP NC 27711; Andrew FM Johnstone⁽¹⁾; Zhengyu Cao⁽²⁾; Sandra Losa⁽¹⁾; Thomas F Murray⁽²⁾. (1) Integrated Systems Toxicology Division, US Environmental Protection Agency, Research Triangle Park NC 27711 (2) Department of Pharmacology, Creighton University, Omaha NE 68178

Patch clamp measurements provide information on how pyrethroids alter the function and kinetics of ion channels, but do not provide information regarding how those alterations ultimately affect other cellular functions, including excitability. We recently have used non-invasive imaging and electrophysiological techniques to determine the ability of 11 pyrethroid compounds (deltamethrin, esfenvalerate, β -cyfluthrin, cypermethrin, λ -cyhalothrin, bifenthrin, permethrin, teflutrin, S-bioallethrin, resmethrin, and fenpropathrin) to alter sodium (SBFI fluorescence) and calcium (fluo-3 fluorescence) flux and spontaneous network activity (MEA recordings) in murine (SBFI/fluo-3) and rat (microelectrode array (MEA) recordings) neocortical primary cultures. Nine of the eleven compounds caused increases in sodium as well as calcium flux; tetrodotoxin blocked pyrethroid-induced influx of both sodium and calcium, indicating that the changes were mediated by voltage-gated sodium channels (VGSC) and that the calcium influx occurred secondarily to activation of VGSC by pyrethroids. These data also demonstrated that the 11 compounds differed in potency and efficacy and that these differences were consistent for sodium and calcium influx measurements. When effects of pyrethroids were examined using MEA recordings, all 11 compounds decreased spontaneous network activity in the presence of bicuculline; however, there were clear differences in the potencies of the pyrethroid compounds. In general, type II pyrethroids were more potent than type I pyrethroids in all three assays, although there were differences between the potency values in each assay. These data provide information on the potency and efficacy of pyrethroid effects on cellular function that can be used for comparisons between pyrethroid effects

on individual channel types as well as *in vivo* actions. (This abstract does not reflect US EPA Policy.)

AGRO 236

Evaluating tools and models used for quantitative extrapolation of in vitro to in vivo data for neurotoxicants

Melissa Chan⁽¹⁾, chanp2@niehs.nih.gov; Michael J DeVito⁽¹⁾; Timothy Shafer⁽²⁾; Michael F Hughes⁽²⁾. (1) National Institute of Environmental Health Sciences, National Toxicology Program, NIH, Research Triangle Park NC 27709 (2) National Health and Environmental Effects Research Laboratory, US Environmental Protection Agency, Research Triangle Park NC 27711

Comparisons of high throughput screening data to human exposures assume that media concentrations are equivalent to steady-state blood concentrations. This assumes the partitioning of the chemical between media and cells is equivalent to the partitioning of the chemical between blood and tissue. The relationship between in vitro effects and in vivo responses was evaluated using deltamethrin as test chemical. In vitro data on chemical-induced decreases in cell firing in rat primary hippocampal cell cultures were compared to in vivo effects on decreased motor activity. Comparing media to blood concentrations indicates that the ED_{50} (effective dose for 50%) in vitro over estimates the ED₅₀ in vivo by approximately an order of magnitude. These findings suggest that media concentration is not directly comparable to blood concentrations. (This abstract does not reflect NIEHS or US EPA policy.)

AGRO 237

Structure-activity relationship models of human CYP450 and UGT metabolism

Robert Fraczkiewicz⁽¹⁾, Robert@simulations-plus.com; Kurt Enslein⁽²⁾. (1) ADMET Cheminformatics, Simulations-Plus, Inc, Lancaster CA 93534-7059 (2) Enslein Research, Inc., Rochester NY

In order to compute effects such as PBPK, V_{max} and K_{mi} , we have developed QSAR (quantitative structure-activity relationships) hydroxylation equations. These models, as finally commercially implemented in the Simulations-Plus ADMET Predictor adaptive neural-network system, consisted of Phase 1 CYP1A2, CYP2C9, CYP2C19, CYP2D6, CYP3A4, and several Phase II UGT glucuronidation (UGT1A1, UGT1A3, UGT1A9, UGT2B7) endpoints. The data were derived from an extensive survey of the open literature; CYP450 consisting of recombinant cDNA data; same for UGT glucuronidation. The performance of these equations resulted in estimates within one-half order of magnitude of the actual value. While the eventual work used recombinant cDNA data, originally we used HLM microsome data, but found that these models performance was unstable, probably due to the noise in the data.

Quantitative structure-activity relationships for organophosphate enzyme inhibition

Christopher Ruark⁽¹⁾, christopher.ruark.ctr@wpafb.af.mil; Eric Hack⁽¹⁾; Peter Robinson⁽¹⁾; Paul Anderson⁽²⁾; Jeffery Gearhart⁽¹⁾. (1) Henry M. Jackson Foundation, Wright-Patterson AFB Ohio 45433-5707 (2) Consortium of Universities, Wright-Patterson AFB OH 45433-5707

Organophosphates (OPs) are a group of pesticides that inhibit enzymes such as acetylcholinesterase. Numerous OP structural variants exist and their toxicity data can be difficult to obtain quickly. To address this concern, quantitative structure-activity relationship (QSAR) models were developed to predict acetylcholinesterase, butyrylcholinesterase, trypsin, and chymotrypsin inhibition, key components in biologically-based dose-response (BBDR) models. The acetylcholinesterase database consisted of 747 structures developed from 69 peer-reviewed publications. AMPAC and CODESSA descriptors (SemiChem, Inc.) were calculated for each compound. The acetylcholinesterase results show that the average nucleophilic reactive index for a carbon atom contributed most significantly to binding. A training R² of 0.73±0.01 and an external test set Q² of 0.62±0.06 was achieved. The QSAR models discussed in this seminar will complement OP BBDR modeling by filling critical data gaps for key parameter values, leading to better risk assessment and prioritization of animal and human toxicity studies especially for OPs lacking experimental data.

AGRO 239

Approach for the assessment of indirect effects to threatened and endangered terrestrial species exposed to herbicides: Glufosinate case study

R. S. Teed⁽¹⁾, steed@intrinsikscience.com; D. R. J. Moore⁽²⁾; T. Hall⁽³⁾; G. Sabbagh⁽⁴⁾; R. L. Breton⁽¹⁾. (1) IES, Intrinsik Environmental Sciences Inc., Ottawa ON K2C 2B5, Canada (2) IES, Intrinsik Environmental Sciences (US) Inc., New Gloucester ME 04260 (3) Ecological Sciences, Bayer CropScience Inc., Research Triangle Park NC 27709 (4) BCS, Bayer CropScience Inc., Stilwell KS 66085

Indirect effects of herbicides on threatened and endangered (T&E) aquatic and terrestrial animals may result from alterations in primary productivity, structure and function of plant communities, and prey availability. A tiered approach was used to assess indirect effects of the herbicide glufosinate to T&E animal species stemming from direct effects to algal and plant community structure and function. Tier 1 was a conservative, screening-level ecological risk assessment (ERA) that followed standard EPA methods for generating risk quotients for algae and terrestrial plants. In Tier 2, exposure distributions were integrated with the preferred effects metric, an SSD for algae and/or plants, to derive risk curves of cumulative probabilities of effects of differing magnitude. Tier 3 relies on ecosystem models to determine how risks from herbicides to algae and plants cascade to other organisms including T&E species that rely on algae and plants for food and habitat. In Tier 4, microcosm and mesocosm tests, and/or field studies were used to determine the magnitude and duration of direct effects to aquatic and terrestrial plants and indirect effects to higher trophic level T&E species. The results of a national endangered species assessment for glufosinate will used to illustrate the tiered approach.

AGRO 240

Demography and modeling to improve pesticide risk assessment of endangered species

John D Stark, starkj@wsu.edu. Department of Entomology, Puyallup Research and Extension Center, Washington State University, Puyallup WA 98374

The ecological risk assessment process for pesticides involves the development of risk quotients (RQ) which are compared to levels of concern. There are several flaws with the current risk assessment process for pesticides including the following: ecological processes and population biology are not considered in this process; data developed for a relatively small number of species is used to predict effects on all other species; and exposure of populations to pesticides can result in lethal and multiple sublethal effects whereby some individual die and the survivors are impaired. Therefore, single measures of effect may miss the total effect on a population. New approaches for ecological risk assessment involving population-level measurements and population modeling have been proposed over the past several years. These include development of demographic data for pesticide-exposed populations followed by population modeling. Recent developments in demographic toxicity and modeling for ecological risk assessment will be discussed.

AGRO 241

Consideration of nontraditional endpoints in the assessment of ecological risk under the Endangered Species Act

Nancy H Golden, Nancy_Golden@fws.gov; George Noguchi. Environmental Contaminants Program, US Fish and Wildlife Service, Arlington VA 22206

As the field of environmental toxicology progresses, research is revealing effects to species that expand beyond the traditional endpoints of survival, growth, and reproduction as measured in single organism lab studies. Exposure to contaminants can result in adverse effects to endocrine function, olfaction, behavior, and other physiological impairments that may be exasperated in combination with ecological stressors. The Endangered Species Act requires us to examine all of the available data regarding the effects of stressors to vulnerable wildlife and make management decisions that error on the side of species conservation. Navigating sets of data that are often incomplete and disparate requires knowledge of both the physiological nature of the observed effect and the life history of the species under review to determine if there may be a linkage between them and to provide protection to vulnerable species facing a myriad of potential threats.

AGRO 242

Using causal analysis to evaluate stressor effects on endangered species

Charles A. Menzie⁽¹⁾, camenzie@exponent.com; Anne Fairbrother⁽²⁾; Nicholas W. Gard⁽²⁾. (1) EcoSciences, Exponent, Alexandria VA 22314 (2) EcoSciences, Exponent, Bellevue WA 98007

Rarity of endangered species is caused by multiple stressors, and conservation will be ineffective if stressors are managed in isolation. However, a reductionist approach is often adopted when government agencies prepare Biological Opinions to rule on "take" allowances permitted under the Endangered Species Act. This fails to recognize that "take"

determinations must be based on the concept that the loss from one stressor does not add to the cumulative effect of all stressors such that the population growth rate becomes < 1. Cumulative effects assessments offer the opportunity to offset "take" due to one stressor by implementing management actions to mitigate the effects of a different stressor. We present a framework for causal analysis of stressor effects that can determine the relative contribution of different stressors to the viability of an endangered species population, with application to assessing relative risks of pesticide-related "takings" and consideration of potential mitigation options.

AGRO 243

Data quality and relevance standards for risk assessment

A Tilghman Hall⁽¹⁾, Tilghman.hall@bayer.com; Jim Gagne⁽²⁾; Bernalyn McGaughey⁽²⁾. (1) Ecotoxicology, Bayer CropScience, Research Triangle Park NC 27709 (2) CSI, Compliance Services International, Lakewood WA 98499

Risk assessments are performed under several different acts or for different regulatory organizations under the same act. Robust assessments rely on: (1) the quality of the studies that support them; (2) the quality and relevance of study endpoints as measures of effect or measures of exposure. supporting assessment endpoints; and (3) the quality and relevance of the chosen assessment endpoints to the attributes being protected. Examples of different quality data will be given, drawing on Reregistration Eligibility Decisions (REDs) for older, oft-tested compounds to show how data quality affects the conclusions. Also, examples of data addressing certain endpoints, such as biomarkers, will be discussed with respect to relevancy when such an endpoint may indicate exposure but not necessarily toxicity. The importance of a weight-of-the-evidence approach will be emphasized.

AGRO 244

Methods for reducing ammonia emissions from poultry litter

Philip A. Moore, Jr, philipm@uark.edu. Poultry Production and Product Safety Research Unit, USDA-Agricultural Research Service, Fayetteville AR 72701

Recent research has shown that ammonia emissions from a typical 50 day old broiler are approximately 46 g/bird. The objective of this paper is to give an overview of methods to reduce ammonia emissions from poultry litter. Research conducted during the past two decades has shown that a simple topical application of aluminum sulfate (alum) to manure can greatly reduce the magnitude of ammonia emissions. Improvements in air quality in poultry rearing facilities due to alum result in heavier chickens which have better feed conversion and lower mortality, making this practice cost-effective. Alum applications also result in reductions in phosphorus runoff and leaching. Another practice that can be used to reduce ammonia emissions is the installation of ammonia scrubbers onto exhaust fans of poultry barns. Incorporation of manure during land application also reduces ammonia emissions while improving water quality.

AGRO 245

Amendments and feed-through additive for gas and odor emission reduction from dairy manure samples

Eileen F. Wheeler⁽¹⁾, efw2@psu.edu; Robin C. Brandt⁽¹⁾; Arlene A. Adviento-Borbe⁽²⁾; Michael L. Hile⁽¹⁾; Alexander N. Hristov⁽³⁾; Patrick A. Topper⁽¹⁾; Herschel A. Elliott⁽¹⁾; Maryann V. Bruns⁽⁴⁾. (1) Department of Agricultural and Biological Engineering, Penn State, University Park PA 16802 (2) Department of Plant Sciences, University of California-Davis, Davis, CA 95616 (3) Department of Dairy and Animal Science, Penn State, University Park PA 16802 (4) Department of Crop and Soil Sciences, Penn State, University Park PA 16802

Amendments are popularly used to reduce air emissions from manure. Seven promising products were studied after a preliminary screening of 22 dairy manure amendments that represented different modes of action. One feed-through additive was evaluated. Gas and odor emissions were simultaneously evaluated from manure (2kg, 1:1.7 feces: urine) stored at two temperatures (10 and 20 °C) for three periods (3d, 30d, 94d). Odor emissions were quantified via olfactometry along with quality characterizations. Amendments demonstrated significant emission reduction compared to untreated manure under certain conditions. For example, acidic (abandoned) mine drainage sediment reduced odor 31% (P=0.032) after 3d at 20 °C while three proprietary products significantly reduced odor by 26 to 47% after 30d at 20 °C. Essential oils tended to increase odor detection but improved odor character descriptors. Gas emission reductions were dependent upon mode of action. Amendments showed promise when administered to reduce certain compounds in a specific timeframe.

AGRO 246

Feeding tannins to dairy cows abates ammonia emissions from barns and soils

J Mark Powell⁽¹⁾, mark.powell@ars.usda.gov; Matias J Aguerre⁽²⁾; Michel A Wattiaux⁽²⁾. (1) US Dairy Forage Research Center, USDA-Agricultural Research Service, Madison WI 53706 (2) Department of Dairy Science, University of Wisconsin-Madison, Madison WI 53706

Dairy cows excrete large amounts of urine, so barns are thought to emit large amounts of ammonia which can adversely impact the health of humans and natural ecosystems. We conducted three studies to determine if feeding more tannin and less crude protein (CP) to dairy cows would reduce urine excretion and ammonia emissions from dairy barns and soil. Relative reductions in ammonia emission from barn floors due to tannin feeding were greatest at the low CP diet due to lower amounts of urine nitrogen excreted and therefore applied. Tannins reduced ammonia emissions from barn floors by 30% at the low CP diet and 16% at the high CP diet. Tannins reduced ammonia emissions by 28 - 49% after slurry application to soils. Although results of the laboratory studies are encouraging, larger scale studies are required to ascertain effectiveness of tannin extracts in abating ammonia loss from commercial dairy farms.

Swine manure odor reduction efficacy of a humic amendment

Robin C. Brandt⁽¹⁾, rcb100@psu.edu; Eileen F. Wheeler⁽¹⁾; Herschel A. Elliott⁽¹⁾; Robert E. Mikesell, Jr.⁽²⁾. (1) Department of Agricultural and Biological Engineering, Penn State University, University Park PA 16802-1908 (2) Department of Dairy and Animal Science, Penn State University, University Park PA 16802-1908

While numerous additives claim to reduce livestock manure odors, supporting research is lacking. We used both laboratory and field olfactometry to evaluate the effectiveness of a commercial product, derived from humic material, to control liquid swine manure odors. Laboratoryincubated (20 °C) amended manure reduced odor emissions significantly (88%, P < 0.0001) (OU cm⁻² hr⁻¹) compared to the untreated control for selected holding times and amendment rates. A follow-up multi-assessor repeat observation field olfactometry experiment was performed to quantify dilutions-to-threshold (D/T) levels at the center of manure rings (3.5 m wide, 61-m in diameter) on grassland. Best estimate odor threshold D/T levels decreased as follows: surface broadcast = aeration infiltration > producttreated surface broadcast > broadcast + chisel incorporation > shallow disk injection > no manure control. Producttreated broadcast manure showed a statistically significant reduction (33%, P < 0.01) in odor D/T compared to untreated surface-broadcast manure.

AGRO 248

Reduction of odorous VOC in phenolics solutions and swine manure slurry using soybean peroxidase and hydrogen peroxide

David B Parker⁽¹⁾, david.parker@ars.usda.gov; Lingshuang Cai⁽¹⁾; Mark Olsen⁽²⁾. (1) US Meat Animal Research Center, USDA-Agricultural Research Service, Clay Center NE 68933 (2) Midwestern University, Glendale AZ 85308

A research project was conducted to evaluate the efficacy of low-activity soybean peroxidase (SBP; 0.75 U/mg) and $\rm H_2O_2$ for reducing emissions of odorous volatile organic compounds (VOC) from standard solutions (phenol and 4-methylphenol; 1 mM each) and swine manure slurry. VOC emissions were measured in a small wind tunnel. Air samples were collected in stainless steel sorbent tubes and analyzed by GC/MS. SBP (2000 mg/L) reduced 4-methylphenol and phenol emissions in standard solutions by 99 and 50%, respectively. The optimum $\rm H_2O_2$ addition was 1.32 mM per mM phenolic substrate. Percent reduction of 4-methylphenol emission was about 25% in swine slurry with SBP addition of 5000 mg/L.

AGRO 249

In silico strategies for modeling stereoselective hydrolysis rates of pyrethroids

Daniel T Chang⁽¹⁾, chang.daniel@epa.gov; Michael-Rock Goldsmith⁽¹⁾; Rogelio Tornero-Velez⁽¹⁾; Ling-Jen Chen⁽²⁾; Elin Ulrich⁽¹⁾; Andrew B Lindstrom⁽¹⁾; Curtis C Dary⁽¹⁾. (1) National Exposure Research Laboratory, Human Exposure and Atmospheric Sciences Division, US Environmental Protection Agency, Research Triangle Park NC 27711 (2) ManTech Environmental Technology, Inc., Research Triangle Park NC 27709

We have been developing in silico methods to estimate stereoselective metabolic parameters in mammals, that makes use of optically-resolved enzyme kinetics data, and illustrated its use for the specific case of carboxylesterase (CE)-mediated hydrolysis of pyrethroids in rats. The methodology involves: (1) a pharmacophore structural qualifier/filter to determine whether a particular stereoisomer is indeed a viable substrate (or not), and (2) a mechanism-specific quantitative structure activity relationship (QSAR) to predict metabolic rate constants. This two-step approach has been trained and validated with in vitro CE hydrolysis rates of 27 individual optically resolved type I and II pyrethroid stereoisomers in rat serum, and extended to human CE1/2 data of pyrethroid analogs (external dataset). Our strategy extends the utility of pharmacophore filters in the reduction of misclassification of mechanistically-competent substrates, while strengthening the QSAR model, useful for both PK/PD model development and sustainable molecular design criteria.

AGRO 250

Computational approaches for developing informative prior distributions for Bayesian calibration of PBPK models

Jimena L. Davis⁽¹⁾, davis.jimena@epa.gov; Rogelio Tornero-Velez⁽²⁾; R. Woodrow Setzer⁽¹⁾. (1) National Center for Computational Toxicology, US Environmental Protection Agency, Research Triangle Park NC 27711 (2) National Exposure Research Laboratory, US Environmental Protection Agency, Research Triangle Park NC 27711

Using Bayesian statistical methods to quantify uncertainty and variability in human PBPK model predictions for use in risk assessments requires prior distributions (priors) which characterize what is known or believed about parameters' values before observing in vivo data. Experimental in vivo data can then be used in Bayesian calibration of PBPK models to refine priors when it exists. However, when little or no in vivo data are available for calibration efforts, parameter estimates and uncertainties can be obtained from priors. We present approaches for specifying informative priors for chemical-specific PBPK model parameters based on information obtained from chemical structures and in vitro assays. Means and standard deviations (or coefficients of variation) for priors are derived from comparisons of predicted values from computational (e.g., QSAR) methods or in vitro assays and experimentally-determined, chemicalspecific values for a data set of chemicals. (This abstract does not necessarily reflect US EPA policy.)

Use of CYP-specific parameters and human biomarker data to develop a human PBPk/PD model for dermal chlorpyrifos exposure

James R Olson⁽¹⁾, jolson@Buffalo.edu; Corie A. Ellison⁽¹⁾; James B Knaak⁽¹⁾; Robin McDougall⁽²⁾; Matthew R. Bonner⁽³⁾; Pamela J Lein⁽⁴⁾⁽⁵⁾; Fayssal M. Farahat⁽⁶⁾; W Kent Anger⁽⁴⁾. (1) Department of Pharmacology and Toxicology, University at Buffalo, Buffalo NY 14214 (2) University of Ontario Institute of Technology, Oshawa ON, Canada (3) Department of Social and Preventive Medicine, University at Buffalo, Buffalo NY 14214 (4) Oregon Health and Science University, Portland OR (5) School of Veterinary Medicine, University of California-Davis, Davis CA (6) Menoufia University, Shibin el Kom, Egypt

Chlorpyrifos (CPF), a widely used OP pesticide, is primarily activated by cytochrome P450 (CYP) 2B6 to CPF-oxon and detoxified by CYP2C19 to trichloro-2-pyridinol (TCPy), while CPF-oxon is metabolically detoxified to TCPy by PON1. Egyptian agricultural workers (n = 37) had urinary TCPy and blood BuChE and AChE activities measured as biomarkers of CPF exposure and effect. Human PBPK/PD modeling was conducted utilizing the exposure and effect biomarker data and CYP-specific kinetic rate constants for CPF metabolism. A statistically-significant inverse correlation was observed between urinary TCPy and blood BuChE and AChE activities. The no effect level or inflection point of the exposure-effect relationships had an average urinary TCPy level of 114 ug/g creatinine for BuChE and 3161 ug/g creatinine for AChE. Human PBPK/PD modeling simulations for a dermal CPF exposure were able to simulate the human exposure and effect biomarkers data accurately. (NIH R01 ES016308 amd EPA Star grant R833454).

AGRO 252

Age-dependent, physiologically based pharmacokinetic/pharmacodynamic (PBPK/PD) modeling of organophosphorus (OP) insecticides in the preweanling rat: Implications of localized brain metabolism

Charles Timchalk, charles.timchalk@pnl.gov. Department of Biological Monitoring and Modeling, Pacific Northwest National Laboratory, Richland WA 99352

Age-dependent PBPK/PD models have been developed for OP insecticides that inhibit acetylcholinesterase (AChE). Studies suggest that OP neurotoxicity occurs at low-doses in the absence of significant brain AChE inhibition. The PBPK/PD model evaluated brain dosimetry in preweanling rats. In vitro metabolism studies were conducted with hepatic and brain microsomes prepared from naïve adult male rats. Brain microsomal metabolism was a fraction (~ 1%) of the liver, yet CYP2D6 was highly expressed. Post-natal day-10 (PND-10), pups were orally administered chlorpyrifos (CPF) at 1 and 5 mg/kg/day (5 doses) and humanely sacrificed 4 hours after the last dose. Brains were analyzed for AChE activity as well as for CPF and trichlorpyridinol (TCPy) levels and compared to adults. Age-, dose-, gender- and brain regional-differences were observed. The importance of localized brain metabolism is highly relevant for lipophilic pesticides that sequester in the brain and can undergo localized metabolism. (CDC/NIOSH grants R01-OH003629 and R01-OH008173)

AGRO 253

Bayesian calibration of carbaryl cholinesterase inhibition using physiologically-based pharmacokinetic and pharmacodynamic modeling

Andy Nong⁽¹⁾, andy.nong@hc-sc.gc.ca; Miyoung Yoon⁽²⁾; Harvey J Clewell⁽²⁾. (1) Environmental Health Science and Research Bureau, Health Canada, Ottawa ON K1A OK9, Canada (2) Center for Human Health Assessment, The Hamner Institutes for Health Sciences, Research Triangle Park NC 27709-2137

Bayesian techniques enable characterization of data uncertainty and variability based on prior and experimental information applicable for risk assessment of pesticides. Amongst *N*-methyl carbamate family of pesticides, carbaryl reversibly inhibits neuronal cholinesterase activity where the extent of knowledge is indeterminate. A hierarchical Bayesian approach was applied to estimate parameters in a physiologically-based pharmacokinetic and pharmacodynamic (PBPK/PD) model from experimental measurements of carbaryl in rats. The model described tissue dosimetry of carbaryl and its metabolites and carbaryl-induced inhibition of cholinesterase activity. In support of model parameterization, kinetic tracer studies were undertaken with rats exposed by oral and intravenous routes. Markov Chain Monte Carlo (MCMC) calibration of rat model parameters was implemented using prior information from literature for physiological distributions together with kinetic and inhibition data on carbaryl. Monte Carlo simulations of the PBPK/PD model with the posterior distribution estimates predicted a 95% confidence interval of tissue doses and cholinesterase inhibition activity in blood and brain within the range of observed data. This initial Bayesian PBPK/PD modeling effort will be used to determine the experimental studies that could provide the highest added value for model refinement.

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Use of *in vitro* data in PBPK models: An example of in vitro to *in vivo* extrapolation with carbaryl

Miyoung Yoon⁽¹⁾, myoon@thehamner.org; Gregory L Kedderis⁽²⁾; Yuching Yang⁽¹⁾; Bruce C Allen⁽²⁾; Harvey J Clewell⁽¹⁾; Zhixia Yan⁽¹⁾. (1) Center for Human Health Assessment, The Hamner Institutes for Health Sciences, Research Triangle Park NC 27709 (2) Independent Consultant, Chapel Hill NC

There is increasing interest in applying in vitro data and physiologically-based pharmacokinetic (PBPK) modeling to improve human risk assessment. In the present study, both pharmacokinetic (PK) and pharmacodynamic (PD) data were collected in vitro to support the development of a human PBPK model for carbaryl. Metabolism of carbaryl was determined in hepatocyte suspensions. Bimolecular inhibition rate constants for carbaryl with cholinesterases (ChEs) were measured in brain and blood. Free fraction of carbaryl in the tissue was determined to derive tissue to blood partition coefficients. These in vitro PK and PD data were extrapolated to whole rats and to humans to describe the disposition and ChE inhibition dynamics of carbaryl with the model. Our work demonstrates a process for developing a human PBPK model for risk assessment based on an animal PBPK model augmented with in vitro to in vivo extrapolation approaches using animal and human tissues.

ENVR DIVISION – Biochar Symposium

ENVR 88

Quality variations of poultry litter biochar generated at different pyrolysis temperatures

Mingxin Guo⁽¹⁾, mguo@desu.edu; Yufang Shen⁽²⁾. (1) Department of Agriculture and Natural Resources, Delaware State University, Dover Delaware 19901, United States (2) Department of Soil and Water Conservation, Northwest Agricultural and Forestry University, Yangling Shanxi 712100, China

Converting to biochar as a soil amendment is a promising method to dispose of excess poultry litter in concentrated poultry production regions. Optimal pyrolysis temperature needs to be determined to produce biochar from poultry litter with acceptable yield and quality. This study explored variations in yield and quality of poultry litter biochar as a function of pyrolysis temperature. Poultry litter granules were completely pyrolyzed at different temperatures from 300 to 600°C. The biochar products were analyzed for yield, carbon content, carbon stability, nutrient availability, water holding capacity, cation exchange capacity, BET surface area, and active functionality. The results show that the yield and nutrient availability of poultry litter char decreased, while BET surface area and cation exchange capacity increased as the pyrolysis temperature was elevated. A pyrolysis temperature of 450°C was selected to convert poultry litter into biochar with desirable yield and quality.

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Ammonia adsorption capacity of biomass and animalmanure derived biochars

Kyoung S Ro⁽¹⁾, kyoung.ro@ars.usda.gov; Gudigopuram Reddy⁽²⁾; Isabel Lima⁽³⁾; Devinder Mahajan⁽⁴⁾; Johnsely Cyrus⁽²⁾. (1) Coastal Plains Soil, Water, and Plant Research Center, USDA-Agricultural Research Service, Florence SC 29501, United States (2) Department of Natural Resources and Environmental Design, North Carolina A&T State University, Greensboro NC 27411, United States (3) Southern Regional Research Center, USDA-Agricultural Research Service, New Orleans LA 70124, United States (4) Department of Chemical and Molecular Engineering, Brookhaven National Laboratory, Stony Brook University, Stony Brook NY 11790, United States

The objective of this research was to characterize and investigate ammonia and hydrogen sulfide gas adsorption capacities of low- and high-temperature biochars made from wood shavings and chicken litter. The biochar samples were activated with steam or phosphoric acid. The specific surface areas and pore volumes of the activated or non-activated biochar samples were evaluated according to the Brunauer, Emmett, and Teller (BET) isotherm model using N2 as an adsorbate. The biochar samples were also characterized with energy-disperse X-ray spectroscopy (EDX) and scanning electron microscopy (SEM). Proximate and ultimate analyses were also performed. The biochar samples were placed in a column made of 13 mm x 120 mm PVC pipe. Calibrated ammonia gas with 20 to 100 ppm concentration was passed through the column at 3 LPM. Effluent gas concentration was monitored via a photoacoustic analyzer in order to establish breakthrough curves. The adsorption capacity of the biochar

was calculated from integrating the breakthrough curves. To date, we found that ammonia adsorption capacities based on 50% breakthrough curves ranged from 0.25 to 0.75 mg/g for non-activated biochars and 0.1 to 36.2 for activated biochars. The adsorption experiments are still ongoing and the final results will be presented at the meeting.

ENVR 90

Characterization of solid pyrogenic black carbon (biochar) by desorption atmospheric pressure photoionization (DAPPI) coupled to Fourier-transform ion cyclotron resonance mass spectrometry

William T Cooper⁽¹⁾, cooper@chem.fsu.edu; David C Podgorski⁽¹⁾; Rasha Hamdan⁽¹⁾; Andrew R Zimmerman⁽²⁾. (1) Department of Chemistry and Biochemistry, Florida State University, Tallahassee FL 32306-4390, United States (2) Department of Geological Sciences, University of Florida, Gainesville Florida 32611, United States

Previous studies have characterized the leachable fraction of pyrogenic black carbon by electrospray ionization coupled to ultrahigh resolution Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometry. However, the parent chars (biochars) have defied molecular characterization because a large fraction is not soluble in common solvents. Here, desorption atmospheric pressure photoionization (DAPPI) has been coupled to 9.4 Tesla FT-ICR mass spectrometry to characterize the molecular composition of parent oak (uncharred), oak combusted at 250°C, and oak pyrolyzed at 400°C. Oak combusted at 250°C exhibits two distinct types of molecules. The first are representative of aromatic compounds from the thermal degradation of lignin and hemicellulose, while the second are molecules associated with cellulose that is not completely degraded. Molecules with high H:C and O:C ratios observed in the parent oak and oak combusted at 250°C were not present in the oak combusted at 400°C.

ENVR 91

Adsorption properties of biochar-based activated carbon

Zhengrong Gu, zhengrong.gu@sdstate.edu; Kasiviswanath Muthukumarappan; James Julson. Department of Agricultural and Biosystems Engineering, South Dakota State University, Brookings SD 57006, United States

Activated carbon (AC) is a valuable product produced from biochar with a price around 1000 to 3000 \$/metric ton. AC is widely used in water treatment, gas separation, air pollution control (such as removal of oxides of sulfur and nitrogen and hydrogen sulfide), as catalyst or support of catalysts, recovery of metal ions in the precious metal industries, and purification processes in food and pharmaceutics industries. Biochar, which is produced from corn stover, prairie cordgrass, and woody biomass feed stocks using MW pyrolysis and fast pyrolysis technologies, was used as the starting material for producing activated carbon (AC) using physical (steam) and chemical (potassium hydroxide) activation processes. The effects of operating conditions for each activation method on the BET surface area of the product and reaction yield were investigated. Adsorption

properties of activated carbons will be evaluated and quantified with adsorption of methylene blue, ammonia, and Cu, Zn, and Ni ions. The mechanism of different adsorption properties from traditional coal or hardwood based activated carbon was investigated using surface titration, XRD, and FTIR.

ENVR 92

Investigation of dissolved organic carbon from water extracts of biochars by electrospray ionization/mass spectrometry

Colleen E. Rostad, cerostad@usgs.gov; David W. Rutherford; Robert L. Wershaw. National Research Program, US Geological Survey, Denver Colorado 80225, United States

Application of biochar to soil has been proposed both as a long-term sink for atmospheric carbon in terrestrial ecosystems and for improving soil fertility. However, the effect on surface runoff of adding water-soluble biochar components to agricultural soil is unknown. Chars from cellulose, lignin, pine, and switchgrass formed under a variety of conditions were extracted with water to determine how formation conditions affect the water-soluble components. Water extracts of chars were analyzed for total organic carbon, dissolved inorganic carbon, and dissolved organic carbon, and by electrospray ionization/mass spectrometry. The total integrated response by electrospray ionization/mass spectrometry correlated well with dissolved organic carbon content. With increasing charring temperature, the average molecular weight increased in the water extracts indicating increased higher molecular weight compounds or decreased lower molecular weight compounds present in the dissolved organic matter. Heating times and durations produce complex changes in biochar and have dramatic effects on water extracts from the biochar as well.

ENVR 93

Effect of pH conditions on nutrients leachability and surface characteristics of biochars

Pyoungchung Kim, pkim1@utk.edu; Nicole Labbe⁽¹⁾; Charles W Edmonds⁽²⁾; Timothy G. Rials⁽¹⁾; Amy Johnson⁽²⁾. (1) Department of Forestry, Wildlife and Fisheries, University of Tennessee, Center for Renewable Carbon, Knoxville TN 37996-4570, United States (2) Department of Biosystem Engineering and Soil Science, University of Tennessee, Soil Science Program, Knoxville TN 37996-4570, United States

Switchgrass-derived biochars produced by auger pyrolysis process at various conditions (450, 600, 800°C for 30 s of residence time) were investigated for the effect of pH (3 -11) and surface characteristics on nutrients leachability. Switchgrass biochars contained 14 - 22% of ash contents. Ash composition consisted mainly of Ca (1.2 – 1.68%), K (1.11 - 1.77%), P (0.26 - 0.45%), Mg (0.30 - 0.43%), S (0.16 - 0.21%), Si (3.54 - 5.21%), and traceable minerals such as AI, Fe, Na, Mn, Ge, and Zn. The sorption reactions of nutrients on biochars characterized by sequential extractions showed that a significant fraction of nutrients was bound to metal oxides. Nutrient leachability of biochars under different pH (from 3 to 11) showed that most of the nutrients were released with decreasing pH values. Only the heavy metals Cr and Cd were released in lower and higher pH values, which is associated with amphoteric behavior. FTIR spectra of biochars subjected to the different pH

treatments showed that surface functionality increased slightly with lower pH.

ENVR 94

Predicting biochar impact on soil carbon dynamics and soil quality in EPIC model

Taras Lychuk⁽¹⁾⁽²⁾, taras.lychuk@pnl.gov; Roberto César Izaurralde⁽¹⁾. (1) Pacific Northwest National Laboratory, College Park MD 20740, United States (2) Department of Environmental Science and Technology, University of Maryland, College Park, College Park MD 20740, United States

Results of simulated impacts of climate change on agriculture envision reductions in crop yields as a result of increased temperature, water, and nutrient stresses and an overall deterioration of soil functions. Biochar is viewed as a potential long-term climate adapting/mitigating technique to reduce GHG emissions, improve soil physical properties, moisture, air and nutrient regimes, as well as sequester large quantities of carbon in the soil and increase crop yields. Most biochar studies have been performed on highly weathered soils, such as Oxisols, with no field studies testing biochar effects on U.S. Midwest soils. We are modifying the EPIC (Environmental Policy Integrated Climate) model to simulate the behavior and functioning of biochar when applied to U.S. Midwest soils in terms of soil carbon sequestration, soil quality, and crop performance. Preliminary literature analysis and algorithm formulations suggest that biochar may have the ability to impact soil properties through positive modification of the soil's carbon and nutrient balances. In the absence of existing full scale field studies of biochar's impact on soils of temperate regions, simulation studies with a biochar-enhanced version of EPIC may be useful to evaluate the potential of this adaptation/mitigation technique and guide the design of much needed field experiments.

ENVR 95

Do soil biochar additions prime or sequester soil organic carbon?

M. Francesca Cotrufo⁽¹⁾, francesca.cotrufo@colostate.edu; Catherine Stewart⁽²⁾; Jiyong Zheng⁽³⁾. (1) Department of Soil and Crop Sciences, Colorado State University, Fort Collins CO 80523, United States (2) Soil Plant Nutrient Research, USDA-Agricultural Research Service, Fort Collins CO 80526, United States (3) State Key Laboratory of Soil Erosion and Dryland Farming on the Loess Plateau, Northwest A & F University, Yangling Shaanxi 712100M, China

Biochar (BC) production has been proposed as a means to mitigate climate change by increasing C sequestration in soils. However, research to date has shown that BC addition can either stimulate or suppress C mineralization in soils, depending on soil type, the BC feedstock and pyrolysis conditions. We are conducting a long-term laboratory incubation where, by means of stable C isotopes and soil organic matter size-fractionation methods, we partition the contribution of BC νs soil organic C to CO $_2$ losses and soil C stores. To assess the effects of BC additions and soil type, we added 0, 1, 5, 10, and 20% oak-derived BC (δ^{13} C = -27% $_0$) by weight to four soils varying for texture class, but all with low δ^{13} C values (-12 to -21% $_0$). Results on CO $_2$ dynamics and soil C size fractions for the first year of incubation will be presented.

Biochar as a carbon sequestration technology for Central Great Plains soils

Francisco J. Calderon, francisco.calderon@ars.usda.gov. Central Great Plains Resources Management Research, USDA-Agricultural Research Service, Akron CO 80720, United States

Agricultural soils in Eastern Colorado have suffered carbon (C) losses due to long-term cultivation. Soil C could be increased quickly by adding amendments that are C-rich, such as biochar and/or compost. We are carrying out research about the following important questions: 1) Can we use biochar to bring back our row crop soils to the level of organic matter present in our native prairie? 2) Can biochar in combination with compost result in better crop yields and nitrogen use efficiency? 3) Will the quality of biochar due to varying feedstocks and pyrolysis conditions have an effect in the performance? Infrared spectroscopy studies indicate that this technology is useful to characterize chars from different temperatures and feedstocks, but not as sensitive to quantify char in soils. Growth chamber studies indicate that additions of char alone are detrimental to crop growth. Use of compost in combination with biochar partially ameliorates this effect.

ENVR 97

Biochar as a soil amendment on two types of Saskatchewan Chernozemic soils

Jocelyn J Stefankiw, jjs384@mail.usask.ca; Jeff J Schoenau; Richard E Farrell. Department of Soil Science, University of Saskatchewan, Saskatoon SK S7N 5A8, Canada

Most research on biochar amended soils has been conducted on old, highly weathered tropical and subtropical soils with few studies on relatively young soils in the cool northern prairie climate. This study examined a biochar as an amendment on two cultivated grassland soils to determine the effect on soil nutrient concentration and nutrient uptake by canola (Brassica napus) in a controlled environment. Canola biomass yield was significantly increased with the addition of fertilizer with and without biochar. However, there was no significant effect on biomass yield that could be attributed to the biochar itself. There was also no significant difference in plant N uptake, N recovery, P uptake, or soil nitrate and phosphate in the biochar plus fertilizer treatment compared to the fertilizer treatment alone. There was a significant increase in soil organic carbon concentration in the treatment with the highest rate of biochar addition on one soil compared to the control. Lack of response of the plant and soil nutrient variables measured to the addition of biochar both with and without fertilizer may be explained by the inherent high organic matter content and nutrient retention ability in these relatively unweathered soils. Future research should focus on longer-term results of biochar addition and its effects on fertilizer use efficiency.

ENVR 98

Impact of biochar addition rate and soil type on greenhouse gas emissions: The importance of long-term data

Catherine Stewart⁽¹⁾, cstewart@nrel.colostate.edu; Jiyong Zheng⁽²⁾; M. Francesca Cotrufo⁽³⁾. (1) Soil-Plant-Nutrient Research, USDA-Agricultural Research Service, Fort Collins CO 80526-8119, United States (2) State Key Laboratory of Soil Erosion and Dryland Farming on the Loess Plateau, Northwest A & F University, 26 Xinong Rd, Yangling Shaanxi 712100M, China (3) Department of Soil and Crop Science, Colorado State University, Fort Collins CO 80523-1499, United States

Biochar addition to soil has been proposed as a means of improving nutrient retention and soil C sequestration in soils. However, research to date has documented net positive, neutral, or negative effects on greenhouse gas emissions after biochar addition to soils, depending on the biochar feedstock, pyrolysis temperature, and soil type. Our objective was to determine the effect of biochar addition rates on trace gas production over a long-term incubation. We added 0, 1, 5, 10, and 20% oak-derived biochar (pyrolyzed at 550°C) by weight to four soils varying from a clay to a sand and measured CO₂, N₂O, and CH₄ over a yearlong incubation. Biochar addition initially suppressed CO₂ production, but after 3 - 4 months, respiration increased in accordance with biochar addition rate. In all soils, N2O emissions were suppressed, although the response to addition rate varied from 20% to 94% reduction in emissions.

ENVR 125

Herbicide sorption in a biochar-amended coastal plain soil under conventional and conservation tillage management

Thomas Potter⁽¹⁾, tom.potter@ars.usda.gov; Paul M White⁽²⁾; Isabel M Lima⁽³⁾. (1) Southeast Watershed Laboratory, USDA-Agricultural Research Service, Tifton GA 31793, United States (2) Sugarcane Research Unit, USDA-Agricultural Research Service, Houma LA, United States (3) Commodity Utilization Research Group, USDA-Agricultural Research Service, New Orleans LA, United States

Commercial cropping systems worldwide depend on herbicides for weed control. Sorption of active ingredients in these products by soil colloids impacts both weed control and soil persistence. Soil organic matter is typically the principal sorption site. Biochar addition to soil increases soil organic matter and will likely increase soil residual herbicide adsorption. There is potential for positive and negative consequences. We investigated biochar impact on soil sorption of three soil residual herbicides, metolachlor, fomesafen, and pendimethalin in a loamy sand soil widely used in the Southeastern USA for cotton (Gossypium hirsutum) production. K_{oc}'s ranged from 50 to 16000 mL g⁻¹. The biochar, produced by pine wood chip pyrolysis at 500°C, was added at rates designed to double the soil organic carbon content. Biochar increased sorption of all compounds by about 50%. Implications for biochar use on herbicide fate in this soil will be discussed.

Biochars from sugarcane trash and sugarcane bagasse as soil amendments

Isabel M Lima⁽¹⁾, isabel.lima@ars.usda.gov; Paul M White⁽²⁾; Kjell T Klasson⁽¹⁾; Minori Uchimiya⁽¹⁾. (1) Southern Regional Research Center, USDA-Agricultural Research Service, New Orleans LA 70124, United States (2) Sugarcane Research Unit, USDA-Agricultural Research Service, Houma LA 70360, United States

In recent years there has been a reduction in the burning of postharvest sugarcane trash in the field due to urban encroachment and air quality concerns. The trash left on the soil surface reduces yields of ration crops due to lower soil temperatures and higher soil moisture. Sugarcane mills occasionally produce excess bagasse during the grinding season. These two organic feed stocks (sugarcane trash and sugarcane bagasse) can be thermochemically converted into biochars that can be brought back to the field to be used as a soil amendment to enhance soil health and water holding capacity and to improve sugarcane yields. This is the first study in a multiple-year study where biochars from sugarcane leaf residue (variety HoCP 96-540), whole plant (variety L79-1002), and sugarcane bagasse are produced, characterized, and applied back to the soil. These feed stocks were chemically characterized for their nutrient content and several physico-chemical and adsorptive properties. Some of them were used in greenhouse experiments with untreated and commercial fertilizer controls included; plant heights are reported. In subsequent years, theoretical recoverable sugar sucrose and ratoon cane yield will also be determined. Possible benefits of biochar include an increase in soil carbon content, improvement of soil drainage and aeration, and addition of nutrients to the growing sugarcane crop. Benefits are expected to both sugarcane growers and processors through the production of valued by-products from pyrolysis of sugarcane trash and bagasse as well as enhancing the sugarcane industry's role in renewable energy markets.

ENVR 127

Sugarcane bagasse and pine wood biochar effects on aerobic soil dissipation of metribuzin and pendimethalin

Paul M White, Jr.⁽¹⁾, paul.white@ars.usda.gov; Thomas L Potter⁽²⁾; Isabel M Lima⁽³⁾. (1) Sugarcane Research Unit, USDA-Agricultural Research Service, Houma LA 70360, United States (2) Southeast Watershed Research Unit, USDA-Agricultural Research Service, Tifton GA 31793, United States (3) Southern Regional Research Center - Commodity Utilization Research Unit, USDA-Agricultural Research Service, New Orleans LA 70124, United States

There is considerable interest in biochar use as an agricultural soil amendment. Positive impacts are increased organic matter, increased herbicide persistence, and improved soil physical properties. Negative impacts may include herbicide carryover and reduced efficacy, increased availability for runoff, and lower crop nutrient availability. Our work focused on impacts on soil dissipation rates of metribuzin and pendimethalin, two common soil-residual herbicides with different sorption characteristics. Biochars produced by pyrolysis of sugarcane bagasse and pine wood were mixed with three soils with different physical and chemical properties. Biochar addition doubled the soil carbon content. Herbicides were added to all soils with and without

biochar. Soils were extracted using methanol after 0, 7, 14, 21, 28, 42, 63, 86, and 111 days incubation at constant temperature and water content. Parent compounds and degradates were analyzed in extracts by LC-MS. Dissipation data and degradate formation will be presented.

ENVR 128

Biochar-mediated reductive transformation of nitro herbicides

Seok-Young Oh⁽¹⁾, quartzoh@ulsan.ac.kr; Jong-Gil Son⁽¹⁾; Pei C Chiu⁽²⁾. (1) Department of Civil and Environmental Engineering, University of Ulsan, Ulsan 680-749, Republic of Korea (2) Department of Civil and Environmental Engineering, University of Delaware, Newark DE 19716, United States

We evaluated biochar as an electron transfer mediator to accelerate the abiotic reduction of nitroaromatic herbicides. We hypothesized that biochar could enhance the reduction of nitroaromatic herbicides because of the adsorptive and conductive graphene moiety. Biochar was produced from poultry litter through pyrolysis at 400°C. We assessed the ability of biochar to catalyze the reduction of two nitro herbicides trifluralin and pendimethaline, using dithiothreitol or H₂S as reductant. 2,4-Dinitrotoluene was included as a model compound for comparison with our previous study (Oh and Chiu, 2009). Similar to the results with graphite and soot from our previous work, reduction of the nitroaromatic herbicides was enhanced by biochar. However, due to the low degree of carbonization, the rate enhancement was less pronounced than that with other black carbon. These results suggest that biochar may be a sorbent and redox catalyst that influences the fate of nitro herbicides in reducing environments.

ENVR 129

Biochar production for use as low-cost adsorbents: Applications in drinking water treatment serving developing communities

Joshua P Kearns⁽¹⁾, joshua.kearns@colorado.edu; Kyle Shimabuku⁽¹⁾; Lauren S Wellborn⁽²⁾; Detlef RU Knappe⁽³⁾; R Scott Summers⁽¹⁾. (1) Civil, Environmental & Architectural Engineering, University of Colorado-Boulder, Boulder CO 80309, United States (2) Environmental Department, Geosyntec, Raleigh NC 27615, United States (3) Civil, Construction, & Environmental Engineering, North Carolina State University, Raleigh NC 27695, United States

Biochar, known traditionally as charcoal, has been used in drinking water treatment for more than 4,000 years. Here we examine applicability of this ancient practice for removal of modern synthetic organic compounds (SOCs), in particular pesticides. We demonstrate the relative influence of feedstock (biochar precursor) and pyrolysis intensity (peak temperature, duration) on herbicide (propanil, 2,4-D) uptake under equilibrium and dynamic steady-state conditions in the presence of dissolved NOM by biochars produced using traditional kiln systems. Three prevalent representative feed stocks (eucalyptus, bamboo, longan wood) are employed for biochar generation at field-scale using a 200-L steel drum kiln and at lab-scale using a programmable laboratory pyrolyzer to simulate typical observed range of pyrolysis intensities. Our findings are relevant to biochar kiln design and operation optimization for production of filter-carbon and implementation of low-cost drinking water treatment systems serving developing communities, as well as to

prediction of SOC fate and transport in agroecosystems under biochar application scenarios.

ENVR 130

Biochar field trials in Zambia, Africa: Doubling growth and understanding why

Gerard Cornelissen⁽¹⁾⁽²⁾, gco@ngi.no; Victor Shitumbanuma⁽³⁾; Gijs D Breedveld⁽¹⁾⁽⁴⁾; Jan Mulder⁽²⁾; Matthijs Van Leur⁽¹⁾; Vegard Martinsen⁽²⁾; Vanja Alling⁽¹⁾; Sarah E Hale⁽¹⁾; Elijah Phiri⁽³⁾; Peter Aagaard⁽⁵⁾; Odd E Arnesen⁽⁶⁾; Jan Erik Studsroed⁽⁶⁾. (1) Department of Environmental Engineering, Norwegian Geotechnical Institute, Oslo 0806, Norway (2) Department of Plant and Environmental Sciences, Norwegian University of Life Sciences, Oslo 0806, Norway (3) Department of Soil Science, University of Zambia, Lusaka, Zambia (4) Department of Geosciences, University of Oslo, Oslo 0806, Norway (5) Conservation Farming Unit, Lusaka, Zambia (6) Norwegian Agency for Development Cooperation, Oslo 0251, Norway

Biochar amendment was combined with conservation farming, where soil is not completely tilled but instead fertilizer/biochar addition and planting occur in hoe basins. The six soils strongly varied in CEC (3 to 28 cmol/kg), pH (3.8 to 7) and TOC (0.3 to 1.8%). Biochars were from waste materials: corn cobs and charcoal dust from the charcoal industry. Testing consisted of chemical screening of soilbiochar combinations as well as pot + field tests with various amounts of biochar. In the first growth season, soils with lowest CEC and pH showed very good effects of biochar on reduction of acid saturation (from 70 to 0%) and maize growth (doubled), already at 4 tons/ha application. Other testing parameters included root-available nutrients measured by in-situ samplers with ion-exchange resin, water holding capacity, pesticide sorption, and total and bioavailable polycyclic aromatic hydrocarbons (PAHs), all aiding in understanding biochar effects in tropical soils.

Soils/chars	рН	CEC	Acid saturation	Acid saturation + 5% charcoal	Acid saturation + 5% corn stover char
Mkushi	4.9	3	61	0	62
Kaoma	5.4	4	55	0	36
UNZA	3.8	9	83	32	72
NRDC	7.0	17	later	later	later
Shimabala	5.2	28	later	later	later
Charcoal dust	7.9	85	0		
Corn stover char	7.6	40	0		

ENVR 131

Nutrient, metals, and organic matter retention in Indonesian and Zambian soils amended with biochar: Batch and column leaching tests

Vanja Alling⁽¹⁾, vanja.alling@ngi.no; Vegard Martinsen⁽²⁾; Gijs Breedveld⁽¹⁾; Jan Mulder⁽²⁾; Sarah Hale⁽¹⁾; Victor Shitumbanuma⁽³⁾; Peter Aagaard⁽⁴⁾; Alex Heikens⁽⁵⁾; Neneng Nurida⁽⁶⁾; Prihasto Setyant⁽⁷⁾; Gerard Cornelissen⁽¹⁾⁽²⁾⁽⁸⁾. (1) Department of Environmental Engineering, Norwegian Geotechnical Institute (NGI), Oslo 0855, Norway (2) Department of Plant and Environmental Sciences, Norwegian University of Life Sciences (UMB), As, Norway (3) University of Zambia, Lusaka, Zambia (4) Conservation Farming Unit, Lusaka, Zambia (5) UNDP, Asia Regional Office, Bangkok, Thailand (6) Indonesian Soil Research Institute, Bogor, Indonesia (7) Indonesian Agricultural Environment Research Institute (IAERI), Pati, Indonesia (8) Department of Applied Environmental Sciences, Stockholm University, Oslo 0855, Norway

Acidic and nutrient-poor Zambian and Indonesian soils have been tested for the effects of biochar amendment on the retention of macro-nutrient, metals and organic matter. Biochar additions to the soils changed their basic properties, e.g. the pH and cation exchange capacity which are of crucial importance for the retention of nutrients (table 1). Sorption isotherms have been constructed for PO₄³⁻, NH₄⁺, and NO₃ on biochar, showing low adsorption of PO₄ 3-. A significant fraction of the PO₄³ in the solution had been added by the biochar. The distribution coefficients for soluble nutrients in the soils with added biochar (0, 1, and 5%) were determined with a batch test. A column leaching experiment will test the long-term biochar-induced effects on leaching of N, P, metals, and organic matter for the soils. These experiments will aid in understanding the mechanisms behind the strong effects of biochar on growth in tropical soils.

Sample	рН	AI(III) mg/L	CEC cmol/kg	BS %	Org. C %	Tot. C %	Tot. N %
UNZA (Zambia)	4.81	1.14	3.49	50.2	0.82	0.85	0.02
UNZA +5% biochar	5.71	0.24	7.36	62.3	2.16	2.16	0.06
Mkushi (Zambia)	6.50	0.18	3.35	35.8	0.39	.039	0
Mkushi +5% biochar	7.04	0.03	5.46	68.2	1.75	1.75	0.02
Kaoma (Zambia)	6.53	0.02	3.47	62.0	0.55	0.58	0
Kaoma +5% biochar	7.33	-	9.63	100	3.08	3.08	0.02
Shimabala (Zambia)	6.45	-	23.54	99.7	1.78	1.79	0.09
Lampung, Sumatra ¹	4		15		1		
Palangka Raya, Kalimantan ¹	3.5		40		30		
Pulang Pisau, Kalimantan ¹	3.5		5		1		

¹ All Indonesian soil values are approximations and will be refined later on

Biochar characteristics and function as a heavy metal sorbent in soil: Role of surface ligands

Minori Uchimiya, sophie.uchimiya@ars.usda.gov. USDA-Agricultural Research Service, Southern Regional Research Center, 1100 Robert E. Lee Boulevard New Orleans, LA 70124, United States

Heavy metal stabilization is an important target function of biochars for both environmental remediation and soil fertilization purposes. Oxygen-containing functional groups of biochars play a vital role in improving CEC and heavy metal retention capacity of soils. In this study, a series of agricultural waste-derived biochars were first characterized for the yield, moisture, ash, volatile matter, and fixed carbon contents, elemental composition (CHNSO), BET surface area, pH, pH_{pzc}, and total acidity, and by ATR-FTIR and ¹H NMR. Selected biochars were activated to introduce carboxyl, hydroxyl, and phosphate groups on increased surface area. Biochars were then screened for their ability to stabilize heavy metals in soils representing a range of CEC, pH, and TOC contents. The results indicate that the biochars can be engineered to improve stability in soil as well as the heavy metal stabilization ability which directly correlates with the amount of metal ion-coordinating surface functional groups.

ENVR 133

Biochar for soil remediation on abandoned mine lands: San Juan Mountains, CO

Christopher D Petlz, cdpeltz@mountainstudies.org. Mountain Studies Institute, Silverton CO 81433, United States

We sought to determine the suitability of biochar as a soil remediation tool for revegetating abandoned mine lands in San Juan County, Colorado. Our study assessed the effects of biochar and straw compost amendments on the mobility, bioavailability, and toxicity of inorganic and organic contaminants in soils at abandoned mine sites. To examine biochar as a soil amendment, we conducted field trials to test for restoration potential, and container trials to examine specific physical and chemical properties of biochar treatments. The biochar field sites were located at elevations between 2,800 and 3,700 meters; site soils conditions ranged from pure waste rock to partially reclaimed forest soils. The field trial segment utilized a randomized block design of three blocks consisting of 2 x 1 meter plots with one seed-only control and three treatments: (1) biochar (30% by volume); (2) biochar and straw mulch; and, (3) straw mulch. The container trials, which were conducted at the Mountain Studies Institute field station, consisted of a seed emergence test, a vegetation biomass accumulation test, and a soil leachate test. Preliminary results indicate that relative to seeding only, the addition of a 30% by volume biochar soil amendment increased vegetation cover on mining affected and acid soils by 57% - 240%. Biochar treatments increased water holding capacity in all soils by 100% - 180%. Above ground biomass was positively affected by biochar additions, with both mine and acid sites respectively showing an increase of 85% - 100%. The results for the effect of biochar on soil leachate chemistry are mixed, with some analytes showing a decrease in leachate concentration at 40 days (Al, Fe, Ni), some showing an increase in concentration (Cu) and most showing very small or no differences (Cd, As, Mn, Pb, Zn).

ENVR 134

Heavy metal adsorption capacity of biomass and animal-manure derived biochars

Isabel M Lima⁽¹⁾, isabel.lima@ars.usda.gov; Kyoung S Ro⁽²⁾; Gudigopuram Reddy⁽³⁾; Devinder Mahajan⁽⁴⁾; Kjell T Klasson⁽¹⁾; Minori Uchimiya⁽¹⁾. (1) Southern Regional Research Center, USDA-Agricultural Research Service, New Orleans LA 70124, United States (2) Coastal Plains Soil, Water, and Plant Research Center, USDA-Agricultural Research Service, Florence SC 29501, United States (3) Department of Natural Resources and Environmental Design, North Carolina A&T State University, Greensboro NC 27411, United States (4) Brookhaven National Laboratory, Stony Brook University, Stony Brook New York 11790, United States

The ability of either plant or manure-based biochars to adsorb heavy metal compounds is highly dependent on the type of feedstock used as well as whether biochars are used as-is or activated. In this study both plant and manurebased biochars were produced and characterized for their capability of removing copper ions from solution. These biochars were further activated either via steam or phosphoric acid and then characterized for various important physico-chemical properties. The objective of this study was to investigate the influence of the feedstock source, pyrolysis temperature, and activation strategy on the adsorption capacity for copper ion. Copper ion adsorption was of particular interest because copper is one of the metals of environmental concern. It is toxic to many animal species and is an environmentally ubiquitous metal found in both drinking water and wastewater. Biochar samples were made by pyrolyzing wood shavings and chicken litter at 250 and 500°C for three minutes and further activating with either steam or phosphoric acid. For the adsorption experiments, a 1% w/v sample was added to 0.01, 0.1, 1, 5, 10 and 20 mM solutions of copper ion for 24 hr. All samples were characterized for their pH, surface area, surface charge, and proximate and ultimate analyses, as well as elemental composition. Adsorption capacity for copper ion was lowest for the biochars and highest for the phosphoric acid activated biochars. Both the biochar and the steamactivated biochar from chicken litter performed significantly better than the corresponding biochar and steam-activated biochar made from wood shavings.

ENVR 316

Biochar reference materials

David W. Rutherford⁽¹⁾, dwruther@usgs.gov; Colleen E. Rostad⁽¹⁾; Robert L. Wershaw⁽¹⁾; Francisco J. Calderon⁽²⁾. (1) National Research Program, US Geological Survey, Denver Colorado 80225, United States (2) USDA-Agricultural Research Service, Akron Colorado 80720, United States

Formation conditions and feedstock composition can significantly alter many physical and chemical properties of biochar. To develop analytical procedures to characterize biochars for research and production control, reference material has been prepared from a mixed pine wood by two representative processes. Biochar Engineering Corporation used a two-stage slow pyrolysis process while the National Renewable Energy Laboratory produced a char by high temperature gasification in a fluidized bed reactor. Each material was homogenized using manual blending techniques followed by cross flow V-blender. The homogenized material was then split into subsamples using

a spinning riffle followed by a Jones Riffle splitter. Random sub-samples of each material were characterized by elemental analysis (ultimate and proximate analysis), surface area and porosity, infrared reflectance. Water extracts were also characterized. These analyses were used to assess the effectiveness of the homogenization and spitting techniques. The reference materials will be available in small quantities to researchers by contacting the authors.

ENVR 317

Carbon isotopic fractionation as a function of charring temperature during the production of biochar

Colleen E. Rostad⁽¹⁾, cerostad@usgs.gov; Robert L. Wershaw⁽¹⁾; David W. Rutherford⁽¹⁾; Nabil M.R. Saad⁽²⁾. (1) National Research Program, U.S. Geological Survey, Denver CO 80225, United States (2) Picarro, Inc., Sunnyvale CA 94085, United States

¹³C/¹²C isotopic fractionation provides a means to study the mechanism of formation of biochar. Chars were prepared from switchgrass and pine wood at different temperatures. ¹³C concentration decreases in both switchgrass and pine wood biochars as formation temperature increases from 200 to 600 °C. The ¹³C concentration then increases as charring temperature increases from 700 to 900 °C. These changes are most likely due to the kinetic isotope effect. From 200 to 600 °C, carbon atoms in the original cellulose, hemicellulose, and lignin structural components react to form graphene structures. Under these conditions, the ¹³C atoms will react slightly more slowly than the ¹²C atoms and therefore, there will be a depletion of ¹³C in the resulting graphene structures. At the higher temperatures, increases in ¹³C concentrations in the chars indicate that the reverse is taking place and that the graphene structures are being degraded to volatile compounds that are depleted in ¹³C.

ENVR 318

Modeling the physical and chemical interactions of natural organic matter in soils: General principles

Robert L. Wershaw, rwershaw@usgs.gov; David W. Rutherford; Colleen E. Rostad. National Research Program, US Geological Survey, Denver Colorado 80225, United States

Soils and sediments are composed of complex mixtures of inorganic minerals and natural organic matter (NOM). The buffering capacity, metal-binding capacity, stability of aggregates of soil particles, water-holding capacity, and sorption capacity for hydrophobic organic compounds of a soil are dependent, to a large extent, on the amount of NOM in the soil. The pool of NOM in soils is vital in maintaining plant fertility; it also serves as a carbon sink in the global carbon cycle. The formalism of thermodynamics provides a framework for modeling the interactions of NOM in soils. Soils are multi-component, multi-phase thermodynamic systems. We propose that as a first step in the modeling of NOM in soils relatively simple, well-characterized artificial (surrogate) NOM phases be prepared in the laboratory, and that the physical and chemical properties of these phases be compared to the physical and chemical properties of soil isolates.

ENVR 319

Effects of biochar amendment in soil on bioenergy crop yield and biomass composition

Charles Warren Edmunds⁽¹⁾, cedmund1@utk.edu; Nicole Labbe⁽²⁾; PyoungChung Kim⁽²⁾; Amy Johnson⁽³⁾; Mark Radosevich⁽³⁾; Timothy Rials⁽²⁾. (1) Department of Biosystems Engineering, Center for Renewable Carbon, The University of Tennessee, Knoxville Tennessee 37996, United States (2) Department of Forestry, Wildlife, and Fisheries, Center for Renewable Carbon, The University of Tennessee, Knoxville Tennessee 37996, United States (3) Department of Biosystems Engineering and Soil Sciences, The University of Tennessee, Knoxville Tennessee 37996, United States

The goal of reducing greenhouse gas emissions and decreasing the usage and dependence on fossil fuels drives research of biofuels and renewable energies. This research investigates the use of biochar, a co-product of biomass pyrolysis, to sequester carbon by incorporating the biochar into agricultural soil. This approach shows great potential to mitigate atmospheric CO2, facilitate the production of renewable energy, and increase crop yield. A greenhouse experiment was conducted to study the effect of biochar as a soil amendment on the growth of two bioenergy feedstock crops, switchgrass and sorghum. Biomass yield and chemical composition will be reported for plants grown using biochars with different properties and two application rates. The goal is to correlate the physical and chemical characteristics and application rate of biochar with the yield and chemical composition of the plants grown in the biochar amended soil.

ENVR 320

Biochar effects on extractable ${\rm NO_3}^{\scriptscriptstyle -}$ and ${\rm NH_4}^{\scriptscriptstyle +}$ and greenhouse gas flux after biochar and fertilizer application to two temperate soils

Jiyong Zheng⁽¹⁾, cstewart@nrel.colostate.edu; Catherine E. Stewart⁽²⁾; M. Francesca Cotrufo⁽³⁾. (1) State Key Laboratory of Soil Erosion and Dryland Farming on the Loess Plateau, Northwest A & F University, Yangling Shaanxi 712100M, China (2) Soil-Plant-Nutrient Research, USDA-Agricultural Research Service, Fort Collins CO 80526-8119, United States (3) Department of Soil and Crop Science, Colorado State University, Fort Collins CO 80523-1499, United States

Biochar may increase soil water-holding capacity, cation exchange capacity and surface sorption capacity which could decrease the leaching losses of available nitrate and ammonium, and reduce the N2O emissions. Despite these properties, the magnitude of the potential benefits depends on the size and individual characteristics of the biochar and the nutrient status of the amended soil. To determine the contribution of biochar to 1) N retention and 2) soil C mineralization, we added two sizes (>250 and <250 mm) of biochar to two soils (sandy, silty-clay loam) with and without fertilizer addition, and measured gas exchange (CO2, N2O, and CH₄) and extractable NO₃ and NH₄⁺. Our data suggest that decreases in N2O after biochar addition to soils can contribute to reducing GHG emissions from soils, but the magnitude of this decrease is determined by the biochar effects on soil CO2 flux, which can either be suppressed or primed.

Distinct phosphorus leaching behaviors of poultry litter (PL) and PL Char

Pei C Chiu⁽¹⁾, pei@udel.edu, 344B DuPont Hall, Newark DE 19716, United States; Yue Wang⁽¹⁾; Paul T. Imhoff⁽¹⁾; Mingxin Guo⁽²⁾. (1) Department of Civil and Environmental Engineering, University of Delaware, Newark DE 19716, United States (2) Department of Agriculture and Natural Resources, Delaware State University, Dover DE 19901, United States

Leaching of phosphorus from manure to surface waters contribute significantly to eutrophication. We hypothesized that converting manure into biochar through pyrolysis could reduce the phosphorus leaching potential and thus represent a potential solution to this problem. Water in contact with poultry litter (PL) and PL char for different durations were analyzed for orthophosphate, acid-hydrolyzable phosphorus, and total phosphorus by colorimetric method and ICP-OES. PL rapidly released large amounts of phosphorus and leaching continued for weeks. Almost all the phosphorus released from PL was dissolved orthophosphate. In contrast, PL char slowly released phosphorus at concentrations orders of magnitude lower than that from PL, despite the higher total phosphorus content of the char. Approximately 80% of the phosphorus released by PL char was orthophosphate, with the remaining phosphorus being particulate (0.025-11 μm). These results supports that PL char may potentially serve as a slow-releasing and sustainable source of phosphorus in soil.

ENVR 322

Ammonia removal using poultry litter and its biochar mixture

Nanh Lovanh, nanh.lovanh@ars.usda.gov; John Loughrin. USDA-Agricultural Research Service, Bowling Green KY 42104, United States

In the era of climate change, conversion of raw materials such as crop residuals and other waste byproducts into biochar could serve as a sink for carbon sequestration which could help reduce carbon footprint in the atmospheric environment. Biochar could also be used for soil amendment to improve soil conditions as liming agent and provide additional micronutrients for crops. In addition, biochar could be used as absorbent for the removal of heavy metals and other environmental pollutants. In this study, biochar from fast pyrolysis of rice-hull poultry litter was used in biofiltration systems for ammonia removal. Columns were packed with poultry litter, combination of poultry litter and biochar, and biochar alone for filtration of synthetic ammonia (500 ppm in air). Ammonia was fed through the columns at flowrates which gave empty bed residence times of one minute. Flow meters were used to monitor the flowrates of the influent and effluent. The influent and effluent ammonia concentrations were monitored using a photoacoustic gas analyzer. The pressure drops across the packed columns were observed to be similar for biochar column (65%) and poultry litter/biochar column (70%). The experiment was carried out over 5000 times the column volumes. Based on the preliminary results, columns packed with biochar alone were able to achieve 90% ammonia reduction. However, the ammonia breakthrough curve was shorter than the breakthrough curve for columns packed with a mixture of biochar and raw poultry litter. The results also showed that the ammonia removal efficiency was about 95% from

columns packed with a mixture of poultry litter and biochar. Thus, it appeared that biotic effect from biochar (and poultry litter) prolonged ammonia removal and increased ammonia removal efficiency. Therefore, biochar could be effective packing materials for biofiltration systems for removing air pollutants from livestock production facilities.

ENVR 323

Characterization of biochars produced under different conditions by 1D and 2D solid-state ¹³C-NMR

Rasha Hamdan⁽¹⁾, rmh07@fsu.edu; Andrew R. Zimmerman⁽²⁾; William T. Cooper⁽¹⁾. (1) Department of Chemistry and Biochemistry, Florida State University, Tallahassee FL 32306-4390, United States (2) Department of Geological Sciences, University of Florida, Gainesville FL 32611-2120, United States

Biochar production is emerging as a potential strategy for mitigating carbon emissions while at the same time increasing soil fertility. However, the effects of combustion conditions and source material on biochar stability in soils are not well understood. We are currently studying the effects of combustion temperature, atmosphere (oxic versus anoxic) and biomass type on the carbon functional groups in biochars. Bulk and surface properties of biochar were characterized using RAMP CP-13C-NMR to assess quantitatively and qualitatively the alteration of the carbon functional groups, while dipolar dephasing (DD)-CP-13C-NMR to study the degree of aromatization and condensation and extent of oxidation. Initial results show that biochars produced at higher temperatures and from grass and hardwood have greater aromaticity and fewer O-containing functional groups. For biochars produced at high temperatures (650 °C), atomic H/C ratios, and the aromatic carbon to hydrogen ratios (F_{aC}/F_{aH}) indicate that the average size of the aromatic units are much smaller than the highly condensed aromatic structures commonly thought to occur in biochars.

ENVR 324

Biochar for soil pH amelioration and improved crop yields

John L Field, john.L.field@colostate.edu; Francesca Cotrufo. Natural Resource Ecology Laboratory, Colorado State University, Fort Collins Colorado 80523, United States

Multiple studies have demonstrated that the addition of biochar to low-productivity agricultural soils can boost crop yield, though underlying mechanisms are poorly understood. A greenhouse experiment investigating the effect of biochar on soil pH and the production of winter wheat (Triticum aestivum 'Hatcher') was established in the spring of 2011. Three agricultural soils of similar texture and chemical properties but different pH (from 5 to 8) were amended with three biochars produced from different feedstocks (pine, corn stover, and wheat straw) and a pH-equivalent liming treatment. Grain and biomass yields will be evaluated, nitrogen use efficiency determined, and tissue ¹³C isotope analysis performed to estimate water use efficiency. This work is intended to elucidate the importance of biochar's liming value relative to its other effects on nitrogen and water dynamics in the given system, as well as investigate the potential benefit of biochar for alkaline agriculture soils.

Thermo-chemical conversion of spent coffee to bio-oil and biochar

Brajendra K Sharma, bksharma@illinois.edu; Wei Zheng; Katie Witkin; Nandakishore Rajagopalan. Illinois Sustainable Technology Center, University of Illinois at Urbana-Champaign, Champaign IL, United States

Energy production from waste biomass/material is a more attractive alternative compared to use of feedstocks such as corn and soybean. This study presents total utilization of waste material- spent coffee grounds through a two-step process. In the first step, triglyceride oil was extracted from spent coffee grounds using hexane soxhlet extraction. The extracted oil properties were studied and found suitable for producing biodiesel. In the second step, the defatted spent coffee grounds was converted into bio-oil and biochar using

a pyrolysis process at 450 °C under nitrogen atmosphere. It was found that spent coffee grounds produced more bio-oil and less biochar compared to defatted coffee ground. The bio-oils were analyzed for their physical properties, such as viscosity, density, elemental composition, heating value, boiling point and molecular weight distribution. Structural characterization of bio-oils was carried out using advanced spectroscopic and chromatographic techniques, such as NMR, FTIR, TLC-FID, and GC-MS to obtain information on carbon and hydrogen distribution, functional groups, and hydrocarbon class type distribution. Two biochars produced from spent and defatted coffee grounds, and their respective feed stocks were characterized for elemental composition, BET surface area, ash, moisture and volatile content. These four samples were then used as soil amendment in a greenhouse experiment to study their effect on crop yields and to investigate if the use of biochar could help reduce the amount of chemical fertilizer, while at the same time maintaining or increasing crop yields.

ENVR DIVISION – Vet Pharm Symposium

ENVR 162

Mechanisms of anabolic steroid-stimulated muscle growth

William R Dayton, wdayton@umn.edu; Michael E White; Marcia R Hathaway. Department of Animal Science, University of Minnesota, St. Paul MN 55108, United States

Anabolic steroid treatment of yearling steers significantly enhances muscle growth; however, there has been no consensus as to the biological mechanism(s) responsible for the anabolic effects of either estrogenic or androgenic steroids. Muscle satellite cells (MSCs) play a crucial role in postnatal muscle growth by fusing with existing muscle fibers and providing the nuclei required for fiber growth. Muscles of yearling steers implanted with a trenbolone acetate (TBA) and estradiol-17b (E2) contain more MSCs than do muscles of nonimplanted steers suggesting that increased MSC number plays a role in anabolic-steroidinduced muscle growth. Treatment for 7 days with TBA/E2 or with E2 alone increases Insulin-like Growth Factor (IGF)-1 mRNA in longissimus muscle of yearling steers as compared to nonimplanted steers. It is likely that increased muscle IGF-1 helps increase the number of MSCs, increased myofiber nuclei, increased hypertrophy and increased muscle growth observed in anabolic steroid treated livestock and humans. Data show G-protein-coupled receptor 30 (GPR30) involvement in increased IGF-1 mRNA expression by cultured bovine satellite cells (BSC). Treatment of cultured BSC with E2 or TBA increases rates of proliferation and protein synthesis and decreases protein degradation. However, in cultures in which Epidermal Growth Factor Receptor (EGFR) activity has been blocked by selective tyrosine kinase inhibitors, E2 has no effect on rates of either proliferation or protein synthesis, but continues to decrease protein degradation. Similarly, E2 does not affect proliferation in BSC cultures in which EGFR expression has been silenced using EGFR siRNA. These results suggest an EGFR requirement for E2 to stimulate BSC proliferation and protein synthesis. Based on these in vivo and in vitro studies, we have begun to define a mechanism for anabolic

steroid-stimulated bovine muscle growth which involves the interaction of muscle IGF-1 level, IGF-1 receptor, estrogen receptor-a, GPR30, EGFR, androgen receptor and specific intracellular signaling pathways.

ENVR 163

Interspecies comparison of the mechanisms of toxicity and effects of veterinary pharmaceuticals with estrogenic or androgenic activity: Are we really living in a sea of estrogens?

Leon E Gray, Jr⁽¹⁾, gray.earl@epa.gov; Vickie S Wilson⁽¹⁾; Phillip Hartig⁽¹⁾; Gerald Ankley⁽²⁾. (1) NHEERL, TAD, Reproductive Toxicology Branch, US Environmental Protection Agency, Durham NC 27713, United States (2) Midwest Ecology Division, US Environmental Protection Agency, Duluth MN, United States

Exposure to veterinary and human pharmaceuticals with estrogenic or androgenic activity can profoundly disrupt development and reproduction in all vertebrate classes ranging from mammals to fish. Effects have been observed in controlled laboratory and in field studies. Field studies demonstrate that exposure to such chemicals individually or as mixtures can disrupt reproductive development and function in aquatic species. Humans also have been severely affected by such chemicals following accidental exposures or with drug usage. Given that these chemicals are present in the environment at levels sufficient to adversely affect fish species and other aquatic species, concern has arisen about their potential to affect humans via exposure through contaminated drinking water. For this reason, the Office of Water, US EPA, has several xenoestrogens on the current Critical Contaminants List. This presentation will review the cellular and molecular events of estrogens and androgens in vertebrates and compare the effects of treatment with estrogens and androgens on mammals to those seen in fish. The talk also will present examples from field studies of how environmental estrogens and androgens disrupt aquatic species as well as examples of untoward effects of these chemicals in humans.

Molecular target homology as a basis for species extrapolation to assess the ecological risk of veterinary drugs

Carlie A. LaLone, LaLone. Carlie@epa.gov; Daniel L. Villeneuve; Christine L. Russom; Joseph E. Tietge; Lyle Burgoon; Gerald T. Ankley. US Environmental Protection Agency, United States

Increased identification of veterinary pharmaceutical contaminants in aquatic environments has raised concerns regarding potential adverse effects of these chemicals on non-target organisms. The purpose of this work was to develop a method for predictive species extrapolation utilizing quantitative molecular homology based approaches for prioritizing pharmaceuticals, including veterinary drugs, based on their potential ecological risk. Because drugs are designed to target specific proteins, similarity of amino acid sequence alignments from molecular targets comparing target species to non-target species may inform predictions of species sensitivity to a pharmaceutical. This strategy was designed to take into account the quality of the alignment and to identify common conserved functional domains. A customized computer tool has been designed that automates the sequence alignments resulting in a quantitative metric that can be used to predict species sensitivity. Case examples of this approach will be presented for veterinary drugs that affect the vertebrate hypothalamic-pituitarygonadal axis.

ENVR 165

In vitro assays for assessment of androgenic and estrogenic activity of defined mixtures and complex environmental samples

Vickie S Wilson, wilson.vickie@epa.gov. Toxicity Assessment Division, US Environmental Protection Agency, ORD, NHEERL, Research Triangle Park NC 27711, United States

Effluents from sources such as wastewater treatment plants and animal feeding operations invariably contain complex mixtures of chemicals. Recent research on effluent from cattle feeding operations in the US have linked morphological alterations in fish with in vitro androgenic activity in associated water samples. Identification of the causative agent in the sample through traditional analytical methods can be cost prohibitive. The use of in vitro assays to identify potential hormonal activity, therefore, is attractive since overall hormonal activity of the water sample is indicated and results can generally be obtained more quickly and at lower cost than analytical methods development or in vivo assays. Further, positive results can be used to target chemical analyses toward hormonally active samples thus conserving valuable resources. Our lab has developed several in vitro assays, including transcriptional activation and receptor binding assays, which have been adapted for screening of environmental samples for estrogenic and androgenic activity. These assays have been successfully used to screen many types of samples including effluents from cattle, dairy, swine and poultry operations and also from different matrices including point (effluent) and non-point (agricultural run-off; groundwater and surface water; combustion by-products) sources. With complex mixtures, it is important to understand how compounds with similar or different mechanisms of action would affect assay results. Several defined mixture studies

have therefore been conducted. These studies indicate that mixtures of hormones act in a dose additive manner. Our results with defined mixtures and environmental samples support the use of these assays as effective tools for assessing hormonal activity in complex environmental samples.

Disclaimer: Abstract does not necessarily reflect US EPA policy.

ENVR 166

Application of steroidal implants in the US beef cattle industry

Jonathon L Beckett⁽¹⁾, jbeckett@beefconsulting.com; Bradley J Johnson⁽²⁾, bradley.johnson@ttu.edu, Box 42141, Lubbock TX 794109, United States . (1) Beckett Consulting Services, Fallbrook CA 93422, United States (2) Department of Animal and Food Sciences, Texas Tech University, Lubbock TX 79409, United States

For over 50 years, beef cattle producers have safely used steroidal implants to enhance productivity and efficiency of beef production. Many different formulations of growth promotants are approved for use in raising cattle, but the most common are anabolic steroid implants administered primarily through small pellets that are placed under the skin on the back of the animal's ear. The active ingredients in these implants belong to one of three major categories of steroid hormones: androgens, estrogens, and progestins. These are the same hormones that are found endogenously (naturally occurring) in all animals. In addition, naturally occurring (zeranol) and synthetic (e.g., trenbolone acetate and melengestrol acetate) analogs of these major classes of hormones have been approved for use in beef cattle production. The active ingredients in the pellets are slowly released to ensure stable hormone delivery during the service life of the implant. The service life can range from 60 to 240 days depending on implant type and drug release technology. Growth promotants such as steroidal implants shift nutrient utilization toward carcass lean tissue deposition at the expense of adipose tissue. These biological effects result in production improvements generally are characterized by an increase in average daily gain ranging from 8% to 28% and improvements in feed conversion efficiency from 5% to 20% in treated cattle compared to non-treated cattle. Steroidal implants have moderate effects of increasing feed intake in ruminants. While responses to implants are relatively consistent within cattle types, factors such as cattle type and growth promotant type, ingredients, and strength of dose affect cattle response to treatment. In conclusion, growth promoting implants have long been used to enhance muscle gain and feed conversion efficiency to provide safe and nutritious beef for consumers at a lower cost while using fewer natural resources.

ENVR 167

Overview of the US Food and Drug Administration Center for Veterinary Medicine environmental risk assessment process for veterinary pharmaceuticals

Holly M Zahner, holly.zahner@fda.hhs.gov; Wesley Hunter; Eric Silberhorn; Charles Eirkson. Center for Veterinary Medicine, US Food and Drug Administration, Rockville MD 20855, United States

The US Food and Drug Administration Center for Veterinary Medicine (CVM) evaluates the environmental impacts of agency actions under the National Environmental Policy Act,

such as conducting investigations on new animal drugs and approving animal drugs for commercial use. Categorical exclusions (CE) and environmental assessments (EA) are used for evaluating the environmental safety of agency actions. A CE from the requirement to prepare an EA is granted for categories of actions that have been predetermined not to typically result in significant environmental impacts. Whereas, an EA is a science-based risk analysis used to determine if significant environmental impacts are expected as a result of an action. The EA should include fate, exposure, and effects data, as well as a risk analysis that compares the ratio of exposure to effects. If a potential risk to the environment is identified, then risk mitigation measures may be necessary. CVM's scientific perspectives regarding the environmental assessment of veterinary drugs will be discussed.

ENVR 197

Quadrupole time-of-flight LC-MS analysis of veterinary drug residues in aquaculture samples

Sherri Turnipseed⁽¹⁾, sherri.turnipseed@fda.hhs.gov; Susan Clark⁽²⁾; Joseph Storey⁽²⁾. (1) Animal Drugs Research Center, US Food and Drug Administration, Denver CO 80225, United States (2) Denver Science Branch, US Food and Drug Administration, Denver CO 80225, United States

Over the past decade, methods for veterinary drug residues in foods have changed significantly. Rather than monitoring for a single drug residue or a specific class of compounds, multi-class screening procedures with large numbers of analytes using LC-MS are now commonly reported. LC-MS with a time-of-flight (TOF) detector is capable of obtaining high resolution data. Virtually an unlimited number of compounds can be simultaneously analyzed with this instrument because full-scan data, rather than preselected ion transitions, are collected. Therefore, in addition to looking for target analytes, additional nontargeted compounds may also be detected. Analytical methods for the analysis of veterinary drug residues in aquaculture samples using quadrupole-TOF LC-MS will be presented. This approach was used to characterize metabolites in catfish dosed with sulfonamides and to detect illegal residues in imported frog legs. Samples were first screened by MS and any drug residues found were confirmed by MS/MS.

ENVR 198

Liquid chromatography mass spectrometry: Analysis of veterinary growth promoters in airborne particulate matter

Brett R Blackwell⁽¹⁾, brett.blackwell@tiehh.ttu.edu; Philip N Smith⁽¹⁾; George P Cobb⁽¹⁾; Michael D Buser⁽²⁾; Bradley J Johnson⁽³⁾; Matthew Baker⁽⁴⁾. (1) Department of Environmental Toxicology, Texas Tech University, Lubbock TX 79409, United States (2) Department of Biosystems and Agricultural Engineering, Oklahoma State University, Stillwater OK 74078, United States (3) Department of Animal and Food Sciences, Texas Tech University, Lubbock TX 79409, United States (4) Department of Agricultural Education and Communications, Texas Tech University, Lubbock TX 79409, United States

Veterinary growth promoters are widely used throughout the United States in livestock production. In beef production, steroid hormones are administered to an estimated 90% of cattle. These include the synthetic steroids trenbolone acetate and melengestrol acetate, as well 17β -estradiol.

Given the endocrine-modulating activity of steroid growth promoters, a sensitive and reliable analytical method is needed to detect trenbolone, melengestrol acetate, estradiol and related residues in environmental matrices. We have developed a method that incorporates solid phase extraction (SPE) and liquid chromatography-tandem mass spectrometry for the simultaneous determination of trendione, trenbolone, melengestrol acetate, estrone, and estradiol in airborne particulate matter samples. Sample preparation involved shaking extraction followed by cleanup on SPE cartridges. Analytes were separated using reversedphase liquid chromatography. Column effluent underwent atmospheric-pressure chemical ionization (APCI) followed by detection using a triple-quadrupole mass spectrometer in SRM mode. Detection limits, recovery and repeatability will be presented and discussed.

ENVR 199

Analysis of steroids in newborn screening by LC-MS/MS

David Klein, dk02@txstate.edu; Mark Fountain. Chemical Threat Laboratory, Texas Department of State Health Services, Austin TX 78714, United States

Texas Department of State Health Services Newborn Screening has approximately 400,000 samples to screen annually. Congenital Adrenal Hyperplasia (CAH) is one of the metabolic disorders that is screened that has a high false positive rate (>30%). The Chemical Threat Lab has employed the emergency response LC-MS/MS to develop steroid metabolite screening in support of developing a second tier CAH screen. The use of the ABSciex 4000 for steroid screning will be discussed.

ENVR 200

Deuterium exchange complicates isotope dilution methods for steroid hormones

William T Foreman, wforeman@usgs.gov; Rhiannon C ReVello; James L Gray. US Geological Survey, Denver CO 80225, United States

Deuterium-hydrogen exchange (D loss) via keto-enol tautomerization from alpha-carbons adjacent to ketone functionalities occurred at one or more labeled positions for androstenedione-d₁, dihydrotestosterone-d₄, estrone-d₄, norethindrone-d₆, progesterone-d₉, and testosterone-d₅ used in our isotope-dilution quantification (IDQ) GC/MSMS method for steroid hormones. Loss occurred in methanol extracts of environmental samples, especially if the extracts were heated during evaporation steps. Deuterium loss even occurred in standard solutions in methanol stored primarily at -15°C. Deuterium-hydrogen exchange for these or structurally similar isotopes might occur in other IDQ methods for hormones (e.g., EPA method 1698 uses norethindrone-d₆ and progesterone-d₉) or pharmaceuticals, and be causing the "odd" isotope and analyte recovery results noted by other research groups that used estrone-d4 or trenbolone-d₂ (or d₃). We describe our observations of isotope D loss and highlight changes employed to minimize this problem in our IDQ method for hormones.

Detection of tetracyclines and tetracycline resistant bacteria in soils under long-term swine effluent application

Inna Popova, inna.popova@okstate.edu; Shiping Deng; Jeffory Hattey. Department of Plant and Soil Sciences, Oklahoma State University, Stillwater OK 74078, United States

Every year in the United Stated more than 11 million pounds of antibiotics are used in the swine industry with approximately 9 million pounds of these antibiotics released into the environment as animal wastes. Limited scientific evidence is available connecting the fate of antibiotics in soils and the development of bacterial resistance. The objective of the presented study is to determine concentrations of four tetracyclines and the persistence of tetracycline resistant bacteria in the soils that have been continuously treated with swine effluent. An analytical protocol based on the ultrasound-assisted extraction and solid phase extraction follwed by HPLC/UV quantification method was developed and optimized. Recoveries of four tetracyclines from soils were 69 - 115% (RSD 0.1 - 5.0%) with detection limits of 0.03 - 0.4 $\mu g/g$ soil. Concentrations of chlortetracycline in 36 soils with different effluent application rates were in the range of 0.04 - 0.26 µg/g soil. The occurrence and degree of bacteria resistance will be presented.

ENVR 202

Particulate matter emissions from animal feeding operations

Ronaldo G Maghirang, rmaghir@ksu.edu. Department of Biological and Agricultural Engineering, Kansas State University, Manhattan KS 66506, United States

Animal feeding operations (AFOs) can emit various gaseous pollutants and particulate matter, including TSP, PM_{10} , and $PM_{2.5}.$ The nature and amount of air emissions depend on a number of factors including the type and number of animals, design, operation of the confinement facility, and climatic and weather conditions. This presentation will deal with current knowledge concerning particulate emissions from open cattle feedlots and other AFOs. Emission rates and abatement measures for mitigating emissions will be discussed.

ENVR 203

Particulate matter sampling strategies for agricultural operations

Derek P Whitelock⁽¹⁾, dwhitelo@nmsu.edu; Michael D Buser⁽²⁾; Lingjuan L Wang⁽³⁾. (1) Southwestern Cotton Ginning Research Laboratory, USDA- Agricultural Research Service, Mesilla Park NM 88047, United States (2) Department of Biosystems and Agricultural Engineering, Oklahoma State University, Stillwater OK 74078, United States (3) Department of Biological and Agricultural Engineering, North Carolina State University, Raleigh NC 27695, United States

Strategies for sampling particulate matter (PM) from agricultural sources vary depending on the type of source, the objective of sampling the particular source, and the PM

characteristics. Agricultural point or area sources may require different categories of samplers, stack or ambient, and those categories are may be further segregated based on the particle size of interest: total suspended particulate, PM_{10} , and $PM_{2.5}$. For ambient PM sampling in particular, sampler array configuration (type, number, and siting) is influenced by the purpose for conducting the sampling. For example, the sampler configuration for evaluating an abatement strategy could differ from that for determining total emissions from a site. The PM size and concentration can impact sampler performance and, thus, influence sampler type and location. This paper presents an overview of the sampler types used for agricultural PM sampling and discusses the factors that influence sampler selection and siting.

ENVR 204

Growth promoters, wind, and human/ecological health: Preliminary feedyard PM analysis

Michael Buser⁽¹⁾, buser@okstate.edu, 214A Agricultural Hall, Stillwater OK 74078, United States; Brett Blackwell⁽²⁾; Phil Smith⁽²⁾; George Cobb⁽²⁾; Brad Smith⁽²⁾. (1) Oklahoma State University, Stillwater OK, United States (2) Texas Tech University, Lubbock TX, United States

[Abstract not available]

ENVR 205

Techniques for determining partial size distribution of particulate matter: Laser diffraction vs. electrical sensing zone

Lingjuan Wang Li⁽¹⁾, Ling_Wang@ncsu.edu; Michael Buser⁽²⁾; Derek P Whitelock⁽³⁾; Zihan Cao⁽¹⁾; Yuanhui Zhang⁽⁴⁾; Calvin Parnell⁽⁵⁾. (1) Department of Biological and Agricultural Engineering, North Carolina State University, United States (2) Department of Biosystems and Agricultural Engineering, Oklahoma State University, United States (3) USDA-Agricultural Research Service, Mesilla Park NM, United States (4) College of ACES and Engineering, University of Illinois, United States (5) Center for Agricultural Air Quality Engineering and Science, Texas A & M University, United States

The study of health impacts, emission estimation of particulate matter (PM), and development of new control technologies require knowledge of PM characteristics. Among these PM characteristics, the particle size distribution (PSD) is perhaps the most important physical parameter governing particle behavior. Various methods and techniques are available for conducting PSD analyses. Advantages and disadvantages associated with each method exist. Unfortunately, there is no single agreed upon method to determine the PSD of PM emitted from difference sources. This paper aims to present full perspectives of PSD measurement techniques through a literature review and a laboratory investigation. In the literature review, different measurement methodologies will be summarized to address their advantages and limitations in application for PSD analysis under different source conditions. The laboratory investigation on PSD measurements was conducted using four PSD analyzers: LS13320 multi-wave length laser diffraction particle size analyzer (Beckman Coulter Inc.), LS230 laser diffraction particle size analyzer (Beckman Coulter Inc.), LA-300 laser scattering particle size analyzer (Horiba Instruments Inc.), and Coulter Counter muiltisizer3 (Beckman Coulter Inc.). PM samples were collected in two

egg production barns using low-volume TSP samplers and were analyzed by the four analyzers for PSDs. In addition to measurements of PM extracted from filters, four types of testing aerosol samples (limestone, starch, #3 micro aluminum, and #5 micro aluminum) were also analyzed by these four PSD analyzers. Differences in MMDs and GSDs of PSDs were statistically tested to discover differences; factors that cause the differences will be reported in this paper.

ENVR 229

Spatial variation in selected veterinary drugs across a cattle feedlot transect from barn to retention basin

Clifford P Rice⁽¹⁾, clifford.rice@ars.usda.gov; Kimberly Cook⁽²⁾; Annesly Netthisinghe⁽³⁾; Becky Gilfillen⁽³⁾; Gabriela Niño de Guzmán⁽⁴⁾. (1) USDA-Agricultural Research Service, Beltsville MD 20705, United States (2) USDA- Agricultural Research Service, Bowling Green KY 42104, United States (3) Department of Agriculture, Western Kentucky University, Bowling Green KY 41066, United States (4) Department of Environmental and Civil Engineering, University of Maryland, College Park MD 20742, United States

Data on the off-site movement and fate of veterinary pharmaceuticals is needed in order to better manage these products. The benefits of these chemicals are well established; however, little information exists on their potential for environmental harm. An essential initial step to understanding this problem is to determine their potential for release and exposure. Three compounds (monensin, lasalocid and doramectin) were specifically studied in this report. These compounds were known to be administered to calves managed in a calving enclosure located on the Western Kentucky Agricultural Research and Education Complex. Their distribution was monitored in soil samples collected across the surface of the enclosure. Initial data show that the majority of the compounds remained in the upper open barn area, while varying amounts of each migrated downslope to a retention basin at the bottom of the facility. Data will also be presented for bacterial density and other compounds.

ENVR 230

Sorption and mineral-promoted transformation pathways of synthetic growth promoters in soil systems

Shen Qu⁽¹⁾, shen.qu@email.ucr.edu; Edward P. Kolodziej⁽²⁾; David M. Cwiertny⁽¹⁾. (1) Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside CA 92521, United States (2) Department of Civil and Environmental Engineering, University of Nevada, Reno, Reno NV 89557, United States

This work examines the fate of trenbolone acetate, melengestrol acetate and zeranol, as well as their primary biological metabolites, in soil. We specifically focus on their interactions with soil organic matter and their susceptibility to mineral-promoted oxidation and hydrolysis. Sorption behavior has been explored in batch experiments with several model soils exhibiting a range of organic carbon contents. Generally, growth promoter sorption is initially rapid followed by a slower rate of uptake over several weeks, is largely irreversible, and tends to scale with soil organic matter content. Growth promoters display a range of sorption affinities even within a family of compounds, as exhibited by markedly different behavior of 17β - and 17α -trenbolone. Experiments with synthetic metal oxides suggest

that manganese and iron oxides oxidize most growth promoters over several hours at pH 6, whereas the hydrolysis of zeranol and its metabolites is catalyzed by certain metal oxides at near-neutral pH.

ENVR 231

Environmental assessment of the antibiotic florfenicol for use in a variety of aquaculture systems

Jane Staveley⁽¹⁾, jstaveley@exponent.com; Richard Endris⁽²⁾. (1) Exponent, Inc., Cary NC 27513, United States (2) Aquaculture Research Program, Intervet/Schering-Plough Animal Health, The Netherlands

Florfenicol® (Intervet International B.V.) is a broadspectrum antibiotic shown to be effective at minimizing disease caused by a variety of fish pathogens. The antibiotic is formulated in feed and authorized in a number of countries under the names Florocol, Aquaflor, or Aquafen. Phase II Tier A and Tier B Environmental Assessment procedures following VICH guidance were used to evaluate the environmental risk of the use of florfenicol in ponds rearing catfish as well as raceways and recirculating systems rearing tilapia. The Tier A assessment involved consideration of physicochemical properties, environmental fate studies, and acute environmental effects studies. Information on the use patterns of florfenicol was used to calculate the Predicted Environmental Concentration (PECs). Initial PECwater values were determined based on both worst-case and typical release parameters and compared to Predicted No Effect Concentrations (PNECs) for freshwater species. Where necessary, refined PECwater values were determined after inclusion of several additional factors affecting the concentrations of florfenicol in the environment (e.g., metabolism in fish, environmental partitioning, etc.). Similarly, the PEC_{soil} values were determined and compared to PNECs for terrestrial organisms. In Tier B, physicochemical properties and environmental fate were again considered, but here chronic environmental effects were evaluated and compared against PECs, reflecting chronic exposures. These assessments are illustrative of the approaches that can be used to characterize the risks of florfenicol under different use patterns. In addition, these assessments can be used to evaluate potential risks associated with other use patterns, fish species, and various treatment dosing regimes.

ENVR 232

Veterinary pharmaceuticals in sewage lagoons of a rural Canadian watershed: The role of phytoremediation for enhanced wastewater treatment

Charles S. Wong⁽¹⁾⁽²⁾, wong.charles.shiu@alum.mit.edu; Jules C. Carlson⁽¹⁾⁽³⁾; Jennifer E. Low⁽¹⁾; Mark L. Hanson⁽³⁾; Pascal Cardinal⁽²⁾. (1) Richardson College for the Environment, University of Winnipeg, Winnipeg MB R3B 2E9, Canada (2) Department of Chemistry, University of Manitoba, Winnipeg MB R3B 2E9, Canada (3) Department of Environment and Geography, University of Manitoba, Winnipeg MB R3B 2E9, Canada

A suite of veterinary compounds (e.g., macrolides, fluoroquinolones, sulfonamides, tetracyclines, tylosin, and trimethoprim) were measured in sewage lagoons and surface reciving waters of Dead Horse Creek, Manitoba, a rural tributary of the Red River draining into Lake Winnipeg. These chemicals were monitored *via* both active grab sampling and passive means using the Polar Organic

Chemical Integrative Sampler (POCIS): 1) to characterize periodic pulse discharges of sewage lagoon wastewaters to the watershed, and 2) to delineate levels and post-release fate of human point sources and veterinary non-point source inputs of these chemicals. Trimethoprim was observed upstream of known wastewater outfalls indicating runoff sources. Time-weighted-average POCIS concentrations were consistent with grab samples. Concentrations of antibiotics decreased significantly in laboratory-based microcosms and field-based mesocosms containing submerged macrophytes, demonstrating that phytoremediation is a viable technology for elimination of such micropollutants in north-central North American aquatic ecosystems.

ENVR 233

Role of reduction-oxidation state on the degradation of synthetic growth promoters

Edward P. Kolodziej⁽¹⁾, koloj@unr.edu; David M. Cwiertny⁽²⁾; Jaewoong Lee⁽¹⁾. (1) Department of Civil and Environmental Engineering, University of Nevada, Reno, Reno NV 89557, United States (2) Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside CA 92521, United States

A range of synthetic growth promoters are commonly used in animal agriculture to improve weight gain. Given their biological potency and observed ability to disrupt endocrine function, the fate of these compounds in the aquatic environment is of concern. The limited number of published studies suggests the particular importance of reductionoxidation state in controlling degradation rates in aquatic systems. This study evaluates the role of redox state on the degradation of synthetic growth promoters, especially focusing on metabolites of trenbolone acetate, by chemically poising heterogeneous microcosms through a range of representative redox states from -400 to +200 mV. Using a sacrificial batch approach, kinetic rates can be determined by analysis of synthetic growth promoter concentration over a time series in the microcosms, while also quantifying the influence of microbial activity and growth on degradation. Observed kinetics, biotransformation pathways, and environmental factors affecting degradation of synthetic growth promoters will be discussed.

ENVR 234

Bioavailability of antimicrobial compounds in sediments

Joel R Coats, jcoats@iastate.edu. Department of Entomology, Iowa State University, Ames IA 50011, United States

Analytical methods were developed to optimize the detection and quantification of the antibiotic erythromycin in surface water and sediment. Extractable and bound residues were determined from water and sediment, using ¹⁴C-erythromycin and two sandy loam sediments, from Iowa and Oklahoma. The optimal extraction solvent was 0.3 M ammonium acetate at pH 4.2: acetonitrile at a 15:85 ratio. Microcosms used pond water and submerged sediment. Total recoveries from the system ranged from 90% - 48% during the 9-week experiment. The presence of sediment in the systems resulted in reductions of erythromycin concentrations in the surface water by one week into the experiment. The availability of aged erythromycin residues

was evaluated by incubating sediment, with and without manure added, 0, 1, 3, or 8 weeks. The manure-amended aged sediments resulted in greater release of the erythromycin from the sediment than did the unamended aged sediments at 1 and 2 weeks.

ENVR 235

Not tonight deer: Determination of an immunocontraceptive peptide in a wildlife vaccine formulation

David A Goldade, David.A.Goldade@aphis.usda.gov; Jeffrey E Kemp; Lowell A Miller. National Wildlife Research Center, United States

Wildlife populations continue to grow despite the use of traditional management efforts. GonaCon™ is an immunocontraceptive vaccine used to reduce reproduction in mammalian species, including white-tailed deer (Odocoileus virginianus). The vaccine consists of synthetic gonadotropin releasing hormone (GnRH) conjugated to a mollusk hemocyanin (Concholepas concholepas) prepared as an emulsion with mineral oil to promote a prolonged immune response. Development of an analytical method for determination of the active ingredient in the vaccine formulation was complicated by the emulsion and conjugation of GnRH to the carrier protein. Breaking the emulsion was achieved chemically by addition of ethyl ether. The aqueous portion containing the GnRH conjugate was cleaved enzymatically with a protease (clostripain) at the arginine-proline site of its peptide sequence. Hydrolysis produced a diagnostic eight amino acid peptide fragment which was unique to GnRH and easily quantified by LC/MS/MS. Typical recoveries of fortified samples at the target concentration exceeded 90%.

ENVR 236

Risk assessment of steroid hormones in veterinary drugs at the US Food and Drug Administration Center for Veterinary Medicine

Holly M Zahner, holly.zahner@fda.hhs.gov; Charles E Eirkson; Eric Silberhorn. Center for Veterinary Medicine, US Food and Drug Administration, Rockville MD 20855, United States

Under the National Environmental Policy Act (NEPA), the US Food and Drug Administration (FDA) Center for Veterinary Medicine (CVM) evaluates the environmental impacts of veterinary drugs containing steroid hormones. Because of the diverse range of hormone compounds, each drug containing hormonally-active compounds is considered on a case-by-case basis to determine whether an Environmental Assessment (EA) will need to be prepared. An EA will generally need to be prepared for many veterinary drugs containing steroid hormones because steroid hormones have been shown to have the potential for serious harm to the environment at low concentrations (ng/L). The EA for steroid hormones should address the risk for environmental impact by comparing the ratio of the cumulative predicted exposure concentration (PEC) in a watershed (i.e., multiple inputs) to the chronic reproductive effects in fish (PNEC). This targeted approach uses appropriate science and mitigations to ensure the safe use of veterinary pharmaceuticals containing steroid hormones.

AGFD DIVISION

AGFD 122

Evaluation of the safety of crop products produced through biotechnology

Wayne Parrott, wparrott@uga.edu.Center for Applied Genetic Technologies, University of Georgia, Athens GA 30602

Products produced through biotechnology are the most highly scrutinized food products on the market. The safety assessment of such food crops involves a multi-pronged approach. The newly introduced gene, its source and its product (the protein it encodes) together with the performance of the plant as well as the inpact of the plant on the environment are all examined in great detail. Both the intended change and possible unintended effects are examined. In the greater than 15 years that biotech products have been grown commercially no safety issues have been attributed to the newly introduced gene. On the other hand, benefits from the technology included reduced pesticide application; less soil erosion because of the more widespread adoption of no or low-till practices; decreased petroleum costs because of the reduced need to enter the field; increased diversity in the field; reduced mycotoxin levels in grain; among others.

AGFD 123

Addressing the safety of crop protection products in a global market

Wendelyn Jones, wjones@croplifeamerica.org; Ray McAllister; Barbara Glenn. CropLife America, Washington DC 20005

Feeding an estimated 9 billion people worldwide by 2050 will require a doubling of food production. This will necessitate more sophisticated technologies within modern agriculture. Products that protect America's food crops are subject to 170 health, safety and environmental tests to ensure safety and effectiveness prior to pesticide registration by the EPA. Development, testing and registration of a new pesticide active ingredient typically takes 9 to 10 years and cost the pesticide manufacturer in excess of \$250 million. On average, only one in 139,000 chemicals screened for pesticide activity successfully makes it through the regulatory process from the discovery laboratory to the farmer's field. Additionally, global trade is dominated by the transfer of agricultural products. It follows that the regulatory process for agricultural chemicals, global harmonization efforts and emerging technical challenges faced by this sector of the chemical industry are key drivers to the global challenge to feed the world.

AGFD 124

Toxicological safety assessment of biotech crops

Carey A Mathesius, carey.mathesius@pioneer.com.DuPont Agricultural Biotechnology, Pioneer Hi-Bred International, Inc., Ankeny IA 50021

The safety assessment process including toxicology will be reviewed for the commercialization of crops derived from biotechnology, which have been modified to express agronomic (including herbicide resistance and insect tolerance) or nutritional traits. The safety assessment pathway for biotech crops is similar to that for individual food ingredients, however the complexities associated with crops as a food or feed lend more to a qualitative assessment between the biotech crop and its non-biotech comparator. The presentation will focus on the mammalian safety assessment principles and discuss specific toxicology studies conducted to ensure the safety of the transgenic proteins and food and feed products derived from biotech crops.

AGFD 125

Allergenicity evaluations of proteins introduced into crop products using biotechnology

Laura S Privalle, laura.privalle@basf.com. Regulatory Science, BASF Plant Science L.P., Research Triangle Park NC 27709

The allergenicity potential of proteins introduced through biotechnology is evaluated as part of the safety assessment of transgenic crop products. Since no single specific parameter can be attributed to a food allergen, the assessment is based on a weight of evidence approach. Characteristics that are considered include sequence homology to known allergenic proteins by applying bioinformatics analyses using an allergen database; resistance to pepsin digestion using simulated mammalian gastric fluid; heat stability measuring loss of functional activity; and exposure as determined by expression levels. Impact on the levels of endogenous allergens by the transformation event is also considered. These may be monitored by immunoblotting techniques using sera from patients allergic to the food. Two dimensional gel electrophoresis followed by mass spectral analysis and gelfree quantitative proteomics methods are being developed as alternative approaches to immunoblots. While the use of animal models have been proposed as a screening tool, to date, none has not been successfully developed and validated to support these safety evaluations.

AGFD 126

Analytical methods for testing biotechnology products

Jingwen Chen, jingwen.chen@syngenta.com. RD Quality Management, Syngenta Biotechnology Inc., Research Triangle Park NC 29560

Since the introduction of genetically modified (GM) crops in the early 1990s, there are about 30 commercial events that are currently cultivated around the world. With the increase in the number of commercial GM events, there will be increased demand for testing agricultural commodities for the presence of products derived from modern biotechnology (GMO's). As major trait providers, biotechnology companies develop, validate, and implement various analytical methodologies in their R&D programs as well as in their stewardship programs. These GMO detection methods are provided to authorities for product registration as part of the regulatory submission. This presentation will provide an overview of analytical methods and applications implemented throughout a product life cycle. The characteristics of both protein- and DNA-based methodologies for analyzing samples from seed/grain and processed food will be discussed. The presentation will also cover regulatory requirements for detection methods and reference materials, and stewardship of Biotechnology products.

AGFD 133

Pesticide residues in food: The role of dietary risk assessment

Mary G. Panek, mary.panek@basf.com. Crop Protection Division, BASF Corporation, Research Triangle Park NC 27709

The media often highlights pesticide residues found in fruits and vegetables. How do scientists outside the agricultural industry interpret this information? Section 408 of the Federal Food, Drug, and Cosmetic Act (FFDCA) authorizes EPA to set tolerances for pesticide residues on foods. The agency can set a tolerance only if EPA scientists determine the tolerance is "safe", i.e. "there is a reasonable certainty that no harm will result from aggregate exposure to the pesticide chemical residue including all anticipated dietary exposure and all other exposures for which there is reliable information" (FFDCA definition). The EPA and industry use U. S. food consumption data and residues measured in field trials and monitoring programs to determine exposure. The exposure for the total population or subpopulation such as children is combined with acute or chronic toxicological endpoints to determine safety levels. This presentation gives a basic overview of dietary risk assessment as performed in the US.

AGFD 134

Secondary standards - barrier or benefit?

Jane M Stewart⁽¹⁾, jane.stewart@basf.com. Environmental and Consumer Safety, BASF, Research Triangle Park NC 27709

The increasing demands of consumers and the influence of non-governmental organizations have driven food retailers to set their own private standards concerning not only food quality, but also pesticide residues in food, and social and environmental issues along the production chain. These private or commercial standards, known as secondary standards, are generally more restrictive (e.g. requiring lower levels of pesticide residues) than official regulatory or import requirements. Secondary standards based on pesticide residue levels are generally based on emotive or hazard-based criteria and not associated to dietary risk evaluations. Some retailers believe that these standards can help suppliers improve the quality of their products and provide a competitive edge. Other stakeholders believe that the costs of complying with these additional standards create an excessive burden for small-scale producers and developing countries, and thus a trade barrier in the market.

AGFD 135

Remediation of fungicide residues on fresh produce using gaseous ozone

Spencer S Walse⁽¹⁾, spencer.walse@ars.usda.gov, 9611 S. Riverbend Ave., Parlier CA 93648, United States . (1) San Joaquin Valley Agricultural Sciences Center, USDA-ARS, Parlier CA 93648, United States

Ozone fumigation was explored as a means for degrading organic fungicide residues on fresh produce. Fungicides sorbed onto model abiotic glass surfaces or onto grape berries were fumigated separately in a flow-through chamber. The relative degradation of fungicides on berries at gaseous ozone concentrations of 900 \pm 12 ppmv (mLL⁻¹) over 2 h was similar to that on glass; reductions were observed for only fenhexamid (~ 64%), cyprodinil (~ 38%), and pyrimethanil (~ 40%). Boscalid and iprodione levels did not change significantly based on a single factor analysis of variance (ANOVA) at the 95% level of confidence (p = 0.05). The kinetics and mechanism of gaseous ozonation, supported by gas chromatography- and liquid chromatography-mass spectrometry product analyses, is discussed in the context of facilitating compliance with maximum residue level (MRL) tolerances.

AGFD 136

Creating and marketing more sustainable food consumer goods

Cristian Barcan⁽¹⁾, cristian.barcan@partners.basf.com. S.E.T. (Sustainability, Eco-Efficiency and Traceability) Initiative, BASF, Elbert CO 80106

Most global predictions indicate that there will be at least 9 billion people in the world by year 2050. This will create additional challenges for the food industry on producing consumer goods that are safe, affordable, socially responsible, and without additional burden on the environment and its resources. To address this challenge, consumer goods/brands have to become more sustainable over time in areas such as safety, environmental impact, social aspects, and costs of ownership. We will explain how a set of traceability and sustainability measurements and selfimprovement tools - combined with an independent product sustainability standard and certification program - can help food manufacturers and brand owners create and market more sustainable goods. The S.E.T.® toolset also helps brand owners comply with the vertical product sustainability standard ProSustain® currently held by Det Norske Veritas (DNV).

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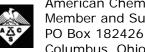
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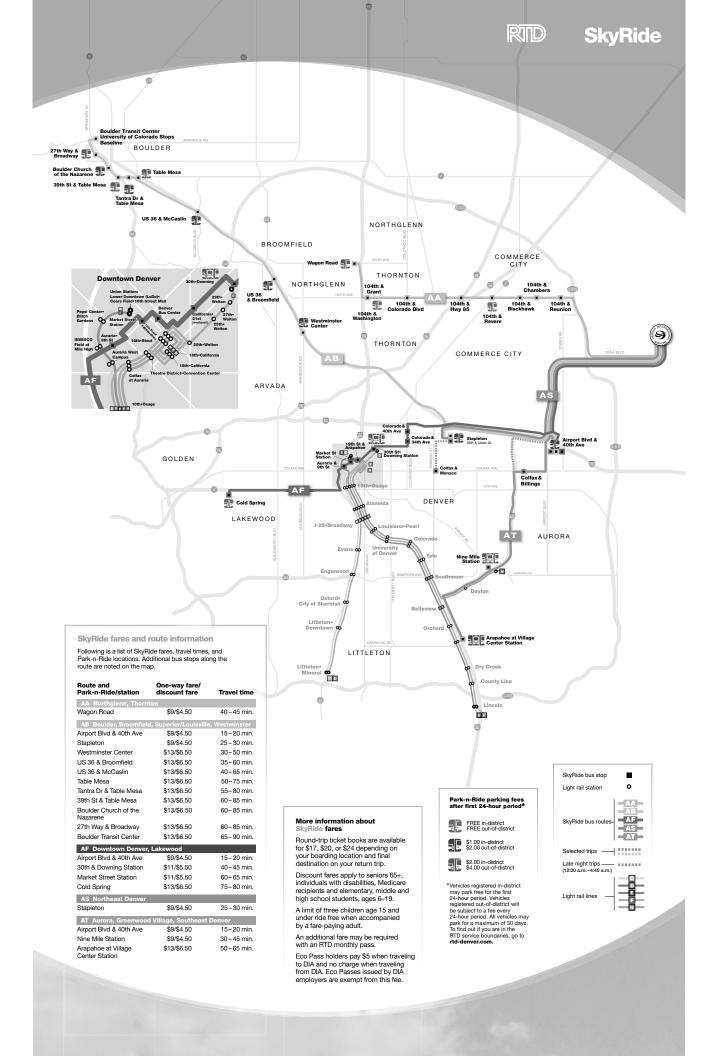
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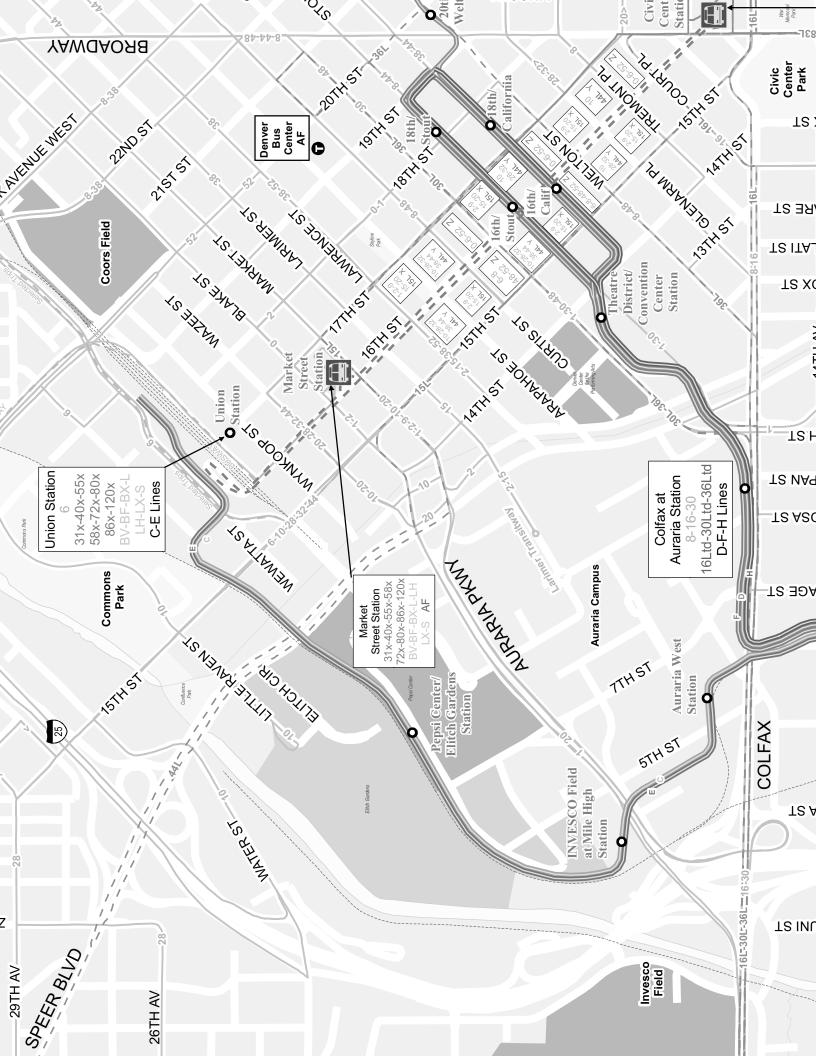
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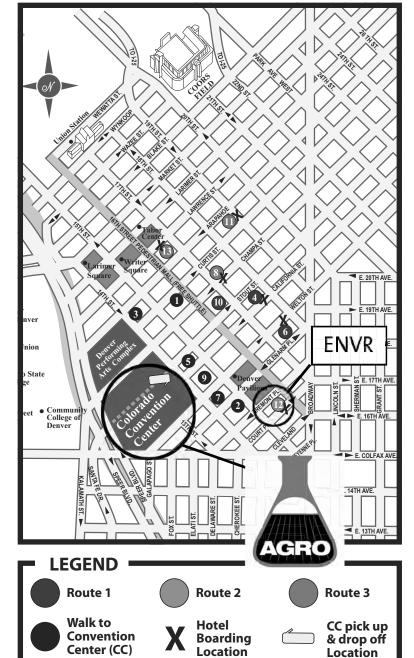


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