PICOGRAM
And Abstracts

AMERICAN CHEMICAL SOCIETY

Division of Agrochemicals

230th ACS National Meeting

August 28 – September 1, 2005, Washington, DC

Fall 2005

Issue No. 69

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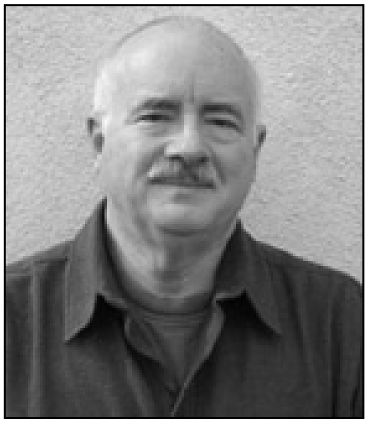

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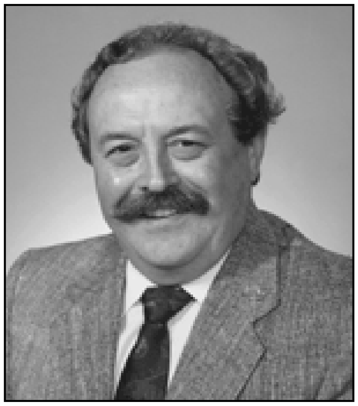

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One-thousand and fifty dollars was donated by six faithful companies in support of the Coffee Lounge in the HORTON GRAND: they were gratefully recognized on the Sponsor Poster near our Desk. We thank them for their generosity - there is no more appreciated gift than the gift of caffeine during our Technical Programming. Please consider encouraging your company to become a sponsor – had the fourth Magi not taken a wrong left at Damascus, his gift would undoubtedly have been coffee.

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THE SOCIAL HOUR – SAN DIEGO

On Tuesday evening at 6:00PM, in the Grand Ballroom of the HORTON GRAND, we again had a joint Social with the Ag & Food Division. All members, speakers and spouses were invited for exotic food, fun, drinks and door prizes – this year's theme was the Cuisine of Donner Pass.

SOCIAL CO-CHAIRS - Al Barefoot & Jeff Jenkins
COFFEE LOUNGE CO-CHAIRS - Terry Spittler & Help Wanted

Message from the Chair

Allan Felsot, AGRO Chair 2005

The Agrochemicals Division welcomes members, guests, and invited speakers to Washington DC for the 230th National Meetings of the American Chemical Society. When asked where I'm from, I respond proudly "from Washington" but then add tongue in cheek, the good Washington not the "evil" one. Speaking as a resident of the Pacific Northwest, and perhaps echoing many fellow westerners to the south, we tend to have a love and hate affair with DC. Similarly, we members of Agrochemicals, whether employed as academics, regulators, consultants, or industry scientists, have a working relationship with and are affected by the political machinations of Washington, DC. Our livelihood depends on grants and contracts from agencies under Congressional mandates, often stimulated by lobbying from so-called special interests. We play the "game" of regulatory science and conduct experiments to produce data that EPA needs to register crop protection products. On the other hand, many of us probably look skeptically upon the pronouncements of the various regulatory agencies, and cry out for more "sound science" before taking action. Perhaps the cliché "can't live with it, can't live without it", describes many feelings in the scientific community for all that Washington, DC has come to represent. But as we embark on yet another biannual pilgrimage for our scientific curiosity and advancement, I think mainly of an idealistic and progressive America embodied overtly and symbolically in Washington, DC.

The AGRO program this fall embodies idealism and progress with diverse symposia and contributed papers discussing the state-of-the-art and tackling thorny issues regarding uncertainty created by exotic pest invasions and the use of public health and crop protection technologies. As usual, attendees will find a diverse array of programming spanning synthetic chemistry, product development, and analytical chemistry to environmental chemistry and toxicology.

I first want to call your attention to our two award symposia. On behalf of our Division, I congratulate Janice E. Chambers, the 2005 ACS International Awardee for Research in Agrochemicals sponsored by DuPont Crop Protection. Janice is a William L. Giles Distinguished Professor and Director of the Center for Environmental Health Sciences in the College of Veterinary Medicine at Mississippi State University. An excellent diverse subject symposium has been organized in her honor starting on Monday morning.

The 2005 Sterling B. Hendricks Award, which is co-sponsored with the USDA-Agricultural Research Service, will be presented to Donald L. Sparks on Wednesday morning. Don holds the S. Hallock du Pont Chair of Plant and Soil Sciences and is currently Chairperson of the Department of Plant and Soil Science at the University of Delaware. An internationally-recognized leading researcher in environmental soil chemistry, Don will give an award address about the challenges and opportunities in environmental sciences. A reception will follow.

As always, we recognize the invaluable contributions of our students through two annual award programs—the Young Scientist Research Recognition Award & Symposium (co-sponsored by Dow AgroSciences and held at the Spring meetings) and the Agrochemical Education Awards for Graduate Student Travel that is held during the Fall meetings. The students will present their research findings as posters on Monday afternoon. Judges will be looking for the best posters and all will be recognized at our traditional Tuesday evening social gathering.

I call your attention to other subject matter symposia including exposure assessment and modeling tools for turfgrass pesticides, QSAR in modern agrochemistry, the importance of pesticide chirality, management of invasive species, biological pest control, and nutrient/soil amendments affecting productivity and environmental quality. At this meeting, AGRO is also co-sponsor of a symposium organized by the Fluorine Chemistry Division (FLUO) on Current Frontiers of Fluoroorganic Chemistry. And don't forget to sample the individual contributed papers and posters that complement the subject matter presentations in the organized symposia. Again, I am astounded by our ability to attract such diversity of subject matter that undoubtedly makes AGRO the most interdisciplinary Division of the American Chemical Society. We may be small in numbers but we are leaders in breaking down the barriers between scientific fields.

Before closing, I'd like to comment on a few issues facing our national Society and our Division. As we all know, accessing current information buried in the ever-burgeoning cache of research literature, conference abstracts, technical reports, and patent licenses is key to our continued progress as scientists in academia, industry, and government. The Chemical Abstracts Service (CAS) Registry has long been the repository of this worldwide information, having developed new tools for searching, acquiring, and displaying the archived records. Recently, the current ACS President, William Carroll, wrote a letter expressing concern of the society over a new venture started by the National Institutes of Health called PubChem (see the letter at http://acswebcontent.acs.org/PDF/PubChem_open_letter.pdf). The original objective of PubChem was to disseminate data that will result from the Molecular Libraries initiative (see the C&EN article at http://pubs.acs.org/cen/government/83/8324gov1.html). As it currently exits, however, PubChem seems to duplicate the efforts of the CAS Registry but with much less staff and uncertainty due to complete dependency on Federal budgetary cycles. On the other hand, CAS has a large dedicated staff and continuous funding through "pay-for-services" agreements with businesses and universities. Discussions between ACS and NIH seem to be ongoing regarding the duplication of efforts and the future of our information storehouse.

Meanwhile, ACS continues its contract with Oxford University Press for producing our popular ACS Symposium Series books. In my discussions with ACS, I've learned that plans are being made to eventually make these books electronically accessible. Such a move should help make the larger scientific community aware of our Division's expertise and contributions at the interface of applied chemistry and biology. We need to encourage ACS to move forward with its e-publishing plans so that the information produced by our Division becomes easily accessible to a wider array of scientists with direct and indirect interests in the fate, effects, and regulation of public health and crop protection technologies.

Finally, agrochemical scientists of all interests have traditionally convened en masse every four years at the IUPAC-sponsored International Congress of Pesticide Chemistry. During the summer of 2006, we will again have this opportunity to exchange new research results and ideas from across the world in Kobe, Japan (see the AGRO website at http://membership.acs.org/a/agro/ for a link to the Congress website). But even before Kobe, planning has to begin for the 2010 Congress. IUPAC will be selecting a proposal from several countries to host that meeting. The AGRO Executive Committee has given approval to submit a proposal to hold the 2010 Congress in the U.S. Presently on the table are ideas for either Washington, DC or nearby Baltimore. I am organizing a committee to prepare a proposal and your input is essential. Thus, please forward to me (afelsot@tricity.wsu.edu) any ideas (and/or concerns) regarding our hosting the Congress after Kobe.

After this Fall meeting, I hand the AGRO Chair responsibilities over to Don Wauchope (USDA-ARS Tifton, GA; don@tifton.usda.gov) who has organized two outstanding meetings during 2005. Dr. Laura McConnell (USDA-ARS Beltsville, MD, mcconnel@ba.ars.usda.gov) will be assuming the Program Chair responsibilities for the following two meetings in Atlanta, GA and San Francisco, CA during 2006. Please submit to Laura ideas for symposia as soon as possible. I also want to acknowledge the chairs and members of our many standing committees. Without all of your participation, we would not exist. I wish you all an informative and productive Fall meeting.

AGRO SOCIAL HOUR

Co-sponsored by the Agrochemicals Division and *Pest Management Science*

YOU ARE INVITED TO THE EVENT OF THE 230^{TH} ACS NATIONAL MEETING
THE AGROCHEMICALS SOCIAL HOUR

When: Tuesday evening, 6:00-8:00 PM

Where: Room 103AV of the Washington DC Convention Center,

Program: 6:30-7:00PM

Welcoming Remarks – Allan Felsot, Division Chair

Introduction of Dr. Steve Duke, New Editor in Chief of *Pest Management Science*

Presentation of Agrochemical Education Awards for Graduate Student Travel by John Johnston, Education Committee Chair

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Professor Janice E. Chambers
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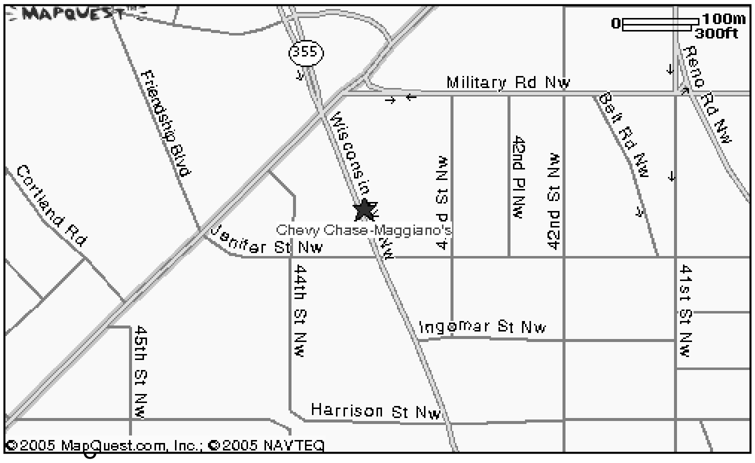

INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

PRESENTED BY THE AGROCHEMICAL DIVISION OF ACS

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Janice E. Chambers is the Director of the Center for Environmental Health Sciences, and is a William L. Giles Distinguished Professor in the College of Veterinary Medicine, Mississippi State University. She is originally from Berkeley, California. She holds an undergraduate degree in Biology from the University of San Francisco, and a Ph.D. in Animal Physiology from Mississippi State University. She held post-doctoral positions at Mississippi State University.

Jan has been the Principal Investigator of over $20 million in federally-funded competitive grants in the field of toxicology, with current or previous support from NIH, EPA, NSF and the American Chemistry Council. She has served on a number of advisory boards and committees, including the National Research Council Board of Toxicology, the International Life Sciences Institute/Health and Environmental Sciences Institute, the Society of Toxicology and the American Chemistry Council. She is or has been a peer review panel member for NIH and NIOSH, and a member of journal editorial boards. She has previously served for 3 years as Secretary for the Agrochemicals Division and has participated in AGRO program planning. She has held a number of committee positions in the Society of Toxicology and is currently the Secretary-Elect. She has received a Burroughs Wellcome Toxicology Scholar Award and a SmithKline Beecham award for Research Excellence, along with research awards at MSU. She is board certified in general toxicology by the American Board of Toxicology and she is a Fellow of the Academy of Toxicological Sciences. She is currently serving as a member of EPA's permanent Scientific Advisory Panel for FIFRA.

The Center for Environmental Health Sciences at MSU, which Jan directs, is an interdisciplinary research center specializing in pesticide toxicology and is supported primarily by the National Institutes of Health. This center has about 30 faculty, staff and students associated with it. Its research areas are neurotoxicology, biochemical toxicology, analytical chemistry, biostatistics, epidemiology, computational chemistry, computational simulation, biochemistry and endocrinology. Jan directs a mechanistic research program specializing in pesticide toxicology with a major emphasis on organophosphorus insecticides, and she has been involved in the training of about 40 graduate students and post-docs. She directs several research projects on the effects of pesticides in mammalian systems to identify the potential human health effects of pesticide exposures, and is primarily interested in the biochemical determinants of toxicity levels in adult and developing animals; her research addresses a number of FQPA issues. Her program emphasizes a consideration of the dose-response relationships, and for making predictions of toxicity based on realistic levels of pesticide exposure. Specifically, there are projects related to the neurochemical and behavioral effects of pesticides in developing organisms; the metabolism of pesticides in developing organisms; effects of chemical mixtures and the development of data related to cumulative risk assessment; mathematical predictions of the effects of mixtures; and exposure assessment of children and adults from contact with a pet dog which has been treated with flea control insecticides.

Jan has a long-term professional relationship with her husband, Howard Chambers, of MSU's Entomology and Plant Pathology Department, which has yielded joint grants, publications, and students, and many mechanistic conversations. The personal side of the relationship has yielded two beautiful and talented daughters, Kristen and Cheryl.

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Good science, no surprises.

2005
STERLING B. HENDRICKS MEMORIAL LECTURESHIP AWARD

Donald L. Sparks is an internationally renowned soil chemist, particularly recognized for his research on the kinetics of soil chemical processes, surface chemistry of soils and soil components using in-situ spectroscopic and microscopic techniques, and the physical chemistry of soil potassium. He is currently the S. Hallock du Pont Endowed Chair of Soil Chemistry and Frances Alison Professor at the University of Delaware.

Dr. Sparks pioneered the application of chemical kinetics to soils and soil minerals including development of widely used methodology, elucidation of rate-limiting steps and mechanisms, and coupling kinetic studies with molecular scale investigations. He was one of the first soil scientists to use synchrotron-based techniques, particularly bulk- and micro-focused x-ray absorption fine structure spectroscopy to directly speciate metals and oxyanions at soil mineral surfaces and in contaminated soils. He is widely recognized as one of the leaders in using these techniques to unravel many important soil chemical reactions and processes. His discoveries in the late 1990's on the formation and role of surface precipitates in the retention, fate and transport of trace metals such as nickel and zinc in natural systems have had major impacts in the areas of sorption models, metal speciation, and soil remediation/contamination. He and his group have recently speciated metals in hyper-accumulator plants.

In addition to carrying out fundamental research, Dr. Sparks has consistently applied his work to agricultural problems such as relating the kinetics of potassium, nitrogen, phosphorous, and boron to soil fertility and environmental quality. He also conducts research on the environmental fate of industrial contaminants as part of an ongoing program to devise safe and effective methods to dispose of these materials.

Dr. Sparks is author, co-author or editor of numerous publications including books, book chapters, and refereed publications. In addition to his research, he is well known as an extraordinary teacher and advisor of graduate students and postdoctoral researchers who are now becoming leaders in the soil and environmental sciences. Among his many honors and awards are President, International Union of Soil Sciences; President, Soil Science Society of America; Fellow, American Association for the Advancement of Science, Soil Science Society of America, and the American Society of Agronomy; Soil Science Research Award; M.L. and Chrystie M. Jackson Award in Soil Chemistry; Environmental Quality Research Award; Francis Alison Award, University of Delaware; and University of Delaware Outstanding Doctoral Graduate Advising and Mentoring Award.

The USDA-Agricultural Research Service will present Dr. Sparks with the Award which is co-sponsored by the Agrochemical and the Agricultural & Food Chemistry Divisions. Dr. Sparks will give an award address entitled, "Grand Challenges and Opportunities in the Environmental Sciences: the Importance of Basic Research and Technology." A reception will follow.

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AGROCHEMICAL EDUCATION AWARDS FOR GRADUATE STUDENT TRAVEL

Twelve graduate students have been awarded AGRO Division travel grants to present their research poster at the ACS National Meeting in Washington, DC. The first place winner will be announced at the Agrochemical Division's Social Mixer. Abstracts can be found on pp 64 – 67, AGRO 61 – 72.

G. E. Schultz	Repellency of catnip and Osage orange essential oils to two mosquito species. **G. E. Schultz**, J. Coats. Department of Entomology, Iowa State University, Ames, IA 50011
L. J. Gereszek	Effects of dietary conjugated linoleic acid on the European corn borer. **L. J. Gereszek**, J. R. Coats, D. C. Beitz. Department of Entomology, Iowa State University, Ames, IA 50011
D. K. Nomura	A brain detoxifying enzyme for organophosphorus nerve poisons. **D. K. Nomura**, D. Leung, K. P. Chiang, G. B. Quistad, J. E. Casida. Molecular Toxicology, University of California, Berkeley, 103 Wellman Hall, UC Berkeley, Berkeley, CA 94720
P. Kulshrestha	AEI: Mechanistic interpretation of molecular interactions of tetracycline with clay and organic matter using nuclear magnetic resonance, mass spectrometry, and attenuated total reflectance Fourier transform infrared spectroscopy. **P. Kulshrestha**, H. S. Atreya, D. Sukumaran, R. F. Giese Jr., T. D. Wood. Department of Geology and Chemistry, University at Buffalo, The State University of New York, 335 Natural Science Complex, Buffalo, NY 14260
Y. Cheng	Anaerobic bacterial degradation of agrochemicals in laboratory microcosms. **Y. Cheng**, A. Ogram. Soil and Water Science Department, University of Florida, 2169 McCarty Hall, Gainesville, FL 32611
K. L. Henderson	Bioavailability of tylosin in environmental matrices. **K. L. Henderson**, T. B. Moorman, J. R. Coats. Department of Entomology, Iowa State University, Ames, IA 50011
K. R. Prihoda	Development and characterization of improved extraction methods for transgenic Bt proteins from soil and sediment. **K. R. Prihoda**, B. W. Clark, B. D. Hopper, A. Jessick, J. R. Coats. Department of Entomology, Iowa State University, Ames, IA 50011
O. Bawardi	Enantiomeric sulfoxidation of the organophosphate pesticide fenthion in fish. **O. Bawardi**, B. Furnes, J. M. Rimoldi, D. Schlenk. Department of Environmental Sciences, University of California Riverside, 2217 Geology Building, Riverside, CA 92521
D. Hu	Environmental fate of tylosin and analysis of immunological cross-reactivity among tylosin isomers. **D. Hu**, K. L. Henderson, J. R. Coats. Dept. of Entomology, Iowa State Univ., Ames, IA 50011
S. K. Mohanty	Evaluation of the transport of selected contaminants in recycled water in tropical soil. **S. K. Mohanty.** Department of Civil and Environmental Engineering, University of Hawaii at Manoa, Honolulu, HI 96822
A. Goel	Modeling the variability in aerial concentrations of atrazine, endosulfan and chlorothalonil at a rural location on the Delmarva Peninsula. **A. Goel**, L. L. McConnell, A. Torrents. Department of Civil and Environmental Engineering, University of Maryland, 1173 Glenn L. Martin Hall, College Park, MD 20742
C. A. Curran	Responses of juvenile salmon to aquatic herbicides. **C. A. Curran**, J. M. Grassley, C. E. Grue. University of Washington, Washington Cooperative Fish and Wildlife Research Unit, School of Aquatic and Fisheries Sciences, Box 355020, Seattle, WA 98195

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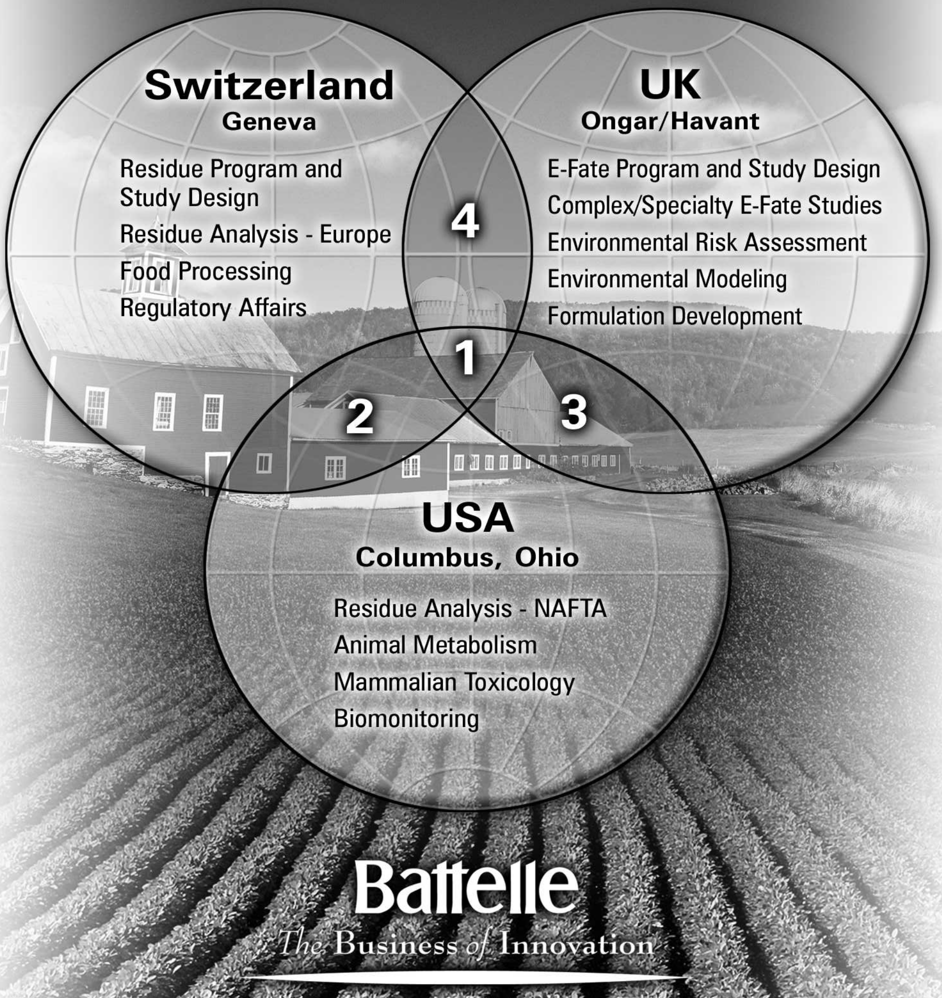

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Major Professor/Supervisor ____

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1. An extended abstract of your presentation (4 pages maximum including figures and tables) that clearly describes the nature of the work (hypothesis, methods, results), its relationship to previous research, and its significance for the field of agrochemicals.
2. An abstract of 150 words (submit directly to http://oasys.acs.org/oasys.htm); this short abstract will be printed in the Agrochemicals Division biannual publication, PICROGRAM.

MAIL OR FAX THIS SIGNED APPLICATION, & FAX OR EMAIL EXTENDED ABSTRACT TO:
Dr. Allan Felsot, Washington State University, FEQL, 2710 University Dr., Richland, WA 99354
(Phone: 509-372-7365; Fax: 509-372-7460; email: afelsot@tricity.wsu.edu)

****Deadline for submittal of application materials: November 5, 2005.**

NOTE: Two awards will be made based on the merits of the submitted applications. Applicants not winning the awards will be invited to present their research in the Young Scientist's Recognition Symposium and will be eligible to receive a small travel grant.

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Magnitude of Residue
Soil Dissipation

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Fish Bioconcentration
Marine & Fresh Water Organisms
Aquatic & Terrestrial Phytotoxicity
Sediment Toxicity Studies
Non-Target Insect Tests
Shellfish Residue Studies
Terrestrial Organisms

Environmental Fate/Metabolism

Photodegradation
Hydrolysis
Aquatic/Soil Metabolism
Aerobic/Anaerobic Metabolism
Plant & Animal Metabolism
AD/DE & Leaching
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Biodegradation Studies
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NOMINATION FORM
ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

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and DuPont Crop Protection (Fall)

I hereby nominate ________________________________ as a candidate for this award.
(First) (Middle) (Last)

Complete the following for your candidate:

1. Birthplace Date of Birth Citizenship
2. Business Address:
3. **IMPORTANT** Please Attach:
   a. A **Curriculum Vitae** for your candidate which describes the individual's career data including, places and nature of employment, professional affiliations, honors received, and a list of publications and patents. Please provide 11 copies.
   b. A **description** (200-1000 words) of the reasons why your nominee should receive this award, stressing the individual's major accomplishments.
   c. Nominations often include one or two letters of support, but this is optional.

Submitted by: ________________________ Date: ______________

Address: ____

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 at the spring meeting of ACS.

The nominating official(s) should be prepared to assist in organizing a symposium and dinner at the National ACS meeting in honor of the awardee.
Please, return this completed form to: Dr. James Seiber
USDA-ARS, WRRC
800 Buchanan St.
Albany, CA 94710
(510) 559-5600 – phone
(510) 559-5963 – fax
jseiber@pw.usda.gov

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CALL FOR NOMINATIONS

2006 STERLING B. HENDRICKS MEMORIAL LECTURESHIP

The Agricultural Research Service (ARS), USDA's primary research agency, is seeking nominations for the 2006 **Sterling B. Hendricks Memorial Lectureship**.

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.

Nominees may be outstanding, senior scientists in industry, universities, or government positions. Current ARS employees are not eligible. Nominations may be made by sending (1) a letter explaining the nominee's contributions to chemistry and agriculture and (2) a current curriculum vitae to:

Kim Kaplan, Lecture Coordinator
at either
kaplan@ars.usda.gov
or
ARS Information Office
Room 1-2253, Mail Stop # 5128
5601 Sunnyside Ave.
Beltsville, MD 20705

Electronic transmission is best; otherwise, use a carrier, such as FedEx. **The deadline for nominations is November 4, 2005**

The Lecture, on a scientific topic, trend, or policy issue of the Lecturer's choice, will be presented at the American Chemical Society Fall Meeting (San Francisco, CA, September 10 – 14, 2006). The Division of Agricultural & Food Chemistry and The Division of Agrochemicals co-sponsor the Lecture which will be held in a joint session of these divisions. The award includes an honorarium of $2000, a bronze medallion, and expenses to attend the meeting.

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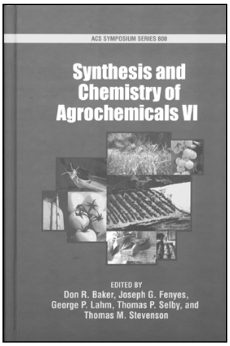

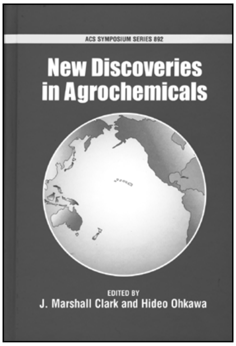

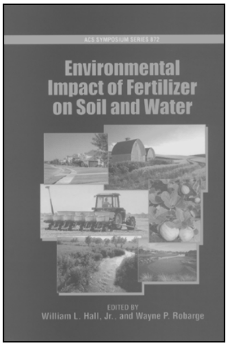

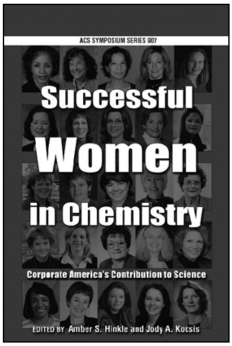

ENVIRONMENTAL FATE AND SAFETY MANAGEMENT OF AGROCHEMICALS

Edited by **J. Marshall Clark**, *University of Massachusetts*, and **Hideo Ohkawa**, *Kobe University*

Environmental Fate and Safety Management of Agrochemicals discusses residue analysis, environmental fate and safety management, environmental risk assessment, metabolism, resistance and management, and advances in formulation and application technology from the academic, government, and industry perspective.

(ACS Symposium Series No. 899)
(An American Chemical Society Publication)
2005 384 pp.
0-8412-3910-X ~~$144.50~~/**$86.70**

NEW DISCOVERIES IN AGROCHEMICALS

Edited by **J. Marshall Clark**, *University of Massachusetts, and* ***Hideo Ohkawa***, *Kobe University*

New Discoveries in Agrochemicals discusses molecular and combinatorial chemistry techniques impacting the aqrochemical sciences. Topics in include biopesticides and transgenic crops, combinatorial chemistry, mode of action, natural products, green chemistry, and human vector control.

(ACS Symposium Series No. 892)
(An American Chemical Society Publication)
2004 440 pp.
0-8412-3903-7 ~~$145.00~~/**$87.00**

ENVIRONMENTAL FATE AND EFFECTS OF PESTICIDES

Edited by **Joel R. Coats**, *Iowa State University*, and **Hiroki Yamamoto**, *Shimane University*

The third of three volumes based on the 2nd Pan-Pacific Conference on Pesticide Chemistry, this book examines metabolism and residue analysis methods of environmental pesticides.

(ACS Symposium Series No. 853)
(An American Chemical Society Publication)
2003 320 pp.
0-8412-3722-0 ~~$145.00~~/**$87.00**

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The goal of this book is to create a resource where women can find a role model, someone with whom they can relate. Profiling women with a wide diversity of experiences and career opportunities allows the reader to find a common connection. This series book highlight both the pleasant and unpleasant career experiences in the corporate arena and includes women whose careers range from the very technical and obvious to those that are not.

(ACS Symposium Series No. 907)
(An American Chemical Society Publication)
2005 208 pp..
0-8412-3912-6 ~~$74.50~~/**$44.70**

ENVIRONMENTAL IMPACT OF FERTILIZER ON SOIL AND WATER

Edited by **William L. Hall Jr.**, and **Wayne P. Robarge**

Fertilizers contribute to the variety, abundance, and low cost of food stuffs available to the public. However, fertilizer misuse can lower air, soil, and water quality. Regulators are scrutinizing fertilizers now more than ever because of their impact on the environment. This book provides an analysis of perchlorate in highly dissolved solid matrices and health issues of trace metals in fertilizers. This book focuses on nutrient impacts to water and the environment.

(ACS Symposium Series No. 872)
(An American Chemical Society Publication)
2003 296pp.
0-8412-3811-1 ~~$125.00~~/**$75.00**

SYNTHESIS AND CHEMISTRY OF AGROCHEMICALS

Edited by **Don R. Baker**, **Joseph G. Fenyes**, **George P. Lahm**, **Thomas P. Selby**, and **Thomas M. Stevenson**

This 30-chapter volume includes current updates and trends in the field of agrochemicals. Topics in the book include herbicides in agriculture, control of insects and acrids in agriculture, and control of fungal disease in agriculture.

(ACS Symposium Series No. 800)
(An American Chemical Society Publication)
2001 368 pp.
0-8412-3783-2 ~~$120.00~~/**$72.00**

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CALL FOR APPLICANTS
AGROCHEMICAL EDUCATION AWARDS

SUPPORT FOR GRADUATE STUDENT POSTER PRESENTATIONS AT THE 2006 FALL MEETING

The Division of Agrochemicals has established an endowment fund that will be used to promote an understanding of the role of chemistry in agriculture as embraced in the following areas related to pest management chemistry: synthesis, metabolism, regulatory, biotechnology, delivery, risk assessment, resistance, residues, mode of action, and fate/behavior. To address this mission, awards will be made through the Division's Education Committee.
Proposals are sought for the 2006 awards. Graduate students will be awarded up to $600 each to help defray costs of attendance to give poster or oral presentations at the ACS 2005 Fall Meeting, which will be held September 10 – 14, 2006, in San Francisco. Posters will be displayed in a special section of the Division of Agrochemicals' poster session as well as the ACS Sci-Mix. A winner and two runners up will be selected for display at the Division's Social. The winner will receive an additional cash award of $500. The subject of the presentation should fall within the areas listed in the introductory sentence.

To apply, a graduate student should submit the following, to be received no later than May 1, 2006:

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.
2. A 2-page extended abstract giving more detail of the research/presentation.
3. A letter of nomination from the faculty advisor.

Please submit the above electronically with the three items as attachments in either Word or Word Perfect to Dr. John J. Johnston at **john.j.johnston@aphis.usda.gov. If there are any questions, please contact Dr. Johnston at USDA/APHIS/National Wildlife Research Center, 4101 LaPorte Ave., Fort Collins, CO 80521, (970)-266-6082.** ***Abstracts will be reviewed by the Education Committee; submitters will be notified of their selection status in May 2006.***

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CALL FOR NOMINATIONS AGROCHEMICALS FELLOW AWARD

The Division has established the Fellow Award to recongnize its members whose deidicated 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 the 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. Contact the Awards Committee for further information.

Dr. James Seiber
USDA-ARS, WRRC
800 Buchanan St.
Albany, CA 94710
510-559-5600 – phone
510-559-5963 – fax
jseiber@pw.usda.gov

Deadline for submitting nominations is May 31 of each year.

PAST WINNERS OF THE AGROCHEMICALS FELLOW AWARD

11971	Dr. Louis Lykken
	Dr. Tom H. (Bucky) Harris
	Dr. Herman Beckman (Posthumous)
1972	Mr. Wendell F. (Bud) Phillips
	Dr. Don G. Crosby
	Dr. Elvins Y. Spencer
1973	Mr. Roger C. Blinn
	Dr. Philip C. Kearney
	Dr. Julius J. Menn
1974	Dr. Morton Beroza
	Dr. James P. Minyard, Jr.
	Dr. Joe C. Street
1975	Dr. Hank F. Enos
	Dr. Maurice B. Green
	Dr. Charles H. Van Middelem
1976	Dr. Marguerite L. Leng
	Dr. Jack R. Plimmer
	Dr. Gerald G. Still
1977	Dr. Gustave K. (Bob) Kohn
1978	Dr. S. Kris Bandal
	Dr. Paul Hedin
1979	Dr. Rodney D. Moss
1980	Dr. G. Wayne Ivie
	Dr. John B. Siddall (Posthumous)
1981	Dr. Robert M. Hollingworth
	Dr. Gino J. Marco
1983	Dr. John Harvey, Jr.
1985	Mr. Henry Dishburger
	Dr. Richard C. Honeycutt
1986	Dr. Gunter (Jack) Zweig
1987	Dr. Willa Garner
1988	Dr. Jan Chambers
	Dr. James Seiber
1990	Dr. Joseph Fenyes
1991	Dr. Nancy N. Ragsdale
1992	Dr. Don Baker
	Dr. Joel Coats
	Dr. Guy Paulson
1993	Dr. Larry Ballantine
1994	Dr. James Heitz
	Dr. Ralph Mumma
	Dr. Willis Wheeler
1996	Dr. John Bourke
1998	Dr. Hank Cutler
	Mr. Paul Giesler
2000	Dr. Barry Cross
2005	Dr. Rodney Bennett

PAST AWARDEES OF
THE STERLING B. HENDRICKS MEMORIAL LECTURSHIP
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1981 Norman E. Borlaug, Nobel Laureate and Director of International Maize and Wheat Improvement Center, Mexico City.
1982 Warren L. Butler, Professor of Biology and Past Chairman, Biology Department, University of California at San Diego.
1983 Melvin Calvin, Nobel Laureate and University Professor of Chemistry, University of California at Berkeley.
1984 Frederick Ausubel, Professor of Genetics, Harvard Medical School and Massachusetts General Hospital.
1985 Alan Putnam, Professor, Department of Horticulture and Pesticide Research Center, Michigan State University.
1986 Ralph Hardy, President, Boyce Thompson Institute for Plant Sciences, Cornell University, and Deputy Chairman, BioTechnica International.
1987 Mary-Dell Chilton, Director of Biotechnology Research for Ciba-Geigy Corporation, Research Triangle Park, North Carolina.
1988 Bruce N. Ames, Chairman, Department of Biochemistry, University of California at Berkeley.
1989 Sanford A. Miller, University of Texas Health Science Center at San Antonio.
1990 Roy L. Whistler, Emeritus Professor of Purdue University.
1991 Peter S. Eagleson, Professor of Civil Engineering, Massachusetts Institute of Technology.
1992 John E. Casida, Professor of Chemistry and Toxicology, University of California at Berkeley.
1993 Philip H. Abelson, Deputy Editor, *Science*, and Scientific Advisor to AAAS.
1994 Wendell L. Roelofs, Liberty Hyde Bailey Professor of Insect Biochemistry, Cornell University.
1995 Winslow R. Briggs, Director Emeritus, Department of Plant Biology, Carnegie Institution of Washington.
1996 Hugh D. Sisler, Professor Emeritus, Department of Plant Biology, University of Maryland.
1997 Ernest Hodgson, Head, Department of Toxicology, North Carolina State University.
1998 Martin Beroza, Chief, Organic Chemicals Synthesis Laboratory, Agricultural Research Service.
1999 Bruce D. Hammock, Professor, Department of Entomology, University of California at Davis.
2000 William S. Bowers, Professor, Department of Entomology and Chemical Ecology at the University of Arizona.
2001 Malcolm Thompson, Research Chemist, USDA-ARS, Beltsville, MD (retired)
2002 Ervin E. Leiner, Professor Emeritus, Biochemistry Department, University of Minnesota.
2003 Dr. Kriton Kleanthis Hatzios, VA Agricultural Experiment Station
2004 Dr. Robert L. Buchanan, Food & Drug Administration

PAST AWARDEES OF THE BURDICK AND JACKSON INTERNATIONAL AWARD

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

PAST WINNERS OF THE ACS INTERNATIONAL AWARD FOR RESEARCH IN AGROCHEMICALS

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1993-Spring	Dr.Morifuso Eto, Kyushu University, Fuoka, Japan
1994-Fall	Dr. Toshio Fujita, Kyoto University, Kyoto, Japan
1995-Spring	Dr. Mohyee Eldefrawi, University of Maryland, Baltimore
1995-Fall	Dr. Koji Nakanishi, Columbia University, New York
1996-Spring	Dr. Günther Voss, Ciba, Basel, Switzerland
1996-Fall	Dr. Klaus Naumann, Bayer, Leverkusen, Germany
1997-Spring	Dr. Fritz Führ, Jülich, Germany
1997-Fall	Dr. Izuru Yamamoto, University of Tokyo, Japan
1998-Spring	Dr. George Levitt, DuPont, Wilmington, DE
1998-Fall	Dr. Leslie Crombie, University of Nottingham, England
1999-Spring	Dr. Don Baker, Zeneca, Richmond, CA
1999-Fall	Dr. James Seiber, University of Nevada, Reno
2000-Spring	Dr. George P. Georghiou, University of California, Riverside
2000-Fall	Dr. Herbert B. Scher, Zeneca
2001-Spring	Dr. Donald Crosby, University of California, Davis
2001-Fall	Dr. Ralph Mumma, Pennsylvania State University
2002-Spring	Dr. Keith Solomon, University of Guelph, Ontario, Canada
2002-Fall	Dr. Marinus Los, American Cyanamid
2003-Spring	Dr. Bob Hollingworth, Michigan State Universtiy
2003-Fall	Dr. Hideo Ohkawa, Kobe University, Japan
2004-Spring	Dr. Stephen Duke, USDA-ARS, Oxford, Mississippi
2004-Fall	Dr. John Marshall Clark, University of Massachusetts
2005-Spring	Dr. Robert Krieger, University of California, Riverside

AWARDS COMMITTEE REPORT

Dr. Janice Chambers, College of Veterinary Medicine, Mississippi State University, will receive the International Award for Research in Agrochemicals at the fall 2005 ACS meeting. This Award is sponsored by DuPont Crop Protection. The award presentation will take place first thing Monday morning, followed by an award symposium on pesticide biochemistry and toxicology organized by Ernest Hodgson.

Laura McConnell should be contacted for information/reservations for the Monday evening Award dinner at 301-504-6298; email: mcconnel@ba.ars.usda.gov. See page 8 for further details.

Dr. Joel Coats, Iowa State University, will receive the International Award for Research in Agrochemicals at the spring 2006 ACS meeting, to be held in Atlanta, GA. This Award is sponsored by DuPont Crop Protection. An award symposium around the general topic of environmental toxicology and chemistry of agrochemicals including insect toxicology is being organized by Aldos Barefoot to recognize Dr. Coat's contributions in these areas.

Dr. Isamu Yamaguchi, Plant Sciences Center, Riken (Japan) will receive the International Award for Research in Agrochemicals at the Fall 2006 ACS meeting to be held in San Francisco, CA for his research in the chemistry of pest management, particularly the biochemistry of fungicidal action. Nancy Ragsdale and Fumio Matsumura will organize the award symposium in Dr. Yamaguchi's honor. This award will be sponsored by BASF Corporation.

Nominations for the 2007 International Award for Research in Agrochemicals are currently being solicited by the Awards Committee. The Awards Committee is accepting new awards nominations for both the International Award for Research in Agrochemicals and for the Division Fellow Award. The nomination forms for both are found in the Picogram. Please consider nominating a deserving colleague. The deadlines each year are December 31 for the International Award and May 31 for the Fellow Award.

Congratulations to Drs. Chambers, Coats and Yamaguchi!

Respectfully submitted,

Jim Seiber

James N. Seiber, Chair
Awards Committee

Notes from the Program Chair

DON WAUCHOPE

The Washington DC AGRO program will have 152 papers—the largest number we have had in some time. This is due to the great work of our special Symposia Organizers, who have corralled speakers and put together a really outstanding, very diverse and timely collection of sessions.:

Thinking Ahead. Laura McConnell will be program chair for 2006: mcconnel@ba.ars.usda.gov. This is the time to think about that symposium you've always wished to see at an AGRO meeting. Give her an email or work up a one-page proposal for the Business Meeting this August. Symposia are the heart of our programs, and *organization of a symposium only happens when some individual gets a bright idea for one and then takes the initiative to propose it.* What area would you like to see highlighted at our next meeting?

I urge you to look over the program in detail, move around the venue, and sample the fare. Note that ALL PROGRAMS WILL BE AT THE CONVENTION CENTER; we are pleased that ACS was able to meet our request to be at the center of things this year, and the AGFD division will also be close by. I look forward to seeing you there. Below is the Fall 2005 schedule (A=AM, P=PM; D=AM & PM, PE=PM & EVE, E=EVE).

SYMPOSIUM OR SESSION	ORGANIZER(S)	Sun	Mon	Tue	Wed	Thu
General Posters	Don Wauchope	A				
Agrochemical Residue and Metabolism Chemistry	Teresa A. Wehner John J. Johnston David Smith	D				
Agrochemical Development from Lab to Field	John W. Lyga George Theodoridis	P				
Biochemical Toxicology of Agrochemicals: Symposium in Honor of Janice Chambers, ACS International Awardee for Research in Agrochemicals Sponsored by DuPont Crop Protection	Ernest Hodgson		D			
Modern Chiral Pesticides: Enantioselectivity And Its Consequences	Wayne Garrison Ron Williams		D			
Agrochemical Education Awards For Graduate Student Travel: Research Poster Presentations	John J. Johnston		P			
Sci-Mix	Don Wauchope		E			
Turfgrass: Pesticide Exposure Assessment and Predictive Modeling Tools	Mary Nett			D	D	
Control of Invasive Species: Regulatory Concerns and Achievements	Anne Leslie			D		
2005 Sterling B. Hendricks Award	Nancy Ragsdale				A	
Biological Pest Control: The Continuum	Paul L. Zubkoff				D	
(Q)SAR in Today's Agrochemistry** (COMP)	Bob Clark					A
General Oral Presentations	Don Wauchope					D
New Nutrient and Soil Amendment Products Impacting Agricultural Production and the Environment	Bill Hall					P
Current Frontiers of Fluoroorganic Chemistry (Primary Sponsor: FLUO)	Koichi Mikami Vadim Soloshonok	PE	D			

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Synthesis-Special Topics Standing Program	J. Fenyes D. Baker	(901) 278-0330 (510) 231-1093	**Biotechnology**	J. Seiber J. Nelson W.P. Ridley	(702) 784-6460 (301) 405-3919 (314) 694-8441
Residues-Special Topics	J.J. Johnston	(970) 266-6082	**Toxicology**	J.M. Clark J. Coats	(413) 545-1052 (515) 294-4776
Standing Program	T.A. Wehner	(732) 729-5713	**Regulation**	N. Ragsdale	(301) 504-4509
Metabolism-Special Topics	H. Cutler	(770) 986-3240	**Special Conferences**	J.M. Clark	(517) 545-1052
Mode of Action	R. Hollingworth J.M. Clark	(517) 533-9430 (413) 545-1052	**ACS Awards Symposia**	J. Seiber	(510) 559-5600
Environmental	R. Honeycutt J. Seiber A. Felsot	(336) 294-5559 (702) 784-6460 (509) 375-9365	**Young Scientists Award**	A. Felsot	(509) 372-7365
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AGRO 2006
CALL FOR SYMPOSIA & GENERAL PAPERS

The following are symposia currently in place for the 2006 ACS National Meetings in Atlanta and San Francisco. Proposals for additional symposia are now being accepted. Please contact:

Dr. Laura McConnell, AGRO Program Chair
Environmental Quality Laboratory
USDA-Agricultural Research Service
10300 Baltimore Ave
Bldg. 007, Rm. 225 BARC-W
Beltsville, MD 20705
e-mail: mcconnel@ba.ars.usda.gov
Phone: (301) 504-6298
Fax: (301) 504-5048

231st ACS NATIONAL MEETING
ATLANTA, GA
MARCH 26 – 30, 2006

Advances in Pesticide Environmental Fate and Exposure Assessments
Organizers: Ellen Arthur, Bayer CropScience, ellen.arthur@bayercropscience.com, (913) 433-5328
Patricia Rice, BASF Corporation, ricep@basf-corp.com, (919) 547-2668
Pamela Rice, USDA-ARS, pamrice@umn.edu, (612) 624-9210
Dan Dyer, Bayer CropScience
Aldos Barefoot, DuPont
K. Balu, Waterborne Environmental Inc.
Glenn Miller, University of Nevada

Pesticide Degradates: Formation, Environmental Occurrence, and Human and Ecological Risks
Organizers: Thomas Potter, USDA-ARS, Tifton, GA; tpotter@tifton.usda.gov; (229) 386-7073
Joel Coats, Iowa State University, Ames IA; jcoats@iastate.edu
Robert Zablotowicz, USDA-ARS, Stoneville, MS; rzablotowicz@ars.usda.gov; (662) 686-5272
Jason Krutz, USDA-ARS, Stoneville, MS; jkrutz@ars.usda.gov; (662) 686-3670

ACS International Award for Research in Agrochemicals
Symposium in Honor of Joel Coats
Organizers: Ralph Mumma, Pennsylvania State University, rom1@psu.edu
Ellen Arthur, Bayer CropScience, ellen.arthur@bayercropscience.com, (913) 433-5328
Pamela Rice, USDA-ARS pamrice@umn.edu, (612) 624-9210

Young Scientist Pre- and Post-Doctoral Research Award Symposium
Organizer: Allan Felsot, Washington State University, FEQL, 2710 University Dr., Richland, WA 99354, Phone: (509) 372-7365; Fax: (509) 372-7460; afelsot@tricity.wsu.edu

General Oral Presentations
Organizer: Laura McConnell

General Posters
Organizer: Laura McConnell

AGRO 2006
CALL FOR SYMPOSIA & GENERAL PAPERS
(continued)

232nd ACS NATIONAL MEETING
SAN FRANCISCO, CA
SEPTEMBER 10 – 14, 2006

Alternatives to the Use of Methyl Bromide in Pre-Plant Soil Fumigation and Stored Commodities
Organizers: Luis Ruzo, PTRL West, (510) 741-3000 ext 228, l.ruzo@ptrlwest.com
Rodney Bennett, Cerexagri, (610) 878-6476, email: rodney.bennett@cerexagri.com

Plant Response to Biotic Insults
Organizers: Ralph O. Mumma, rom1@psu.edu
James H. Tumlinson, jht2@psu.edu
Gary W. Felton, gwf10@psu.edu
Department of Entomology, Chemical Ecology Laboratory, Pennsylvania State University

Agricultural Impacts on Air Quality: Pesticides, Pharmaceuticals, PM, VOCs, and Odors
Organizers: Laura McConnell, USDA-ARS, mcconnel@ba.ars.usda.gov (301) 504-6298
Cathleen Hapeman, USDA-ARS, hapemanc@ba.ars.usda.gov
James Seiber, USDA-ARS, jseiber@pw.usda.gov
Michael Majewski, USGS, majewski@usgs.gov

ACS International Award for Research in Agrochemicals
Symposium in Honor of Isamu Yamaguchi
Organizer: James Seiber, USDA-ARS, jseiber@pw.usda.gov

Sterling B. Hendricks Memorial Lecture
Organizer: Kim Kaplan, USDA-ARS, kaplan@ars.usda.gov

Agrochemical Education Awards For Graduate Student Travel
Research Poster Presentations
Organizer: J. J. Johnston, USDA-APHIS, john.j.johnston@aphis.usda.gov, (970) 266-6082

General Oral Presentations
Organizer: Laura McConnell

General Posters
Organizer: Laura McConnell

CALL FOR PAPERS

Pesticide Degradates: Formation, Environmental Occurrence, and Human and Ecological Risks

American Chemical Society 231st National Meeting
Atlanta, GA
March 26 – March 30, 2006

This symposium is designed as an update to the symposium sponsored by the Agrochemical Division in 1990 at the 200th National Meeting held in Washington, D.C.

Pesticide degradates in the environment remains a significant topic. Advances in instrumentation in particular HPLC-MS and nationwide monitoring programs such as the USGS NAQWA program have greatly expanded knowledge and understanding of this topic.

This symposium is intended to bring together current knowledge. Papers are requested on the following topics:

- Identification of degradates of novel and conventional active ingredients
- Mechanisms and kinetics of degradates formation and dissipation
- Environmental occurrence of degradates - soil, sediment, water, atmosphere
- Use of environmental forensic techniques in degradate assessments
- Other related topics including assessments of human and ecological risks

To submit proposed papers or posters, please contact one of the co-organizers:

Thomas Potter, USDA-ARS, Tifton, GA; tpotter@tifton.usda.gov; (229) 386-7073
Joel Coats, Iowa State University, Ames IA; jcoats@iastate.edu
Robert Zablotowicz, USDA-ARS, Stoneville, MS; rzablotowicz@ars.usda.gov; (662)686-5272
Jason Krutz, USDA-ARS, Stoneville, MS; jkrutz@ars.usda.gov; (662) 686-3670

CALL FOR PAPERS

Advances in Pesticide Environmental Fate and Exposure Assessments

American Chemical Society 231st National Meeting
Atlanta, GA
March 26 – March 30, 2006

The Agrochemicals Division is pleased to sponsor a symposium addressing the advances made in assessment of pesticide environmental fate and exposure. The focus of this symposium is on advances in environmental fate research, study designs, modeling, and monitoring that affect pesticide environmental risk assessments.

Some suggested topics are:

Environmental Fate

- Dissipation of pesticides in watersheds, field-scale studies, small-scale outdoor studies or laboratory studies
    - Degradation, hydrolysis, photolysis, metabolism in soil and aquatic systems, characterization and effects of biological activity in soil, kinetic analysis of degradation and dissipation rates, evaluation of major and relevant metabolites, impact of research advances on regulatory guidelines and harmonization
- Translocation and availability
    - Infiltration, runoff, volatilization, sorption/aged sorption, column leaching, and lysimeters

Exposure Assessments

- Use of data in exposure and risk assessments
    - Model inputs, comparisons of lab and field data and/or model results

To submit proposed papers or posters, please contact one of the co-organizers:

Ellen Arthur, Bayer CropScience, ellen.arthur@bayercropscience.com, (913) 433-5328
Patricia Rice, BASF Corporation, ricep@basf-corp.com, (919) 547-2668
Pamela Rice, USDA-ARS, pamrice@umn.edu, (612) 624-9210
Dan Dyer, Bayer CropScience
Aldos Barefoot, DuPont
K. Balu, Waterborne Environmental Inc.
Glenn Miller, University of Nevada

CALL FOR PAPERS

Plant Response to Biotic Insults

American Chemical Society 231st National Meeting
Atlanta, GA
March 26 – March 30, 2006

Purpose of Symposium

Plants chemically respond to biotic insults (insects, bacteria, fungi, and animals) by stimulating their defensive mechanisms. Sometimes the defense response occurs even though the stimulus is to an adjacent plant. These unique complex chemical signals result in tritropic interactions. There has recently been tremendous activity and accomplishments in this field and already several companies have commercial products stimulating plant defenses. As we further understand the fundamental relationships between plants and their environment, only then can we incorporate these data in our pest management schemes.

Possible Topics
- Insect, Bacteria, Fungi-Plant Interactions
- Tritropic Insect-Plant Interactions
- Chemical Signals
- Biotic/Abiotic Relationships
- Plant Defensive Chemistry
- Mechanisms of Plant Response to Stress
- Commercialization of Products

For additional information contact the organizers:

Ralph O. Mumma, rom1@psu.edu
James H. Tumlinson, jht2@psu.edu
Gary W. Felton, gwf10@psu.edu
Department of Entomology
Chemical Ecology Laboratory
Pennsylvania State University
University Park, PA 16802

CALL FOR PAPERS

Alternatives to the Use of Methyl Bromide in Pre-Plant Soil Fumigation and Stored Commodities

American Chemical Society 232nd National Meeting
San Francisco, CA
September 10 – 14, 2006

Purpose of Symposium

To examine the various chemicals and processes being currently evaluated as potential methyl bromide replacements from the point of view of their chemical and environmental behavior, efficacy and toxicology

Suggested Topics:

For chemicals used as fumigants:

- Physico-chemical properties, environmental fate and metabolism, analytical techniques
- Environment monitoring and exposure, emission control, efficacy and toxicology
- Regulatory requirements and registration status

For processes:

- Methodology and efficacy of solarization, heat treatment, composting and other procedures aimed at minimizing or eliminating the need for chemical treatment of soils and stored products

For additional information contact the organizers:

Luis Ruzo, PTRL West, (510) 741-3000 ext 228, l.ruzo@ptrlwest.com
Rodney Bennett, Cerexagri, (610) 878-6476, rodney.bennett@cerexagri.com

PACIFICHEM 2005

PACIFICHEM 2005

Honolulu, Hawaii, USA, December 15-20, 2005

SYMPOSIUM 225

Rational Methods for the Selection and Use of Agrochemicals: Risk Modeling, Monitoring and Management

This symposium will examine the behavior in the environment of insecticides, herbicides and pharmaceuticals and the development of rational methods aimed at reducing their overall impacts on trade and human and environmental health, whilst promoting their efficacy.

The three half-day sessions of oral presentations and an evening poster session will cover the following themes,

i) Risk assessment using fugacity modeling and other methods to estimate the risk of exposure of produce, the environment and humans,

ii) Improving analytical techniques for monitoring contaminants, emphasizing rapid methods derived from biotechnology such as ELISA to supplement instrumental methods, providing feedback allowing better choices to be made,

iii) Risk management as a guide to environmental policy, seeking practical solutions through better practice and remediation.

The overall aim of the symposium will be to generate a set of rational principles for selection of the best agrochemicals to use in particular scenarios and to encourage the registration of new chemicals with reduced risks. Each session will begin with an invited keynote speaker and subsequent papers will develop the main theme, ranging from research chemistry, regulatory methods, and the role of better methods encouraging commerce and trade.

Speakers include Don Mackay, Keith Solomon, Chris Hall, Gerry Stephenson (CA), Bruce Hammock (USA), Nick Schofield, Mark Silburn, Bruce Simpson, Alice Lee, Angus Crossan (AUS), Shuo Wang (CH), and Paco Sanchez-Bayo (JP).

Please visit the Pacific Basin website http://www.pacifichem.org/ for a complete listing of symposia in the Agrochemical as well as other divisions and for registration and housing information.

11th IUPAC International Congress of Pesticide Chemistry, Kobe, JAPAN, 2006

Evolution for Crop Protection,
Public Health and Environmental Safety

Sunday, August 6 to Friday, August 11, 2006
Kobe International Conference Center and Kobe Portopia Hotel

The Congress aims to bring together scientists who study chemistry, biology, toxicology and environmental science of crop protection, vector control and environmental health issues from all over the world in order to present achievements of science and technology, and exchange opinions about pesticide chemistry and bioscience. The sessions will include plenary and session lectures, workshops, poster presentations, luncheon/evening seminars and a commercial exhibition.

Sponsoring Organizations
The International Union of Pure and Applied Chemistry
Pesticide Science Society of Japan

The meeting will be split into topic areas (Categories I, II, & III) and workshops on emerging issues. Each will be comprised of session lectures, poster sessions, selected poster and oral presentations, and discussions.

Category I: Drug Design Based on Agrogenomics, Biopesticides and Transgenic Crop, New Chemistry, Natural Products, Bioregulator for Crop Protection (PGR, Fertilizers etc), Control Agents for Vectors of Communicable Diseases

Category II: Mode of Action and Resistance Mechanism - insect control, Mode of Action and Resistance Mechanism - weed control, Mode of Action and Resistance Mechanism - plant disease control, Advanced in Formulation and Application Technology, Metabolism and Toxicology, Resistance Management and IPM

Category III: Environmental Chemistry/Residue Analysis, Environmental Risk Assessment, Regulatory Aspects, and Risk Communication, Environmental Fate and Ecological Effect, Monitoring and Remediation of Persistent Organic Pollutants,

Workshops on Emerging Issues: Emerging Technologies in Crop Protection and Production, Genomics, Proteomics, and Metabolomics, Emerging Global Food Quality and Human Health Protection Issues, Global Food Safety and Trade Issues

Application forms and deadlines will be announced in the 3rd Circular
and on the official home page in August 2005.

www.iupac2006.jtbcom.co.jp

OFFICERS AND COMMITTEES OF THE DIVISION OF AGROCHEMICALS

AGRO Division Officers

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Dr. Laura L. McConnell, **Vice Chair**	(301) 504-6298	(301) 504-5048	mcconnel@ba.ars.usda.gov
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Dr. Terry Spittler, **Treasurer**	(315) 787-2283	(315) 787-2320	tds2@cornell.edu

FERT Subdivision Officers

Dr. Wayne Robarge, **Chair Elect**	(919) 515-1454	wayne_robarge@ncsu.edu
William Herz, **Vice Chair**	(202) 515-2706	wcherz@tfi.org
Herb MacKinnon, **Secretary**	(813) 989-2267	hmackin1@tampabay.rr.com

Executive Committee

2003-2005	**2004-2006**	**2005-2007**
Dr. Todd Anderson	Dr. Randy Weintraub	Dr. Matthew Brooks
Dr. Kevin Armbrust	Dr. Jeff Bloomquist	Dr. Marty Kovacs
Dr. Jeff Jenkins	Dr. John Clark	Dr. Ann Lemley
Dr. Laura McConnell	Dr. Kenneth Racke	Dr. Teresa Wehner
Dr. Scott Senseman	Dr. Pamela Rice	Dr. Paul Zubkoff
Dr. Luis Ruzo		

Councilors

2004-2007	2005-2008
Dr. Barrington Cross, Councilor	Dr. Joel Coats, Councilor
Dr. Judd Nelson, Alt. Councilor	Dr. Nancy Ragsdale, Alt. Councilor

Division Committees

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Dr. Don Baker
Dr. John M. Clark
Dr. Joel Coats
Dr. Barry Cross
Dr. Allan Felsot
Dr. Rick Grazzini
Dr. Robert Hollingworth
Dr. Mark S. Lee
Dr. Judd Nelson
Dr. James Seiber
Dr. David J. Smith

FERT Program Committee

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Dr. Wayne Robarge
Ms. Michelle Nutting
Dr. Gary Pierzynski
Mr. William Herz

Nominating Committee

Dr. Jeanette Van Emon, **Chair**	(702) 798-2154	(702) 798-2243	vanemon.jeanette@epa.gov

Dr. Jeff Jenkins
Dr. Terry Spittler

Membership Committee

Dr. Randy Weintraub, **Co-Chair**	(610) 878-6472	(610) 878-6475	randy.weintraub@cerexagri.com
Dr. Christopher Peterson, **Co-Chair**	(662) 338-3104	(662) 338-3101	cjpeterson@fs.fed.us

OFFICERS AND COMMITTEES OF THE DIVISION OF AGROCHEMICALS

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Dr. Terry Spittler, Ex Officio	(814) 272-1039	(814) 272-1019	ROM1@psu.edu
Dr. Don Baker	Dr. Willis Wheeler		Dr. Willa Garner
Dr. Ralph Mumma			

Awards Committee

Dr. James Seiber, **Chair**	(510) 559-5600		jseiber@pw.usda.gov
Dr. John Casida	Dr. Ernest Hodgson		Dr. Fritz Fuehr
Dr. Bruce Hammock	Dr. Jim Tumlinson		Dr. Nancy Ragsdale
Dr. Robert Hollingworth	Dr. Willis Wheeler		Dr. Izuru Yamamoto
Dr. Ralph Mumma			

Publications Committee

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Dr. Cathleen Hapeman	(301) 504-6451	(301) 504-5048	hapemanc@ba.ars.usda.gov

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Dr. Aldos Barefoot, **Social Hour**	(302) 451-5856	(302) 451-5941	aldos.c.barefoot@usa.dupont.com
Dr. Jeff Jenkins, **Social Hour**	(541) 737-5993	(541) 737-5001	jeffrey.jenkins@orst.edu

Special Committees

By-laws Committee

Dr. Don Baker, **Chair**	(925) 254-108

Committee on Patron Relations

Dr. Luis Ruzo, **Chair**	(510) 741-3000	(510) 741-3030	l.ruzo@ptrlwest.com
Mr. Paul Giesler			

Future Special Conference Committee

Dr. John M. Clark, **Chair**	(413) 545-1052	Dr. Robert Hollingworth

Public Relations Committee

Dr. Jeff Jenkins , **Chair**	(541) 737-5993	(541) 737-5001	jeffrey.jenkins@orst.edu
Dr. James Seiber	Dr. Ann Lemley		

Education Committee

Dr. John Johnston, **Chair**	(970) 266-6082	(970) 266-6089	John.J.Johnston@aphis.usda.gov
Dr. John Bourke**, Investment Coordinator**			
Dr. Allan S. Felsot, **Young Scientist Recognition Coordinator**	(509) 372-7365	(509) 372-7460	afelsot@tricity.wsu.edu
Dr. John M. Clark	Dr. Joel Coats		Dr. Barry Cross
Dr. Vincent Hebert	Dr. Ann Lemley		Dr. Glenn Miller
Dr. Judd O. Nelson	Dr. Jack R. Plimmer		Dr. Nancy Ragsdale
Dr. William Ridley	Dr. David Barnekow		Dr. J. Harold Falls

Long Range Planning Committee (Ad Hoc)

Dr. Don Wauchope	(229) 386-3892	(229) 386-7215	don@tifton.usda.gov
Dr. Rod Bennett	Dr. Allan Felsot		Dr. Dave Barnakow

MINUTES FROM THE AGROCHEMICAL DIVISION COMBINED GOVERNANCE MEETING

ACS 229th ACS Annual Meeting – San Diego
Sunday, March 13, 2005, 5:00 pm – 10:05 pm
Agrochemicals Division – Allan Felsot, Chair

Program Planning

Allan Felsot called the meeting to order at 5:00 pm. Members in attendance introduced themselves, and the Secretary passed around a sign up sheet. The sign-up sheet is retained in the archives. Terry Spittler asked for volunteers for the AGRO desk to answer questions about the division, sell books, and seek new members. The meeting continued with a presentation on programming.

San Diego Update - Don Wauchope

There are 115 papers & posters in 8 symposia. The program includes the International Award Symposium (sponsored by BASF) in honor of Robert Krieger, a symposium on *Metabolomics*, a general paper session and general poster session. The Young Scientist Award Symposium has 15 posters, and FERT organized two symposia on *Organic Farming and Nutrients* and *Monitoring of Specialty and Agricultural Products affecting Air, Water and Soil.* Don organized a symposium on *Agricultural Chemistry in the Classroom* for the Chemical Education Division.

Washington Program – 230th ACS National Meeting, August 28 – Sept 1, 2005 - Don Wauchope

There are 13 symposia proposed for Washington. OASys is open with a deadline of end of April for abstracts. The Sterling Hendricks Memorial Lectureship Award will be presented to Donald Sparks. The International Award symposium (sponsored by DuPont) will be held in honor of Janice Chambers. The program will include the Graduate Student Research Poster Competition, and 12 other symposia covering biological pest control, agrochemical discovery, residue and metabolism chemistry, chiral pesticides, invasive species, pesticide exposure assessment and predictive modeling and fate of turf grass nutrient in urban environment and FERT organized symposia on air monitoring programs, homeland security in agriculture and water quality protection.

Atlanta and Beyond - Don Wauchope, Laura McConnell, Wayne Robarge

The symposium on Advances in pesticide environmental fate has been moved to Atlanta to minimize overlap with other symposia planned for Washington. Ralph Mumma is working on a symposium on plant stress and chemical responses or on plant insect interactions. Joel Coats and Tom Potter are planning a session on Metabolites of Veterinary Chemicals in the Environment. Will Ridley, Doug Sammons and Allan Felsot will organize Weed Resistance to Herbicides. The Young Scientist and International Award will be held as usual.

Two symposia were proposed for the San Francisco meeting: FERT will organize a program on perchlorate, while Luis Ruzo and Rod Bennett propose a symposium on fumigants.

Special Programming

Pan-Pacific Conference - 2004

John Clark reported that ACS Symposium Series books from the conference have been published and should be available at the AGRO table. AGRO sustained about a $4000 loss, as there were unexpected costs up to the last minute.

Pan Pacific Conference - 2008

The new ACS Office of Congress Management and Vendor Relations will be able to assist with the conference. Barry has a sample contract letter from Nancy Todd of ACS OCMVR. We expect the conference to attract 100-175 people. Barry proposes that AGRO begin planning for the conference and meet with Nancy in June, 2005 to begin the process. The Pan Pacific conference organizing committee should include representatives from the Japanese Pesticide Society, Korean Pesticide Society, Australian Pesticide Society, and Chinese Pesticide Society. The following motion was made by Barry Cross, seconded by John Clark, and passed by the executive committee:

Motion:

The Agrochemicals Division agrees to co-sponsor the 4th Pan Pacific Conference in 2008 and authorized the Treasurer to sign a contract with ACS Office of Conference Management and Vendor Relations to manage the logistics.

Al Barefoot agreed to be Conference Chair; Joel Coats, Program Chair.

Mid-Atlantic Regional Meeting, Rutgers, May 22-25, 2005, www.marmacs.org

AGRO agreed to support the meeting and send AGRO representatives.

2006 IUPAC International Pesticide Congress

Ken Racke gave a presentation on IUPAC, the status of the 2006 Congress and a proposal for hosting the 12th Congress. The 2006 Congress will be held in Kobe and has been organized into topics in three areas with workshops, poster sessions, and an exhibition. Further information can be found at http://www.iupac2006.jtbcom.co.jp/.

The deadline for submitting a proposal (2-3 pages) for hosting the 2010 congress is October. The proposal should include theme, dates (reminder: August is EU holiday month), estimated size, venue, housing, co-sponsoring organizations, Chair and members of Organizing Committee, Chair of Scientific Committee, provisional budget (including planning funds). The IUPAC decision will come by the end of the year. A proposal must be ready for approval at the Fall 2005 annual meeting of the Division. Allan Felsot, Don Baker, Jeanette van Emon, and Rod Bennett agreed to work on the proposal.

Rod Bennett proposed the motion below which was seconded by Don Wauchope and passed without dissent.
Motion:
The Agrochemicals Division will engage in an agreement with Nancy Todd, ACS Office of Conference Management, to:

- work on a pre-proposal for the 12th IUPAC Pesticide Conference,
- help the exploratory committee to prepare the proposal, and
- handle logistics for the conference if the proposal is accepted by IUPAC.

If the proposal is approved by IUPAC, then the Office of Conference Management will open an account and pay up-front expenses from that account.

AGRO sponsored workshop in China
Phil Lee proposed a workshop in Beijing, August, 2006 following IUPAC meeting. The host would be the Chinese Agricultural University. Topics would include technology for evaluating pesticide risks, benefits; food safety, formulation and application technology, laws and regulations governing pesticide use, MRL harmonization, future interactions between China and US, Pan-Pacific conference. The AGRO delegation should consist of representatives from government, industry, and academia. Phil will present a proposal for approval at the Washington meeting.

ACS Office of Conference Management and Vendor Relations
The ACS has established a new Office of Conference Management and Vendor Relations. Nancy Todd described the rationale for the new office and described the services. The office must pay for itself and will charge $35/attendee and seek commissions from hotels.

Executive Committee
Update from The Chair
Allan Felsot gave review of the SETAC meeting. There were about 4000 people at the conference with a large number of papers on pesticides. Allan reminded us that ACS expects the Division to participate in local and regional activities. For instance our participation in the Southeast regional meeting, Mid-Atlantic meeting, and Western Regional meeting in February 2006 would meet ACS expectations.

Secretary's Report - Aldos Barefoot

Al reported that he forwards membership lists for AGRO to membership chair and lists for FERT to subdivision officers. He worked with the membership chair to collect information from activity lists during the past two years. The secretary scheduled the business meeting and provided an agenda and announcement for distribution via the email list. He asked for reports in an electronic form prior to the meeting for display during the business meeting and to facilitate preparation of the minutes after the meeting.

Treasurer's Report - Terry Spittler
Terry provided a summary of the AGRO financial status. The Treasurer usually must take $10,000-15,000 from the endowment each year to cover AGRO expenses.

Fertilizer Subdivision Report - Wayne Robarge
FERT has been active in sponsoring workshops on trace metals, analytical methods and perchlorate. Wayne and Bill are now listed as reviewers for ES&T.

Councilor's Report - Joel Coats, Barry Cross
Barry and Joel reported that the ACS had a budget surplus of $68,000 in 2004 and projects a $5.1 million surplus in 2005. The programming guidelines have been simplified, and ACS has produced an ethics report. Divisions are encouraged to appoint a regional meeting coordinator. Co-sponsored symposia will be in both Division programs – proposed for DC, but may not be ready in time.

Publications Committee - Laura McConnell
The PICOGRAM was successfully published for the Spring 2005 meeting with 5 half-page ads and 6 full-page ads. As a new feature, the names of new division members were added just after the message from the Division Chair. This feature will be continued in future issues. The list of previous award winners returns in this issue as requested. This list will be run at least once a year. Thank you to Allan Felsot and Judy Rupert for working very hard to launch the new AGRO division website. Allan and Judy would appreciate any feedback on the organization or information included.

The PICOGRAM will be posted on the website in adobe format for the convenience of our members. Beginning in Fall 2005, the PDF will be posted as soon as it is submitted to the printers. Content for the Fall PICOGRAM will be due in mid-June. Please forward announcements regarding upcoming conferences or workshops, pictures taken at the Spring meeting, biographical information on award winters, etc.

E-mail Communications System - Tim Ballard & Terry Spittler
Tim has located a programmer to work on a directory. Tim noted that to be in the directory, members must provide information. He also proposed cleaning up the email addresses.
Motion: Don Wauchope made a motion to authorize $500 for correcting email addresses. Al Barefoot seconded the motion. Motion passed.

Awards Committee - Jim Seiber

DuPont will sponsor the International Award for Janice Chambers in Fall 2005. The International Award will be presented to Joel Coats and Isamu Yamaguchi in 2006. Ralph Mumma is organizing the symposium for Joel.

Finance Committee - Barry Cross

Barry reported that we have approximately $200,000 in working funds and $400,000 in the education fund. Barry noted that these funds should be used to advance the activities of the Division.

Hospitality Committee - Jeff Jenkins, Terry Spittler

Six companies supported the coffee lounge for this meeting. Please take note of the sponsors listed on the board at the AGRO desk and thank them for their contributions. Other supporters have committed to a contribution, so please check the AGRO desk for updates. AGRO and AGFD will hold a joint Social Hour on Tuesday, March 15, 2005, 6-8 pm at the Horton. The cost breakout was discussed and no changes in the allocation were proposed. Currently, AGRO contributes about $4000 to the joint social, while AGFD contributes $2500.

Nominating Committee - Jeanette Van Emon (2005 election), Rodney Bennett (2006 election)

Jeanette informed us that 168 ballots were returned in the last election. Rod is hoping to have ballots by the end of May so that election results can be announced at the Fall meeting.

Public Relations Committee - Jeff Jenkins

Press releases were sent to five news organizations to publicize the presentation of the International Award for Research in Agrochemicals to Dr. Robert Krieger. The web-site has a media button.

Education Committee - John Johnston

Young Scientist Research Award:
There were 15 entries for the Young Scientist Award. Dow continues to sponsor the award. Jianguo Tan, Michigan State University, won the competition. Michelle Haldik, Johns Hopkins University, was the runner-up. John encouraged all members to interact with the students at the poster competition on Tuesday, the Sci Mix and the AGRO social. The next Graduate Student Research Poster Competition is scheduled for the Fall meeting in Washington, DC. The next Young Scientists Research Award will be presented at the 2006 meeting in Atlanta. Applications should be sent to Allan Felsot.

By-Laws Committee - Don Baker

Don continues to look for needed changes in the by-laws. A useful change would be to standardize membership categories across Divisions.
AGRO Division Procedures Manual - Nancy Ragsdale
Nancy will incorporate all comments by the Washington meeting.

New Business

Dues were reviewed and approved with no changes. Rod Bennett proposed that the budget for symposia be increased to allow greater flexibility for funding invited speakers. The Treasurer, program chair and symposium organizer must agree on the appropriate funding.
Motion:
Allan Felsot moved that the budget for each session be increased to $900. Rod seconded the motion, which passed unanimously.
Allan suggested that the Agrochemicals Division should consider a change in name to better reflect the scientific disciplines represented by the members. He proposed Division of Crop and Public Health Protection.
Allan adjourned the meeting at 9:15 pm.

Respectfully submitted,
Aldos C. Barefoot, Secretary

[*]BYLAWS OF THE DIVISION OF AGROCHEMICALS
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 date 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 ~~national~~ 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 ~~him~~ 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, and the Chairs, the Chairs-Elect, Councilors and Alternate Councilors, 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.

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

Section 9. The officers of the Division other than the Chair and the Chair-Elect, Division Councilors and Alternate Councilors, 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 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 officers, 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 Members-at-Large shall be elected each year.

Section 14. The terms of Councilors and 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 will 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 Division 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 the 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
DIVISION OF AGROCHEMICALS

PROGRAM

230th ACS National Meeting
Washington, DC, August 28 - September 1, 2005

R. D. Wauchope, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

The Role of Analytical Chemistry in State and Federal Regulation (see *ANYL*, Thu)

Studying the Metabolome (see *BIOL*, Sun)

Environmental Chemistry: Green Chemistry, Pollutants and Sustainability (see *CHED*, Sun)

Chemical Information and Open Access (see *CINF*, Mon)

Where Toxicology Meets the Law-Focus on Dioxin (see *TOXI*, Wed)

Characterization and Properties of Environmentally Relevant Black Carbon Particles (see *ENVR*, Sun, Mon, Wed)

Global Environmental Regulation: Regulation of Chemicals – A View towards 2015 (see *ENVR*, Mon)

Perchlorates: Science and Policy (see *ENVR*, Wed, Thu)

Current Frontiers of Fluoroorganic Chemistry (see *FLUO*, Sun, Mon)

Advanced Characterization of Natural Organic Matter (see *GEOC*, Tue, Wed, Thu)

SOCIAL EVENTS:
see invitations (pp 7 & 8) for locations and information
Award Banquet: Mon 6:00 pm
Social Hour: Tue 6:00 – 8:00 pm

BUSINESS MEETING:
Sun 5:00-10:00 pm
Washington DC Convention Center -- 303

SUNDAY MORNING

Section A: Washington DC Convention Center, Hall A

General Posters
R. D. Wauchope, *Organizer*

9:00 - 11:00
1. Enantiomer-specific fate and effects of chiral pesticides. **A. W. Garrison**, J. K. Avants

2. Factors influencing pesticide runoff from warm-season turfgrasses. **P. A. Ampim**, J. H. Massey, B. A. Stewart, M. C., Smith, A. B., Johnson, K. L. Armbrust, A. A. Andrews

3. Evaluation of the leaching models LEACHP and RZWQM for predicting turf pesticide concentrations in tile drains. **N. Peranginangin**, J. Purdy, T. Estes, A. Wadley

4. Imidacloprid content of the eluate of vegetated and non-vegetated soil columns. **C. J. Peterson**

5. Elucidating the leaching and transformation of benzoxazinone allelochemicals in soil when using rye and wheat sprouts as green manure. **S. S. Krogh**, **S. J. M. Mensz**

6. New sources of information on pesticide chemical properties: A summary of current activities. **R. D. Wauchope**, J. E. Bagdon, J. Edwards, I. G. Ferris, D. G. Shaw, J. B. Unsworth

7. International standards for pesticide chemical and physical properties: An IUPAC project. **D. G. Shaw**, R. D. Wauchope

8. EPA pesticide fate database for risk assessment. **S. L. Liu**, M. T. Shamim, J. Holmes, T. Nguyen, L. Hoot, D. S. Spatz, A. N. Shamim

9. Novel class insecticide, flubendiamide: Synthesis and biological activity. **M. Tohnishi**, H. Nakao, T. Furuya, A. Seo, H. Kodama, K. Tsubata, S. Fujioka, H. Kodama, T. Hirooka, T. Nishimatsu

10. Patterns of inhibition of cholinesterase and carboxylesterase following *in vivo* exposure of rats to binary mixtures of organophosphorus insecticides. **E. C. Meek**, J. E. Chambers, H. Chambers, R. L. Carr, J. Kamykowski

11. Synthesis of substituted quinazolines as insecticides. **S. Sehgel**, T. G. Cullen, J. Dixson, Z. M. Elshenawy, S. ElMarakby, L. LaLfrance, E. G. Rowley, D. Warkentin

12. 5,4'-Dihydroxy-3,7,3'-trimethoxyflavone interaction at donor site on spinach thylakoids. **B. King-Díaz**, R. González-Vázquez, M. I. Aguilar, N. Diego, J. R. de Santiago-Gómez, B. Lotina-Hennsen

13. Evaluation of chiral HPLC mobile phase composition for the separation of Brodifacoum enantiomers. **R. S. Stahl**, J. J. Johnston

14. Toxicity of Fipronil enantiomers to the water flea and black fly. **B. J. Konwick**, A. W. Garrison, A. T. Fisk, M. C. Black, J. P. Overmyer

15. Development of an immunoassay for monitoring environmental and animal/human exposure to persistent organic pollutant polybrominated diphenyl ethers (PBDES). **K. C. Ahn**, S. J. Gee, H -J. Tsai, B. D. Hammock

16. Development of immunoassays for urine biomarkers to study human exposure to the pyrethroid insecticide permethrin. **K. C. Ahn**, H. J. Kim, S. J. Gee, B. D. Hammock

Section B: Washington DC Convention Center, 302

Agrochemical Residue and Metabolism Chemistry
T. A. Wehner, J. J. Johnston, and D. Smith, *Organizers*

9:00 — Introductory Remarks.

9:05 —17. Diphacinone and diphacinone metabolites in Wistar Norway rats exposed to diphacinone/tetracycline baits. **T. M. Primus**, S. F. Graves, J. J. Johnston

9:25 —18. Early stage assessment of fungicide metabolic stability. **R. I. Baloch**, C. Yerkes, B. Jesse, J. M. Renga

9:45 —19. Generation of pharmacokinetic data for PBPK modeling. **M. E. Krolski**, T. Nguyen, R. T. Lopez, S -L. Ying, W. Roensch, J. K. Campbell, C. Lunchick

10:05 — Intermission.

10:25 —20. Identification and characterization of adducts of chloroaromatic pesticides with guanosine. **D. W. Boerth**, E. Eder, M. Medeiros, D. Coulombe, R. Mauro

10:45 —21. Measurement of pyrethroid residues in environmental samples by enhanced solvent extraction/supercritical fluid extraction coupled with gas chromatography-tandem mass spectrometry. **G. Xiong**, J. M. Van Emon

11:05 —22. Method for the determination of chlorpyrifos in black oil sunflower seeds. **R. E. Mauldin**, T. M. Primus, G. M. Linz, T. L. Buettgenbach, J. J. Johnston

SUNDAY AFTERNOON

Section A: Washington DC Convention Center -- 303

Agrochemical Development from Lab to Field
J. W. Lyga and G. Theodoridis, *Organizers*

1:00 — Introduction Session I. Translation of pesticidal activity from lab to greenhouse to field.

1:05 —23. Innovation opportunities in the crop protection industry. **A. Orth**, G. Theodoridis, J. W. Lyga

1:25 —24. Carbamoyloxadiazolidinedione herbicides. **T. M. Stevenson**

1:45 —25. Phthalic acid diamides activate ryanodine-sensitive calcium release channels in insects. **P. Lümmen**, U. Ebbinghaus-Kintscher, N. Lobitz, T. Schulte, C. Funke, R. Fische

2:05 — Intermission.

2:25 —26. Pharmacokinetics, toxicodynamics and activation to clothianidin of thiamethoxam in Colorado potato beetles. **R. Nauen**, U. Ebbinghaus-Kintscher, P. Jeschke

2:45 —27. Insecticidal 3-arylpyrimidin-2,4-diones: A case study of translation from target site to lab to field. **J. W. Lyga**, S. F. Ali, L. P. Kinne, F. L. Marek, M. A. Wusaty

3:05 —28. Factors involved in the field translation of a class of mitochondrial Qi inhibitor fungicides. **J. W. Owen**, Y. Adelfinskaya, Z. Benko, C. T. Schobert

3:25 — Intermission.

3:40 — Introduction Session 2. Synthesis of agrochemicals: Good ideas that never made it to products.

3:45 —29. A structure-based design approach to plant selective 4-hydroxyphenylpyruvate dioxygenase inhibitors. **D. L. Camper**, M. H. Parker

4:05 —30. Polycyclic dinitriles: Low nanomolar GABA-ergic insecticides, a pharmacophore and a new radioligand for insect GABA receptors. **C. W. Holyoke Jr.**, M. H. Howard, J. J. Rauh, M. Kline, D. A. Kleier, D. Cordova, E. A. Benner, D. Bai, D. B. Sattelle

4:25 —31. 2,4-Diaminoquinazoline insecticides. **E. G. Rowley**, T. G. Cullen, L. V. LaFrance, S. Sehgel, S. A. ElMarakby, D. Warkentin

4:45 — Concluding Remarks.

Section B: Washington DC Convention Center -- 302

Agrochemical Residue and Metabolism Chemistry
T. A. Wehner, J. J. Johnston, and D. Smith, *Organizers*

1:30 — Introductory Remarks.

1:35 —32. Use of SPME for measuring bioavailable concentrations. **J. Gan**, W. Yang, W. Hunter

1:55 —33. SPE strategies for determination of nitrofuran antibiotic metabolites in honey and tissue. **M. Young**

2:15 —34. Stability and degradation of antibiotic residues in honey. **J. Kochansky**

2:35 — Intermission.

2:50 —35. Streamlining sample preparation and LC-MS/MS multiresidue analysis of antibiotics in animal tissues. **K. Mastovska**, S. J. Lehotay, A. R. Lightfield

3:10 —36. Tissue binding and metabolism of the avicide 3-chloro-4-methylaniline hydrochloride in red-winged blackbirds and dark-eyed juncos. **D. A. Goldade**, J. D. Tessari, J. Johnston

3:30 —37. HPLC determination of Nicarbazin in avian whole blood, blood solids, and plasma fractions. **R. S. Stahl**, C. A. Yoder, L. A. Miller, T. M. Primus, J. J. Johnston

3:50 — Concluding Remarks.

MONDAY MORNING

Section A: Washington DC Convention Center -- 209C

Biochemical Toxicology of Agrochemicals: Symposium in Honor of Janice Chambers, ACS International Awardee for Research in Agrochemicals Sponsored by DuPont Crop Protection
E. Hodgson, *Organizer*

8:40 — Introduction and Award Presentation.

9:00 —38. Award Address. Metabolism and effects of organophosphorus insecticides. **J. E. Chambers**

9:45 — Intermission.

10:00 —39. One source of genetic variability affecting the detoxication of chlorpyrifos and diazinon. **C. E. Furlong**, T. B. Cole, C. Pettan-Brewer, D. M. Shih, A. Tward, A. J. Lusis, L. G. Costa

10:35 —40. In vitro studies using human tissues as a tool to identify inter- and intra-species differences in pesticide metabolism. **J. Tang**

11:10 —41. Metabolic interactions of agrochemicals in humans. **E. Hodgson**

Section B: Washington DC Convention Center -- 208B

Modern Chiral Pesticides: Enantioselectivity and Its Consequences
W. Garrison and R. Williams, *Organizers*

8:30 — Introductory Remarks.

8:35 —42. Key questions when addressing the efficacy, environmental behavior and side effects of chiral pesticides. **T. Poiger**

9:00 —43. Chiral switch from metalaxyl to metalaxyl-M: Lessons learned from a registration authority perspective. **M. D. Müller**

9:25 —44. Modern chiral pesticides: Chirality and its significance in some currently used chiral herbicides in Nigeria. **P. N. Gbaruko**, J. C. Igwe, J. O. Gbaruko, C. A. Ntima, C. Ogbonna, B. C. Gbaruko

9:50 —45. Bioaccumulation and enantioselective biotransformation of fipronil and selected conazole fungicides. **B. J. Konwick**, A. T. Fisk, J. K. Avants, J. F. Kenneke, A. W. Garrison

10:15 — Intermission.

10:35 —46. Chirality in currently used insecticides and its environmental implications. **J. Gan**, W. Liu, S. Qin, D. Schlenk

11:00 —47. Degradation of Indoxacarb and its R-enantiomer in soil, sediment and water. **S. K. Singles**

11:25 —48. Degradation of Indoxacarb and its R-enantiomer in rats, livestock and fish. **M. T. Scott**

MONDAY AFTERNOON

Section A: Washington DC Convention Center -- 209C

Biochemical Toxicology of Agrochemicals: Symposium in Honor of Janice Chambers, ACS International Awardee for Research in Agrochemicals Sponsored by DuPont Crop Protection

E. Hodgson, *Organizer*

1:15 — Introductory Remarks.

1:20 —49. Human carboxylesterases and their role in pyrethroid metabolism. **M. K. Ross**, A. Borazjani, P. M. Potter

1:55 —50. Exactly the same but different: Analysis and implications of the promiscuity of ligand-dependent activation of the Ah receptor signaling pathway. **M. S. Denison**

2:30 —51. Predictive xenobiotic metabolomics: Integrating biochemical toxicology with computer modeling. **R. S. H. Yang**, A. N. Mayeno, B. Reisfeld

3:05 — Intermission.

3:20 —52. Comparative detoxication of organophosphates by serum and liver esterases of neonatal, juvenile and adult rats. **H. Chambers**, E. C. Meek, J. E. Chambers

3:55 —53. Multi-step model for the molecular mechanism of organophosphates binding with acetylcholinesterase. **S. R. Gwaltney**

4:30 —54. Mechanism of selective toxicity of insecticides in mammals and insects. **T. Narahashi**, X. Zhao, T. Ikeda, J. Z. Yeh

Section B: Washington DC Convention Center -- 208B

Modern Chiral Pesticides: Enantioselectivity And Its Consequences

W. Garrison and R. Williams, *Organizers*

1:30 — Introductory Remarks.

1:35 —55. Mathematical manipulations of enantiomeric data. **E. M. Ulrich**, D. R. Helsel, W. T. Foreman

2:00 —56. Investigating the enantioselective toxicity of conazole fungicides in rainbow trout through the use of NMR-based metabonomics. **D. R. Ekman**, B. J. Konwick, A. W. Garrison, J. F. Kenneke, A. T. Fisk

2:25 —57. In vitro phase I metabolism of the triazole fungicide bromuconazole and its four enantiomers. **J. F. Kenneke**, C. S. Mazur, A. W. Garrison

2:50 — Intermission.

3:10 —58. Determination of metolachlor ethanesulfonic acid (ESA) enantiomers in water by chiral LC/MS/MS. **A. K. Kabler**, S. Chen

3:35 —59. Determination of the ratio of the 1'S and 1'R diastereomers of metolachlor and S-metolachlor in soil and water by stereoselective immunoassays. **J. F. Brady**, J. A. Key

4:00 —60. Selectivity in aquatic toxicity and biodegradation of the herbicide Metolachlor. **W. Liu**, Q. Fang, Y. Ma

4:25 — Concluding Remarks.

Section C: Washington DC Convention Center -- Hall A

Agrochemical Education Awards For Graduate Student Travel: Research Poster Presentations

J. J. Johnston, *Organizer*

2:00 - 5:00

61. Repellency of catnip and Osage orange essential oils to two mosquito species. **G. E. Schultz**, J. Coats

62. Effects of dietary conjugated linoleic acid on the European corn borer. **L. J. Gereszek**, J. R. Coats, D. C. Beitz

63. A brain detoxifying enzyme for organophosphorus nerve poisons. **D. K. Nomura**, D. Leung, K. P. Chiang, G. B. Quistad, J. E. Casida

64. AEI: Mechanistic interpretation of molecular interactions of tetracycline with clay and organic matter using nuclear magnetic resonance, mass spectrometry, and attenuated total reflectance Fourier transform infrared spectroscopy. **P. Kulshrestha**, H. S. Atreya, D. Sukumaran, R. F. Giese Jr., T. D. Wood

65. Anaerobic bacterial degradation of agrochemicals in laboratory microcosms. **Y. Cheng**, A. Ogram

66. Bioavailability of tylosin in environmental matrices. **K. L. Henderson**, T. B. Moorman, J. R. Coats

67. Development and characterization of improved extraction methods for transgenic Bt proteins from soil and sediment. **K. R. Prihoda**, B. W. Clark, B. D. Hopper, A. Jessick, J. R. Coats

68. Enantiomeric sulfoxidation of the organophosphate pesticide fenthion in fish. **O. Bawardi**, B. Furnes, J. M. Rimoldi, D. Schlenk

69. Environmental fate of tylosin and analysis of immunological cross-reactivity among tylosin isomers. **D. Hu**, K. L. Henderson, J. R. Coats

70. Evaluation of the transport of selected contaminants in recycled water in tropical soil. **S. K. Mohanty**

71. Modeling the variability in aerial concentrations of atrazine, endosulfan and chlorothalonil at a rural location on the Delmarva Peninsula. **A. Goel**, L. L. McConnell, A. Torrents

72. Responses of juvenile salmon to aquatic herbicides. **C. A. Curran**, J. M. Grassley, C. E. Grue

MONDAY EVENING

Section A: Washington DC Convention Center -- Hall A

Sci-Mix
R. D. Wauchope, *Organizer*

8:00 - 10:00
6-8, 61-72. See previous listings.

TUESDAY MORNING

Section A: Washington DC Convention Center -- 209C

Control of Invasive Species: Regulatory Concerns and Achievements. New Approaches for Prevention, Regulation and Assessment of Invasive Species
A. Leslie, *Organizer*

8:30 — Introductory Remarks.

8:40 —73. Overview of permitted and prohibited listing approaches for new and emerging invasive plants. **R. G. Westbrooks**

9:00 —74. Proposed revisions to U.S. Department of Agriculture's Animal and Plant Health Inspection Service Quarantine on Plants for Planting. **A. V. Tasker**

9:20 —75. Developing a U.S. national invasive plant list. **T. S. Killeffer**

9:40 — Intermission.

10:00 —76. Regulatory and cooperative responses to noxious and invasive exotic plants by the Maryland Department of Agriculture. **R. H. Tichenor**

10:20 —77. Probabilistic risk assessment for identifying acceptable methods to control invasive species. **J. J. Johnston**

10:40 —78. Invasive species challenges and perceptions in the horticultural industry: Regulative and legislative. **J. P. Thompson**

11:00 —79. Registration of aquatic herbicides: A new model. **K. D. Getsinger**, D. R. Stubbs, M. D. Netherland

11:20 —80. Inclusion of noxious weed management in the reform of the Endangered Species Act. **J. Bean**, J. L. Vollmer, G. A. Thies

11:40 — Concluding Remarks.

Section B: Washington DC Convention Center -- 208B

Turfgrass: Pesticide Exposure Assessment and Predictive Modeling Tools. Exposure Assessments for Turf Pesticides
Cosponsored with Turf Umbrella Workgroup
M. Nett, *Organizer*
P. J. Rice, *Presiding*

8:30 — Introductory Remarks.

8:45 —81. Research on the fate of pesticides applied to turfgrass: A perspective by a scientist, administrator and emeritus. **A. Smith**

9:10 —82. Farmer's perspective on modern turf farming. **C. Harbourt**, L. DeLalio

9:35 —83. Impact of lawn care practices on aquatic ecosystems in suburban watersheds: EPA STAR grant research findings. **K. L. Armbrust**

10:00 — Intermission.

10:20 —84. Effects of lawn-care chemicals on macroinvertebrate communities. **J. P. Overmyer**, R. Noblet, K. L. Armbrust

10:45 —85. Missing links in ecological risk assessment: Use of biomarkers in freshwater bivalves to establish causal relationships between pesticide exposures from turfgrass runoff and effects on stream ecosystems. **D. E. Conners**, M. C. Black

11:10 —86. Aesthetics and practice of maintaining the ideal lawn in Peachtree City, GA. **T. L. Gragson**, A. Keeler

11:35 — Concluding Remarks.

TUESDAY AFTERNOON

Section A: Washington DC Convention Center -- 209C

Control of Invasive Species: Regulatory Concerns and Achievements. The Federal Response and Coordination, Extension and Partnerships to Address Invasive Plants

A. Leslie, *Organizer*

1:00 — Overview of weed control by federal agencies: Introduction.

1:05 —87. Lessons learned from invasive species management in the National Wildlife Refuge System. **M. Lusk**

1:25 —88. National Park Service exotic plant management teams: An innovative model for wildland weed control. **L. R. Drees**

1:45 —89. Overview of NEPA requirements for federal invasive species management. **G. Ramos**

2:05 —90. USDA Forest Service national strategy and implementation plan for invasive species management. **M. Ielmini**

2:25 —91. Overview of the Giant Hogweed eradication project in Pennsylvania. **A. V. Tasker**

2:45 —92. The Department of Defense Invasive Species Management Program. **P. J. Egan**

3:05 — Intermission.

3:20 — Coordination, extension and partnerships to address invasive plants: Introduction.

3:25 —93. National Invasive Species Council update. **C. P. Dionigi**

3:45 —94. Development of an early detection and rapid response system for the Pink Hibiscus Mealybug through education, training, and implementation of Integrated Pest Management. **R. M. Nowierski**

4:05 —95. Achieving the goal that invasive plant removal is standard in natural areas. **M. J. Imlay**

4:25 —96. Progress on development of a National Early Detection and Rapid Response System for Invasive Plants in the United States. **R. G. Westbrooks**

4:45 — Concluding Remarks.

Section B: Washington DC Convention Center -- 208B

Turfgrass: Pesticide Exposure Assessment and Predictive Modeling Tools. Field Studies for Turf Pesticide Modelling

Cosponsored with Turf Umbrella Workgroup
M. Nett, *Organizer*
J. H. Massey, *Presiding*

1:30 — Introductory Remarks.

1:40 —97. Determination of transferable residues of carbaryl from turf. **M. E. Krolski**, V. Standart, J. K. Campbell

2:05 —98. Surface drinking water assessment and monitoring for oxadiazon herbicide on golf courses. **U. B. Nandihalli**, R. Allen, R. L. Jones, T. S. Ramanarayanan, G. J. Sabbagh

2:30 —99. Monitoring residues from use of an agrochemical product on golf courses at the watershed scale. **S. H. Jackson**

2:55 —100. Differential application of fluorobenzoic acids to evaluate surface runoff from turfgrass. **P. J. Rice**, B. P. Horgan

3:20 — Intermission.

3:40 —101. Cyazofamid Turfgrass dissipation studies with modifications to measure loss from clipping removal. **J. L. Wiedmann**

4:05 —102. Reducing pesticide residues in finished compost resulting from urban applications onto turfgrass. **S. A. Cryer**, M. P. Tolley, C. Blewett, D. W. Roberts

4:30 —103. Overview of a project to improve pesticide runoff estimation from turfgrass. **J. H. Massey**

4:55 — Concluding Remarks.

WEDNESDAY MORNING

Section A: Washington DC Convention Center -- 209C

2005 Sterling B. Hendricks Award
Cosponsored with USDA-Agricultural Research Service
N. Ragsdale, *Organizer*

8:30 — Introduction of Presenter.

8:35 — Presentation of Sterling B. Hendricks Award.

8:45 —104. Award Address. Grand challenges and opportunities in the environmental sciences: The importance of basic research and technology. **D. L. Sparks**

9:30 — Reception.

Section B: Washington DC Convention Center -- 208B

Turfgrass: Pesticide Exposure Assessment and Predictive Modeling Tools. Modeling of Turf Pesticides
Cosponsored with Turf Umbrella Workgroup
M. Nett, *Organizer*
M. Carroll, *Presiding*

9:00 — Introductory Remarks.

9:10 —105. Modeling approaches to address turf and golf course scenarios. **J. Lin**

9:35 —106. New thatch and subsurface drainage components in PRZM. **J. M. Cheplick**, C. Harbourt, W. Northcott

10:00 —107. The development of a standard turf scenario. **A. Wadley**, M. Nett

10:25 — Intermission.

10:45 —108. Modeling 2,4-D transport in turfgrass thatch and soil. S. Raturi, R. L. Hill, **M. Carroll**

11:10 —109. Development and testing of a comprehensive model of pesticide losses from turf. **A. Magri**, D. A. Haith

11:35 —110. Regional analyses of pesticide runoff from turf. **D. A. Haith**, M. W. Duffany

Section C: Washington DC Convention Center – 302

Biological Pest Control: The Continuum. Early Stages
P. L. Zubkoff, *Organizer*

10:00 — Introductory Remarks.

10:15 —111. Biopesticides meet the marketplace: Opportunities for eco-products in agriculture and communities. **T. A. Green**

10:40 —112. Nematode-antagonistic natural products. **D. J. Chitwood**, S. L. F. Meyer, I. A. Zasada

11:05 —113. Plant volatiles: From compounds to metabolic pathways and their regulation. **N. Dudareva**

WEDNESDAY AFTERNOON

Section A: Washington DC Convention Center -- 209C

Biological Pest Control: The Continuum
P. L. Zubkoff, *Organizer*

1:30 — Introductory Remarks.

1:35 —114. Insect semiochemicals and their applications in pest management. **A. Zhang**

2:00 —115. Detection of genetically modified plant material: Analytical methods. **C. Etsitty**, J. Kough, M. B. Rindal

2:25 —116. Regulatory issues with the development of biological pesticides. **A. H. Reynolds**, T. Milofsky

2:50 — Intermission.

3:05 —117. Strategies for incorporation of biopestides into IPM programs. **S. Bacchus**, M. Braverman, D. Horne

3:30 —118. The application of green chemistry to crop protection. **P. Marrone**

4:00 —119. The future of natural products in pest management. **S. O. Duke**

4:30 — Concluding Remarks.

Section B: Washington DC Convention Center -- 208B

Turfgrass: Pesticide Exposure Assessment and Predictive Modeling Tools. Modeling of Turf Pesticides
Cosponsored with Turf Umbrella Workgroup
R. D. Wauchope and M. Nett, *Organizers*
M. Carroll, *Presiding*

1:30 — Introductory Remarks.

1:45 —120. A comparison of two turf modeling approaches. **A. Wadley**

2:10 —121. Modeling offsite transport of turf-applied pesticides: model and data needs. Q. Ma, **S. Z. Cohen**, N. L. Barnes

2:35 — Intermission.

3:00 — Open Working Meeting: Research for Improving Risk Assessment for Turf-Care Chemicals.

4:30 — Concluding Remarks.

THURSDAY MORNING

Section A: Washington DC Convention Center -- 209C

General Oral Presentations
R. D. Wauchope, *Organizer*
L. Schwartz, *Presiding*

9:00 — Introductory Remarks.

9:05 —122. Bioavailability of phytotoxins in multisolute systems as influenced by soil competitive sorption properties. **N. Tharayil**, P. C. Bhowmik, B. Xing

9:25 —123. Multiple-inlet irrigation plus intermittent flooding reduces NPS runoff in rice production. **M. C. Smith**, J. H. Massey, A. A. Andrews, J. G. Thomas, P. L. Tacker, E. D. Vories, S. Lancaster

9:45 —124. Predicting soil fumigant acute, sub-chronic, and chronic air concentrations under diverse agronomic practices. **S. A. Cryer**, I. J. van Wesenbeeck, P. L. Havens, J. A. Knuteson

10:05 —125. Managing 1,3-D exposure and risk in the high use regions of Merced and Ventura California: Results of SOFEA(C) modeling. **I. J. van Wesenbeeck**, S. A. Cryer, P. L. Havens, B. A. Houtman

10:25 — Intermission.

10:40 —126. Improving Day Zero recoveries in field soil dissipation studies. **A. K. Sharma**, H. Strek, A. C. Barefoot

11:00 —127. Pesticidal activity of phytochemicals produced by arid land flora. **S. Clark**, B. Woodard, C. Wallace, F. Abdel-Rahman, M. A. Saleh

11:20 —128. Photolysis of [14C] furfural in aqueous solutions and indentification of photoproducts by HPLC/RAM and LC/MS. **M. F. Kovacs Jr.**, A. C. Katz, S. P. McLaughlin, G. J. Burger, J. A. Norton

Section B: Washington DC Convention Center -- 208B

(Q)SAR in Today's Agrochemistry Methodology
Cosponsored with COMP
B. Clark, *Organizer*

8:15 — Introductory Remarks.

8:20 —129. Enzymatical hydrolysis of chiral dichlorprop-methyl effecting by beta-cyclodextrins. **W. Liu**, Y. Wen, Z. Fang

8:40 —130. Quantitative structure activity relationship of antifungal terpenoids. **B. Woodard**, S. Clark, M. A. Saleh

9:00 —131. Estimation of the ADME characteristics for putative insecticides using time/dose/response relationships. **M. G. Ford**, D. W. Salt

9:30 —132. Estimation of tissue:blood partition coefficients of carbamates and organophosphorous (OP) pesticides using relative lipid content and Log P as the mechanistic determinants. **J. B. Knaak**, D. Chang, C. C. Dary, R. Tornero-Velez, M. Okino, F. Power

9:50 — Intermission.

10:05 —133. Molecular transformations as a way of finding and exploiting consistent local QSAR. R. P. Sheridan, J. C. Culberson, **P. A. Hunt**

10:35 —134. Putting the "Structure" in (Q)SAR into context. **R. D. Clark**, B. B. Masek

11:05 —135. A new software-aided approach to agrochemical structure optimization. **K. Kassam**, R. Sasaki, M. Hachey

11:25 —136. Organism-based QSAR models for various toxicological outcomes. **A. Holder**, M. D. Miller, L. Ye, C. Li, J. D. Eick, C. Chappelow, E. Kostoryz, D. M. Yourtee

THURSDAY AFTERNOON

Section A: Washington DC Convention Center -- 209C

General Oral Presentations
R. D. Wauchope, *Organizer*
M. F. Kovacs Jr., *Presiding*

1:15 — Introductory Remarks.

1:20 —137. Evaluation of water balance components and nitrate-N losses from a Southeastern Coastal Plain Field using the Root Zone Water Quality model. **L. Schwartz**, R. D. Wauchope, R. K. Hubbard

1:40 —138. Tebuconazole ozonation in water: By-products and dissipation kinetics. **T. Potter**, T. Manning, D. Folsom, L. Hardin, D. Wauchope

2:00 —139. Evaluation of the evaporation potential of components of agricultural products. **I. J. van Wesenbeeck**, D. J. H. Driver, J. Ross

2:20 —140. Kinetic model and optimization of DEET degradation by flow-though anodic Fenton treatment (FAFT). **H. Zhang**, A. T. Lemley

2:40 —141. Statistically-based method for establishing NAFTA-harmonized tolerances. **P. S. Villanueva**, D. J. Miller

3:00 —142. Molecular interactions of Demeton S and Hg(II) by NMR. **S. O. Pehkonen**, Z. Judeh

3:20 —143. Organophosphate induced chronic neurotoxicity: Health, environmental and risk exposure issues in developing nations of the world. **E. I. Ogwo**, P. E. Gbaruko, B. C. Gbaruko, E. Odo, J. C. Igwe

Section B: Washington DC Convention Center -- 208B

New Nutrient and Soil Amendment Products Impacting Agricultural Production and the Environment

B. Hall, *Organizer*

1:00 — Introductory Remarks.

1:10 —144. Development of a new Standard Reference Material: SRM 695 Trace Elements Multi-nutrient Fertilizer. **E. A. Mackey**

1:35 —145. Performance characteristics of urea-based polymeric controlled release fertilizers. **I. J. Hill**, B. Guertal, J. Wargo, S. Wertz

1:55 —146. Review and summary of the IFA Conference on Enhanced Efficiency Fertilizers. **W. L. Hall Jr.**

2:20 —147. Artificial fertilizers and climate change impacts on crop yields. **D. M. László**

2:50 —148. Kinetics of radionuclides and heavy metals behavior in soils: Implications for plant growth. **J. C. Igwe**, C. V. Ukaegbule, B. C. Gbaruko, E. Odo, C. U. Iroh

3:10 — Intermission.

3:20 —149. Agrochemical and morphological characteristics of city hard domestic wastes (HDW). **S. B. Pardaev**

3:50 —150. The ecological consequences of application of high rates of nitrogen fertilizers in Zaravshon Walley. **F. K. Khashimov**, T. K. Ortikov

4:20 —151. Effect of polyethylene film mulching on agrochemical change in Serozem soils under irrigation. **T. C. Goziev**

4:40 —152. Ecological consequences of humus mineralization in Uzbekistan. **T. K. Ortikov**, F. K. Khoshimov

DIVISION OF AGROCHEMICALS

1. Enantiomer-specific fate and effects of chiral pesticides

Arthur W. Garrison and Jimmy K. Avants, National Exposure Research Laboratory, U.S. Environmental Protection Agency, Ecosystems Research Division, 960 College Station Rd., Athens, GA 30605, Fax: 706-355-8202, garrison.wayne@epa.gov

Up to 25% of all pesticides and many other pollutants are chiral, existing as 2 (or more) mirror image isomers called enantiomers. Enantiomers usually differ in their biological properties, especially in their interactions with enzymes, leading to differences in their microbial transformation rates and in their toxicities. This poster provides examples of the techniques used for enantiomer separation, a necessity for measurement of enantioselectivity. Examples are also given of selectivity in soil and water microbial transformations with a variety of pesticides, including metalaxyl, dichlorprop, ruelene (cruformate), and others. A set of rules is provided for guidance in research on the enantioselective transformation of pesticides. Finally, several examples are given of differences in the effects of pesticide enantiomers using a variety of endpoints. The ultimate goal of this research is to provide data for help in determining whether the manufacture and use of single-enantiomer pesticides is of benefit to the environment.

2. Factors influencing pesticide runoff from warm-season turfgrasses

Peter A. Ampim[1], Joseph H. Massey[1], Barry A. Stewart[1], M. Cade Smith[1], Alton B. Johnson[2], Kevin L. Armbrust[3], and Ashley A. Andrews[1]. (1) Mississippi State University, 117 Dorman Hall, Mississippi State, MS 39762, Paa24@pss.msstate.edu, (2) Alcorn State University, (3) Mississippi State Chemical Laboratory, Mississippi State University

Understanding the fate of turf applied pesticides and predicting possible environmental concentrations requires knowledge of the factors affecting their transport. This on-going research is part of a larger effort designed to improve the understanding and modeling of pesticide runoff from turf. Following a standardized field protocol, 2, 4-D herbicide, flutolanil fungicide, and chlorpyrifos insecticide were applied to two grass species (bermuda or zoysia) maintained as either golf course fairways or residential lawns. The 3.65 m x 9.14 m plots had 3% slope and the treatments were arranged as a split design. Simulated rainfall (2.5 cm/h) was applied to the plots to generate runoff within 24 h of pesticide application. Runoff from the plots was collected at 5 min intervals and analyzed by HPLC-UV. To date, average runoff rates for the three pesticides were 25% for 2,4-D, 2% for flutolanil, and 0.5% for chlorpyrifos. These results correlated well with the soil-water distribution coefficients that were determined for the Brooksville silty clay soil at the runoff site. The KOC values were 73 ml/g for 2,4-D, 576 ml/g for flutolanil, and 3551 ml/g for chlorpyrifos. A function of application rate, maximum observed concentrations in turf runoff were 962 ppb for 2,4-D, 1336 ppb for flutolanil, and 23 ppb for chlorpyrifos. Efforts to determine the effects of grass species, mowing height, and plot size on pesticide runoff continue.

3. Evaluation of the leaching models LEACHP and RZWQM for predicting turf pesticide concentrations in tile drains

Natalia Peranginangin[1], John Purdy[2], Tammara Estes[3], and Adrian Wadley[3]. (1) Environmental Fate, Syngenta Crop Protection, P. O. Box 18300, Greensboro, NC 27419-8300, (2) Syngenta Crop Protection Canada, (3) Stone Environmental, Inc

Predicting pesticide leaching concentrations in turf is a challenge. Literature has shown that the current field-scale process-based leaching models LEACHP and RZWQM have been widely tested for leaching predictions from traditional agricultural crop pesticides but have been minimally tested for those from non-traditional agricultural environments such as turf. The objective of this study is to test these models' ability to predict pesticide concentrations in tile drains where two experimental turf plots studies were performed. In these studies, a "worst-case" field scenario was simulated by applying pesticide at maximum number of allowed applications in conjunction with the maximum single labeled use rate. In addition to natural rainfall, the plots received irrigation according to local agricultural practice for survival of the turf at the site. Tile drain water samples were collected at volume intervals and analyzed for the parent and its major metabolite concentrations. The observed concentrations were then compared with simulated concentrations from LEACHP and RZWQM. Selections of input parameters are discussed and models' performance is evaluated.

4. Imidacloprid content of the eluate of vegetated and non-vegetated soil columns

Chris J Peterson, Wood Products Insect Research Unit, USDA Forest Service, 201 Lincoln Green, Starkville, MS 39759, Fax: 662-325-6645, cjpeterson@fs.fed.us

The imidacloprid content of eluate from vegetated and non-vegetated soil columns was measured. Premise® 2 (Bayer Environmental Sciences) was applied to soil at the labeled rate for termite prevention in perimeter treatment and the soil put into six-inch cone plots. Bermuda grass, *Cynodon dactylon*, was used as the vegetation and was planted from seed. Cones were watered once per week with 30 ml water to simulate a 1-inch rain event. Once per month for six months, the eluate was collected and the content of imidacloprid was measured. Imidacloprid in the cone plot eluate peaked at one month, declined rapidly by month two, then entered a lagging phase with no significant decreases for the next four months. There was no statistical difference in eluate concentration between vegetated and non-vegetated plots. The concentration of imidacloprid in the cone plot soil declined by about 80% in the six month period. Despite the decline, treated soil was toxic to termites initially and after six months, and toxicity was not significantly affected by the presence of vegetation.

5. Elucidating the leaching and transformation of benzoxazinone allelochemicals in soil when using rye and wheat sprouts as green manure

Stine S. Krogh and **Susanne J. M. Mensz**, Department of Crop Protection, Danish Institute of Agricultural Sciences, Research Centre Flakkebjerg, Slagelse DK-4200, Denmark, stinesteen.krogh@agrsci.dk, susannejohannemiriam.mensz@agrsci.dk

Abstract text not available.

6. New sources of information on pesticide chemical properties: A summary of current activities

R. Don Wauchope[1], Joseph E. Bagdon[2], Jesse Edwards[3], Ian G. Ferris[4], David G. Shaw[5], and John B Unsworth[6]. (1) Southeast Watershed Research Laboratory, USDA - Agricultural Research Service, 2316 Rainwater Road, PO Box 946, Tifton, GA 31794, don@tifton.usda.gov, (2) Natural Resources Conservation Service, US Department of Agriculture, (3) Department of Chemistry, Florida A&M University, (4) FAO - IAEA, (5) University of Alaska, (6) Chelmsford, Essex, IUPAC Agrochemicals Advisory Commission

A variety of government agency and NGO projects are in progress designed to provide critical information needed for describing the behavior and fate of pesticide active ingredients in the environment. These are (a) INFOCRIS, a unique FAO open-source, cooperative web-based system which will include (among much other agriculture-related information) pesticide active ingredient chemical properties information developed in cooperation with the IUPAC Agrochemicals Advisory

Committee (ACC); (b) the IUPAC "pesticide compendium," a critical review of pesticide physical properties which is a cooperative project of the IUPAC-Environmental Chemistry Division and Analytical Chemistry Division (a presentation on this project in included in the IUPAC Analytical Chemistry Division poster session); (c) the IUPAC "Global Pesticide Information" project of the IUPAC-ACC, which will also provide web-based information on pesticide products; (d) an updating of the ARS/NRCS pesticide properties database slated to be complete in 2005; (e) a cooperative project between USDA-ARS and Florida A. & M. University to develop a critical compilation of pK_a and pK_b values for acidic and basic pesticides; (f) a new environmental fate pesticide properties database being compiled by the EPA Office of Pesticide Programs. Although there is overlap between these projects, they serve to complement and reinforce each other, and the results will provide a greatly improved database of fundamental property information which will be useful for many purposes, especially environmental impact assessments, risk management and simulation modeling. We will present an overview of the progress and status of each of these projects, with a view toward attracting additional volunteer collaborators to work on some of them.

7. International standards for pesticide chemical and physical properties: An IUPAC project

David G. Shaw[1] and R. Don Wauchope[2]. University of Alaska, Fairbanks, AK 99775, ffdgs@uaf.edu, (2) Southeast Watershed Research Laboratory, USDA - Agricultural Research Service

Reliable values for fundamental physical and chemical properties of pesticides are essential for prediction of biological and environmental fate and behavior of these widely used materials. Although such data are available in numerous compilations, in many cases information is provided with little or no indication of data quality and without reference to the method of determination or to the source of the data. This has led to a worldwide situation in which users of pesticide information are often unaware of discrepancies, uncertainties and errors in compiled data. IUPAC, the International Union of Pure and Applied Chemistry is engaged in a joint Project of the Division of Chemistry and the Environment and the Division of Analytical Chemistry to exhaustively compile and critically evaluate all available experimental data for a suite of physical and chemical properties and to produce a Compendium of Fundamental Physical and Chemical Properties of Selected Pesticides. We are compiling value, precision and accuracy estimates for aqueous solubility, vapor pressure, melting point, vapor pressure, Henry's law constant, n-octanol/water partition constant, acid-base constant(s), and solubility in acetone, toluene and hexane for 60 important pesticide chemicals. Forms have been developed and an internet-based system has been set up. We encourage interested scientists to contact the authors for additional information and possible collaboration in this project.

8. EPA pesticide fate database for risk assessment

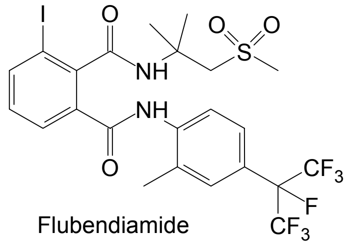
S. L. Liu, M. T. Shamim, J. Holmes, T. Nguyen, L. Hoot, D. S. Spatz, and A. N. Shamim, Office of Pesticides Programs, US Environmental Protection Agency, 401 M St. SW, Washington, DC 20460, LIU.LARRY@EPA.GOV

The Office of Pesticide Programs (OPP) in the Environmental Protection Agency (EPA) has developed a web-based Pesticide Fate Database, which will be available on EPA's Web site this spring. The database contains summary information on the physical/chemical properties and the chemical fate and transport of pesticide active ingredients found in products registered in the United States. It also contains information on the degradates or breakdown products of these pesticides. Using a query-based system, the Pesticide Fate Database allows users to search, sort, and retrieve up-to-date pesticide fate and chemistry information, which has been derived from studies submitted by pesticide manufacturers in support of the registration/reregistration of their pesticide products. Some of the important pesticide endpoint information in the current database include: 1) basic physical and chemical properties, 2) biotic and abiotic degradation half-lives in soil and water, 3) adsorption/desorption constants, and 4) bioconcentration factors in fish. For non-agricultural chemicals such as antifoulants and wood preservatives, aqueous availability and leaching data are also included. These endpoints can be used as inputs for developing drinking water and environmental exposure assessments. Currently, the database is populated with about 188 pesticide active ingredients and will be expanded to include more chemicals in the future. This presentation includes details of the database structure and its applications.

9. Novel class insecticide, flubendiamide: Synthesis and biological activity

Masanori Tohnishi[1], Hayami Nakao[1], Takashi Furuya[1], Akira Seo[1], Hiroki Kodama[1], Kenji Tsubata[1], Shinsuke Fujioka[1], Hiroshi Kodama[1], Takashi Hirooka[1], and Tetsuyoshi Nishimatsu[2]. (1) Research & Development Division, Nihon Nohyaku Co., Ltd, 345, Oyamada-Cho, Kawachi-Nagano 586-0094, Japan, Fax: +81 721 56 9090, (2) Marketing Division, Nihon Nohyaku Co., Ltd

Flubendiamide (N^2-[1,1-dimethyl-2-(methylsulfonyl)ethyl]-3-iodo-N^1-[2-methyl-4- [1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-phenyl]-1,2-benzenedicarboxamide) is a novel class insecticide having a quite unique chemical structure as an insecticide and is now being developed. The uniqueness of the structure results from the molecule mainly consisting of the three novel parts having the following substituents; heptafluoroiso-propyl group in the anilide moiety, sulfonylalkylamine group in the aliphatic amide moiety, and iodine atom at the 3-position of phthalic acid moiety. Flubendiamide provides extremely high insecticidal activity especially against a broad spectrum of lepidopterous insect pests, and is safe to non-target organisms. Flubendiamide, furthermore, shows unique biological mode of action, which results in no cross-resistance to the existing insecticides. The structure activity relationships, the synthetic method, and biological activity will be presented.



Flubendiamide

10. Patterns of inhibition of cholinesterase and carboxylesterase following *in vivo* exposure of rats to binary mixtures of organophosphorus insecticides

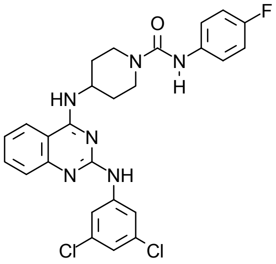
Edward C Meek[1], Janice E. Chambers[1], Howard Chambers[2], Russell L Carr[1], and Jeff Kamykowski[1]. (1) College of Veterinary Medicine, Mississippi State University, P.O. Box 6100, Mississippi State, MS 39762, Fax: 662-325-1031, emeek@cvm.msstate.edu, (2) Department of Entomology and Plant Pathology, Mississippi State University

The patterns of inhibition of target and non-target esterases following exposure of rats to binary mixtures of organophosphorus insecticides were investigated. Brain and serum cholinesterase (ChE) and serum carboxylesterase (CbxE) inhibition following exposure to individual and simultaneous or sequential mixtures of dimethyl (azinphosmethyl and methylparathion) or diethyl (chlorpyrifos and parathion) phosphorothionate insecticides were studied. Insecticides were administered by oral gavage in corn oil. The dose levels of each insecticide that would inhibit 10% of brain ChE at the time of peak inhibition were used. Sequential exposures were performed with the first insecticide administered followed by the second insecticide at the peak inhibition time for the first. Tissue samples were collected at 2, 4, 8, 10, 12, and 24 hr following exposures. Brain and serum ChE levels were determined by continuous spectrophotometric assay, and serum CbxE levels were determined by discontinuous spectrophotometric methods. One dimethyl (azinphosmethyl) and diethyl (parathion) mixture yielded additive effects on brain ChE, indicating no apparent interactions between the compounds. Simultaneous administration of another dimethyl (methyl parathion) and diethyl (chlorpyrifos) mixture also yielded additive effects on brain ChE, however sequential administration yielded a greater-than-additive-effect. Sequential exposure of two diethyl insecticides (parathion followed by chlorpyrifos) indicated greater-than-additive inhibition on brain ChE and interactions that appeared to be dependent on the order of administration. To predict the *in vivo* response of mixtures of organophosphorus insecticides will require knowledge of both activation and detoxication potentials, potencies of the oxons, and sequence of exposure (Supported by American Chemistry Council CRAM 2a-99).

11. Synthesis of substituted quinazolines as insecticides

Saroj Sehgel[1], Thomas G. Cullen[2], John Dixson[1], Zeinab M. Elshenawy[3], Sayed ElMarakby[2], Lou LaLfrance[2], Elizabeth G. Rowley[3], and Dennis Warkentin[1]. (1) Agricultural Products Group, FMC Corporaion, R & D Centre, P. O. Box 8, Princeton, NJ 08543, Fax: 609-951-3603, Saroj_Sehgel@FMC.Com, (2) (3) Agricultural Products Group, FMC Corporation

Substituted 2,4-diaminoquinazolines are very active against tobacco budworm in a surface treated diet assay. These were synthesized by displacing chloride from 2,4-dichloroquinazolines by various amines. The synthesis, biological activity, and structure activity relationship will be presented.



12. 5,4'-Dihydroxy-3,7,3'-trimethoxyflavone interaction at donor site on spinach thylakoids

Beatriz King-Díaz[1], Raquel González-Vázquez[1], Maria Isabel Aguilar[2], Nelly Diego[3], Jesús R. de Santiago-Gómez[3], and Blas Lotina-Hennsen[4]. (1) Department of Biochemistry, Universidad Nacional Autónoma de México, Fac. de Química, Edificio E, Ciudad Universitaria, Coyoacan, Distrito Federal 04510, Mexico, Fax: 55-56-225-329, kingbeat@servidor.unam.mx, (2) Department of Pharmacy, Universidad Nacional Autónoma de México, Fac. de Química, (3) Laboratorio de plantas vasculares, Universidad Nacional Autónoma de México, Fac. de Ciencias, (4) Departamento de Bioquímica, Universidad Nacional Autonoma de México

Croton ciliatoglanduliferus Ort. from the Euphorbiaceae family, is a wild plant commonly found in the Tehuacan region (Puebla, Mexico) and the Guerrero State where it is used as a repelent against insects and also for medical purposes [1]. Bioactivity-guided chemical study of the hexanic extract of Croton ciliatoglanduliferus led to the isolation a mixture of two flavonoids. They were separated by thin layer chromatography and characterized by spectroscopic methods as 5-hydroxy-3,7,3',4'-tetramethoxyflavone (1) and 5,4'-dihydroxy-3,7,3'-trimethoxyflavone (2). Only (2) showed photosynthetic electron transport interaction on spinach chloroplast. Since it inhibited ATP-synthesis (I50 = 51 μM) and electron flow, its interaction site was found to be located at the donor side on PSII.

13. Evaluation of chiral HPLC mobile phase composition for the separation of Brodifacoum enantiomers

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Brodifacoum, an anti coagulant rodenticide, has two chiral centers, and thus four enantiomers. We evaluated the effect of varying mobile phase composition on the separation of these four enantiomers on a β-cyclodextrin, 5 μm spherical solid phase, 250 x 4.6 mm column. The mobile phase combinations and solvent volume percent ranges we evaluated were: 1. acetonitrile (89.5 – 98.5%): methanol (1 – 10%): triethyl amine-acetate, 0.5%, pH 4.0 (0.5%). 2. methanol (60 – 98%): triethyl amine-acetate, 0.5%, pH 4.0 (2 – 40%). 3. methanol (95 – 98%): acetic acid, 0.2 N (0.5 – 5%): water (0 – 1.5%). 4. Methanol (80 – 99%): ammonium nitrate, 0.5 M, pH 4.0 (1 – 20%). 5. acetonitrile (80 – 99%): ammonium nitrate, 0.5 M, pH 4.0 (1 – 20%). The methanol: triethylamine acetate and methanol: acetic acid mobile phases provided the best resolution between the enantiomer pairs associated with each chiral center. The study was useful in elucidating the role of mobile phase composition in the chiral separation of multiple enantiomers. These mobile phase combinations will be used to permit the isolation and subsequent bioactivity determination of individual Brodifacoum enantiomers.

14. Toxicity of Fipronil enantiomers to the water flea and black fly

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Fipronil is a phenylpyrazole-class insecticide widely used in rice culture, turf grass management, and residential pest control. As a chiral molecule, fipronil exists as two non-superimposable mirror image forms called enantiomers, which can have different toxicological activity. Because of fipronil's high toxicity to invertebrates, information is needed to assess whether a difference in toxicity of its enantiomers warrants the production and use of only the target-active enantiomer. In this research, we analyzed the enantiomer-specific toxicity of fipronil using two aquatic invertebrate species. Acute toxicity to Ceriodaphnia dubia (water flea) indicated that the (+) enantiomer was significantly more toxic than the (-) enantiomer, with about a 3-fold difference in LC50 values. For Simulium vittatum IS-7 (black fly), both fipronil enantiomers were equally toxic. However, the response to fipronil was markedly different between the two invertebrate classes with the black fly being nearly 2 orders of magnitude more sensitive than the water flea.

15. Development of an immunoassay for monitoring environmental and animal/human exposure to persistent organic pollutant polybrominated diphenyl ethers (PBDEs)

Ki Chang Ahn, Shirley J. Gee, Hsing-Ju Tsai, and Bruce D. Hammock, Department of Entomology, University of California, Davis, 1 Shields Avenue, Davis, CA 95616, kahn@ucdavis.edu

Polybrominated diphenyl ethers (PBDEs) are ubiquitously used as additive flame retardants. Their quantities detected in the environment and biota samples are currently increasing. The aim of the study is to develop a competitive indirect enzyme-linked immunosorbent assay (ELISA) to monitor environmental and biological samples exposed to PBDEs. 2,2',4,4'-Tetrabromodiphenyl ether (BDE-47) that is the most abundant among many PBDE congeners in animal/human tissues and human breast milks was established as the target analyte. The three groups of immunizing haptens with a carbon-carbon double bond linker introduced on the different 2', 4', or 5' positions of the target molecule were designed to allow effective hapten presentation on the carrier protein for antibody production. These haptens were synthesized along with a group of coating haptens mimicking a characteristic fragment of the target molecule. Twelve polyclonal antibodies produced against each immunizing hapten-KLH conjugate coupled by the mixed anhydride method were screened against numerous hapten-BSA conjugates as coating antigens. A heterologous immunoassay showed a high sensitivity for the target analyte. At optimized ELISA conditions, the detection range in the assay buffer including a high content of DMSO was from 0.7-17 μg/mL and an IC50 value of 3.5 μg/L BDE-47. Little or no cross-reactivity to some PBDEs, PCB, TCDD, and halogenated phenols was measured. The ELISA suggests a convenient tool for a preliminary screening of the flame retardant BDE-47 persistent in environmental/biota samples.

16. Development of immunoassays for urine biomarkers to study human exposure to the pyrethroid insecticide permethrin

Ki Chang Ahn, Hee Joo Kim, Shirly J. Gee, and Bruce D. Hammock, Department of Entomology, University of California, Davis, 1 Shields Avenue, Davis, CA 95616, kahn@ucdavis.edu

The insecticide permethrin is one of the most commonly used pyrethroids in agriculture and public health. For risk assessment of human exposure to permethrin, we have developed competitive indirect immunoassays based on polyclonal antibodies for the detection of possible major human urinary metabolites of permethrin. The target analytes, 3-phenoxybenzoic acid (3-PBA), cis/trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-1-carboxylic acid (DCCA), glycine conjugates of 3-PBA and DCCA and a glucuronide conjugate (3-PBAlcG) of 3-phenoxybenzyl alcohol (3-PBAlc) are proposed as permethrin biomarkers in human urine. ELISAs had IC50 values of 2 µg/L for 3-PBAlcG and 11-22 µg/L for cis/trans-DCCA, respectively. An improved automatic immunoassay using a chemiluminescent reporter and magnetic separation technique showed an IC50 value of 0.3 µg/L for 3-PBA in the buffer. These assays are being improved to provide a useful monitoring tool for evaluating human exposure to the insecticide in terms of rapidity, sensitivity and practicality.

17. Diphacinone and diphacinone metabolites in Wistar Norway rats exposed to diphacinone/tetracycline baits

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Diphacinone is an anticoagulant used in formulated products to control populations of pest species such as ground squirrels and pocket gophers. To assess the potential secondary hazard to scavengers, the residues of diphacinone in the carcasses must be determined and a risk assessment completed. A study was conducted to assess the effect of tetracycline hydrochloride in conjunction with the anticoagulant diphacinone as a means of lowering diphacinone residues and associated non-target secondary hazards while maintaining bait efficacy. Wistar Norway rats were the test species for the study. The residues in liver and whole body tissue samples were typically determined by ion-pairing reversed-phase high performance liquid chromatography (HPLC) after liquid extraction of the sample combined with a solid phase extraction (SPE) clean-up procedure with the addition of chlorophacinone as a surrogate. The hydroxy metabolites of diphacinone were also observed and their ratio to the parent peak measured. Identification of these hydroxy metabolites were confirmed by HPLC/mass spectrometry (HPLC/MS) with atmospheric pressure chemical ionization and an ion trap detector. Extracts were analyzed in full scan and MS/MS modes, to confirm the presence of diphacinone and to identify the metabolites of diphacinone.

18. Early stage assessment of fungicide metabolic stability

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Residual field performance is a highly desirable attribute for comercially successful fungicides. It is certainly an attribute that the Discovery chemists would like to design in to their molecules as they synthesize potential fungicide candidates. Most plant metabolism information is historically generated much later in the fungicide development process and certainly after radioactive material is available. At an early stage in Discovery the issues of determining metabolic stability and identification of metabolites formed in the plant system are two fold. Firstly, the lack of radiolabeled material which facilitates detection of metabolites formed and secondly the resource and the time required to generate metabolism data. A medium throughput wheat metabolism assay has been developed at Dow AgroSciences which has ensured rapid turnaround allowing rate of metabolism data to be generated in a matter of days without the use of radiolabeled material. The poster presentation will discuss the usefulness and limitations of the assay for assessing metabolic stability and generation of metabolites using commercial fungicides as examples.

19. Generation of pharmacokinetic data for PBPK modeling

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In response to the USEPA reregistration risk assessment process specific to liquid formulations of carbaryl broadcast applied to residential turf, Bayer CropScience proposed to refine the post application risk assessment using pharmacokinetic data. A series of rat metabolism studies were designed and performed to determine the kinetic behavior and metabolic profile of carbaryl in target tissues as a function of both the dose rate and route of administration. The kinetic results were compared to values of carbaryl and cholinesterase inhibiting metabolites of carbaryl in the target tissues. Data from these experiments were then used to develop and refine a physiologically-based pharmacokinetic (PBPK) model in support of the carbaryl risk assessment. This program was the first application of PBPK data to a risk assessment submitted to the USEPA. This paper will describe the kinetic experiments performed and some of the challenges faced in developing input data sets for PBPK modeling.

20. Identification and characterization of adducts of chloroaromatic pesticides with guanosine

Donald W. Boerth[1], Erwin Eder[2], Melissa Medeiros[3], Danielle Coulombe[3], and Ryan Mauro[3]. (1) Department of Chemistry and Biochemistry, University of Massachusetts, North Dartmouth, MA 02747, Fax: 508-999-9167, dboerth@umassd.edu, (2) Institute of Toxicology, University of Würzburg, (3) Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth

Plant DNA studies show evidence of direct and indirect adducts from pesticide use. In addition to indirect adducts formed by products of lipid peroxidation from oxidative stress, evidence from 32P post-labeling studies indicates direct binding of the pesticide molecules with DNA bases in the case of diazinon, chlorothalonil, and other pesticides. Nucleophilic aromatic substitution reactions have been investigated as the possible mechanism for the binding of chloroaromatic and other aromatic pesticides with DNA bases. Molecular modeling via semi-empirical, ab initio, and density functional calculations support this binding pathway. Experimental studies of in vitro reactivity of a variety of aromatic pesticides with guanosine, a reactive nucleoside, resulted in identification of adducts with chlorothalonil, 2,4-dichlorophenoxyacetic acid, dichlobenil, and several other pesticides. Putative adduct structures were evaluated by molecular computational methods. Structural characterization was carried out by LC-MS and NMR methods. Experimental reactivities were correlated with theoretical binding potentials from molecular modeling studies at various levels of theory.

21. Measurement of pyrethroid residues in environmental samples by enhanced solvent extraction/supercritical fluid extraction coupled with gas chromatography-tandem mass spectrometry

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Environmental exposure to synthetic pyrethroids has been attracting increasing attention due to the possible carcinogenicity of these compounds as well as their growing use in agriculture, forestry, public health, as well as domestic and veterinary applications. For the trace analysis of pyrethroids, gas chromatography-mass spectrometry (GC-MS), especially gas chromatography-tandem mass spectrometry (GC-MS/MS), provides excellent sensitivity and selectivity. Solvent-saving techniques such as the enhanced solvent extraction (ESE, or pressurized fluid extraction) and supercritical fluid extraction (SFE) have been extensively studied for the analysis of multiresidue pesticides in complicated samples. However, applying these methods to the extraction of pyrethroids, especially the use of ESE for pyrethroid sample preparation, has not been thoroughly investigated. In our work,

ESE and SFE of pyrethroids were addressed by conducting solvent selection, minimization of extraction times and the optimization of other instrument parameters. Permethrin, cypermethrin, and deltamethrin were the three pyrethroids chosen for study. 3-Phenoxybenzoic acid was employed as the internal standard for the analysis. The samples included soils and baby food. An Ion Trap GC-MS/MS instrument was used for the quantitation of individual pyrethroids. Employing ESE/SFE with GC-MS/MS provides a simple and selective analytical method. Notice: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

22. Method for the determination of chlorpyrifos in black oil sunflower seeds

Richard E. Mauldin[1], Thomas M. Primus[1], George M. Linz[2], Teresa L. Buettgenbach[1], and John J. Johnston[1]. (1) USDA/APHIS/WS/National Wildlife Research Center, 4101 LaPorte Avenue, Fort Collins, CO 80521, richard.e.mauldin@aphis.usda.gov, (2) Great Plains Field Station, USDA/APHIS/WS/NWRC

Damage to ripening sunflower crops by blackbirds is an important agricultural problem in the northern Great Plains. Chlorpyrifos (an organophosphate pesticide) is a registered insecticide and acaricide commonly used to control insects on sunflower. In an effort to reduce crop loss by non-lethal means, chlorpyrifos was evaluated for its potential as a bird repellent and found to be highly successful in feeding studies with caged blackbirds. To support further evaluation of chlorpyrifos repellency in field trials, a rapid, simple, high performance liquid chromatographic (HPLC) analytical method was developed to assess residues in sunflower achenes which had been aerially sprayed. Control black oil sunflower seeds were cryopulverized, fortified at 5 µg g^{-1}, 50 µg g^{-1}, and 500 µg g^{-1}, and extracted in a 75% acetonitrile/25% 10 mM phosphate buffer (pH 3.5) mobile phase. Extracts were filtered and analyzed by HPLC using an ODS3 C-18 column with UV detection at 230 nm. The method was rugged and reliable, with chlorpyrifos recovery > 80% at all fortified concentrations. The method limit of detection was 0.84 µg g^{-1}, and no chromatographic interferences were observed.

23. Innovation opportunities in the crop protection industry

Ann Orth, George Theodoridis, and John W. Lyga, Agricultural Products Group, FMC Corporation, P.O.Box 8, Princeton, NJ 08543-0008

A discussion of the current crop protection industry, its challenges, and innovation opportunities will be presented.

24. Carbamoyloxadiazolidinedione herbicides

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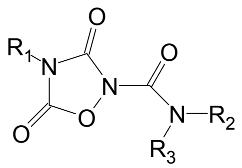
Carbamoyloxadiazinediones (COD's) are a novel class of herbicides with excellent pre-emergence activity on a wide spectrum of grass and broadleaved weeds. We were able to develop a number of different methods for the synthesis of COD's. This enabled us to use a variety of different kinds of precursors for rapid optimization of the R1, R2 and R3 substituents. Systematic study of the substituents allowed us to identify several viable candidates for maize, soybeans, rice and specialties. This talk will focus on the synthesis of the COD's, their herbicidal activity and structure-activity relationships of this class. We will also discuss key learnings from metabolism and hydrolysis studies which helped guide our efforts toward selection of successful field candidates.



25. Phthalic acid diamides activate ryanodine-sensitive calcium release channels in insects

Peter Lümmen[1], Ulrich Ebbinghaus-Kintscher[1], Nicole Lobitz[1], Thomas Schulte[1], Christian Funke[2], and Rüdiger Fischer[2]. (1) Research Biology Insecticides, Bldg. 6220, Bayer CropScience AG, D-40789 Monheim, Germany, peter.luemmen@bayercropscience.com, (2) Research Chemistry Insecticides, Bayer CropScience AG

Flubendiamide represents a novel chemical family of substituted phthalic acid diamides with potent insecticidal activity. So far, the molecular target and the mechanism of action were not known. Here we present for the first time evidence that phthalic acid diamides activate ryanodine-sensitive intracellular calcium release channels (ryanodine receptors, RyR) in insects. With calcium imaging, we showed that flubendiamide and related compounds induced ryanodine sensitive cytosolic calcium transients that were independent of the extracellular calcium concentration in isolated neurons from the pest insect Heliothis virescens as well as in transfected CHO cells expressing the ryanodine receptor from Drosophila melanogaster. Binding studies on microsomal membranes from Heliothis flight muscles revealed that flubendiamide and related compounds interacted with a site distinct from the ryanodine binding site and disrupted the calcium regulation of ryanodine binding by an allosteric mechanism. This novel mode of action seemed to be insect specific because flubendiamide had no measurable effect on mammalian type 1 ryanodine receptors.

26. Pharmacokinetics, toxicodynamics and activation to clothianidin of thiamethoxam in Colorado potato beetles

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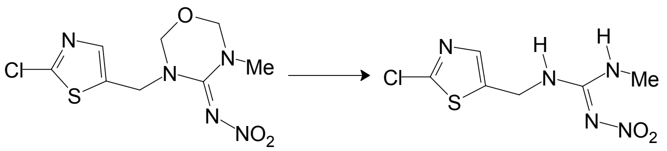
It has recently been demonstrated that the neonicotinoid insecticide thiamethoxam (THIAM) undergoes rapid activation to clothianidin (CLOTHI) in fall armyworm larvae, western corn rootworm larvae and adults and cotton plants, thus suggesting a pro-drug nature of THIAM. CLOTHI is known as a potent agonist of insect nicotinic acetylcholine receptors. We expanded our investigations to one of the most relevant species targeted by neonicotinoid insecticides, i.e. Leptinotarsa decemlineata (Colorado potato beetles, CPB). Pharmacokinetic studies revealed rapid conversion to CLOTHI of THIAM applied topically and orally to CPBs when analyzing hemolymph samples by LC-MS/MS. Toxicodynamic studies using head membrane preparations (radioligand displacement studies) and isolated nerve cells (whole-cell voltage clamp electro-physiology) of CPB adults strongly support the pro-insecticide nature of THIAM. Furthermore, CLOTHI concentrations determined ex vivo correlate seemingly well with the on-set of poisoning symptoms in intoxicated phenotypes. Additional evidence for CLOTHI being the active principle of THIAM was provided by considering neonicotinoid cross-resistance data.

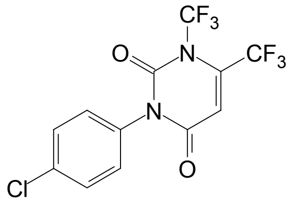


THIAM CLOTHI

27. Insecticidal 3-arylpyrimidin-2,4-diones: A case study of translation from target site to lab to field

John W. Lyga[1], S. F. Ali[2], Lyle P Kinne[2], F. Larry Marek[2], and Mark A Wusaty[2]. (1) Agricultural Products Group, FMC Corporation, P. O. Box 8, Princeton, NJ 08543, Fax: 609-951-3835, john_lyga@fmc.com, (2) Discovery Research, FMC Corporation Agricultural Products Group

The 3-arylpyrimidin-2,4-diones were identified as an early lead class from a GABA screening program at FMC. Compound 1 had moderate activity in our GABA [3H]EBOB binding assay (IC_{50} = 10 μM) with measurable whole organism activity against mosquito (*A. aegypti*), however, it caused sever phytotoxicity in our herbicide screen. Although we were able to increase the in vitro activity to nM levels, reduce phytotoxicity, and achieve whole organism activity below 10 ppm, we were still challenged by soil degradation and mammalian toxicity issues. Work toward addressing these translation issues will be presented.



28. Factors involved in the field translation of a class of mitochondrial Qi inhibitor fungicides

John W Owen, Yelena Adelfinskaya, Zoltan Benko, and Christian T Schobert, Discovery Research, Dow AgroSciences, L.L.C, 9330 Zionsville Road, Indianapolis, IN 46268, wjowen@dow.com

Translation of fungicidal efficacy from lab and/or greenhouse testing to the field situation can be quite complex, but is certainly impacted by such factors as compound potency, spectrum, application frequency, metabolic & environmental stability, delivery systems, rainfastness, physical properties and their impact on redistribution in host plants and crop canopies, and pathogen biotypes. A number of these factors will be illustrated with examples from within classes of fungicidal chemistries that inhibit mitochondrial electron transport, but primarily from a series of potently Oomycete active N-formylaminosalicylamides. This class of chemistry inhibits mitochondrial respiration at the Qi site, orientated towards the inner surface of the inner mitochondrial membrane. Multiple field trial data indicated inconsistent foliar uptake and plant distribution as a significant activity translation barrier for this chemistry, supported by the necessity for the use of a penetrating adjuvant (such as crop oil concentrate) as a tank mix in order to deliver curative efficacy vs Plasmopara. Data generated on the physical properties and membrane permeation in particular of individual N-formylaminosalicylamides suggest a clear basis for their inadequate redistribution behavior in grape-vines. Subsequent laboratory studies pointed to xylem unloading rather than bioavailability of 'in tissue' located active ingredient as a key obstacle to delivering robust systemic protectant activity with this chemistry.

29. A structure-based design approach to plant selective 4-hydroxyphenylpyruvate dioxygenase inhibitors

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A high degree of selectivity toward the target site of the pest organism is a desirable attribute for new safer agrochemicals. To assist in the design of novel herbicides, we determined the crystal structures of the herbicidal target enzyme 4-hydroxyphenylpyruvate dioxygenase (HPPD; EC 1.13.11.27) from the plant Arabidopsis thaliana with and without herbicidal inhibitors and from a mammalian (rat) HPPD in complex with an inhibitor. Detailed comparisons of the plant and mammalian HPPD-ligand structures suggest a structural basis for the high degree of plant selectivity of certain HPPD inhibitors and point to design strategies to obtain potent and selective inhibitors of plant HPPD as agrochemical leads. The design, synthesis, and testing of a set of novel tetramic acid inhibitors will be described.

30. Polycyclic dinitriles: Low nanomolar GABA-ergic insecticides, a pharmacophore and a new radioligand for insect GABA receptors

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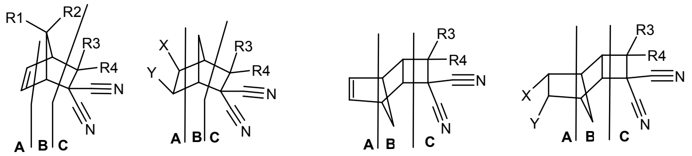
The polycyclic dinitriles are a potent class of insecticides which are non-competitive GABA antagonists acting at the convulsant site. This class of compounds displaces TBPS and EBOB from both insect and rat brain tissue with Ki's in the low nanomolar range. We will discuss comparative in vitro and in vivo potencies in insect and mammalian species. Using molecular modeling we have developed a pharmacophore model that unifies this class and some previous classes of GABA antagonist convulsants. Key pharmacophore elements are a polarizable functionality separated by a fixed distance from two electrophilic elements. These compounds are prepared by cycloaddition of dienophiles with substituted cyclopentadienes or quadricyclanes. Using a variety of cycloaddition partners and post-cycloaddition modifications we have been able to thoroughly explore substituent space. In addition, we have discovered a novel radioligand which is a useful probe for the GABA convulsant site in pest insect species.



31. 2,4-Diaminoquinazoline insecticides

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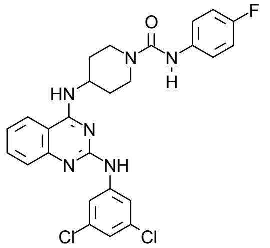
2,4-Diaminoquinazolines are easily prepared and optimized to high activity against tobacco budworm in a surface treated diet assay. 2,4-Dichloroquinazoline was treated with an appropriately protected 4-aminopiperidine, followed by reaction with an aniline at high temperature to prepare the desired targets. These compounds were 10 to 100-fold less active than expected in a foliar assay. A number of possible reasons for this poor diet to foliar translation were explored including metabolism and formulations.



32. Use of SPME for measuring bioavailable concentrations

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In multi-phase matrices, phase distribution determines the bioavailability and hence the ecotoxicological effects of a chemical. For a hydrophobic compound, it is well recognized that its availability for bioaccumulation or toxicity is reduced due to association with colloidal particles and dissolved organic matter (DOM). As fine colloidal particles and DOM are essentially inseparable from the aqueous phase, quantifying bioavailable concentrations is a great challenge. This presentation will discuss the use of solid-phase microextraction (SPME) for detecting bioavailable concentrations in various matrices, with a focus on pyrethroid insecticides. Our studies show that SPME fibers mimic membranes or lipids of aquatic organisms, and chemical accumulation in the SPME fiber is parallel to bioaccumulation or toxic effects observed in test animals. SPME can therefore be used as a “biomimetic” surrogate to estimate chemical bioavailability in sediment porewater, soil, runoff effluents, or “brown” surface water.

33. SPE strategies for determination of nitrofuran antibiotic metabolites in honey and tissue

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Antibiotics such as oxytetracycline are approved for use in beekeeping for treatment of bacterial bee infections such as American foulbrood (AFB). However, AFB bacteria have developed significant resistance to oxytetracycline. Unfortunately, in search for alternative treatments, some beekeepers have resorted to the use of unapproved antibiotics for control of AFB and other bee infections. Among the antibiotics illegally used in beekeeping is nitrofurazone, a nitrofuran antibiotic. When nitrofurazone is administered to a bee colony, semicarbazide, a metabolite, may be found in trace levels in the honey product. Other nitrofuran antibiotics, furaltadone, furazolidone and nitrofurantoin are illegally used in veterinary agriculture. In this presentation, we will review current procedures for determination of these compounds in honey and demonstrate improved sample preparation suitable for tandem LC-MS as well as LC-TOF analysis. Also, the suitability or those procedures will be investigated for some very different sample matrices such as shellfish and poultry.

34. Stability and degradation of antibiotic residues in honey

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Oxytetracycline (OTC) has been used since the 1950s for control of American Foulbrood, a devastating bacterial disease of honey bees, but bacterial resistance is now widespread. Tylosin has been selected as an alternative, and FDA approval is pending. Tylosin, however, is more stable than OTC, with a half-life in sucrose syrup of from 75–186 days at 34C (hive temperature) depending on the purity of the sugar in the syrup. The lack of UV-absorbing impurities in sugar syrup allowed direct injection of syrup samples onto the HPLC column. This was not possible with honey, but solid phase extraction of tylosin from honey, followed by HPLC determination enabled measurement of the rate of decomposition of tylosin in honey at the same temperature. Tylosin is hydrolyzed to desmycosin (a related antibiotic with equal biological activity) with a half-life of approximately 4 months at 34C.

35. Streamlining sample preparation and LC-MS/MS multiresidue analysis of antibiotics in animal tissues

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For enforcement and surveillance purposes, the multiresidue analysis of antibiotics in samples of animal origin has been traditionally done mainly by semi-quantitative microbial inhibition assays. Microbial assays offer relatively low-cost and high-throughput detection, but they do not work sensitively for all antibiotics classes (aminoglycosides and aminocyclitols, beta-lactams, fluoroquinolones, lincosamides and macrolides, sulfonamides, tetracyclines etc.) and cannot usually distinguish particular analytes within a class. Also, the assays are prone to unidentifiable microbial inhibitions, which occurrence complicates the situation even further. Confirmatory identifications based on physico-chemical techniques are necessary to verify the results, but their scope is often limited to a particular analyte or class. Thus, it is highly desirable to develop and implement reliable and cost-effective physico-chemical (instrumental) methods for multiclass, multiresidue analysis of antibiotics (and other veterinary drugs), which should provide a more efficient way to conduct regulatory monitoring of the food supply. Recent advances in liquid chromatography-tandem mass spectrometry (LC-MS/MS) have provided the opportunity to identify and quantify most of the veterinary drugs (potentially even in one analytical run). Development of a uniform sample preparation strategy remains a very challenging task because of the relatively wide range of analyte properties and complexity of animal matrices, mainly due to different sample types (muscle, liver, kidney, hair, urine or blood from different animals, and also milk or eggs). This leads to the presence of different matrix co-extractives and diverse analyte-matrix interactions, thus different problems in terms of analyte extractability, stability and detectability. This presentation will discuss the above challenges and describe streamlined analytical approaches used in our laboratory, such as dispersive solid-phase extraction for fast sample clean-up or the echo peak technique for improved quantitation and data processing in the LC-MS/MS analysis.

36. Tissue binding and metabolism of the avicide 3-chloro-4-methylaniline hydrochloride in red-winged blackbirds and dark-eyed juncos

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The avicide 3-chloro-4-methylanaline hydrochloride (chloro-p-toluidine hydrochloride, CPTH, DRC-1339) is used to control pest bird species which damage agricultural crops. This chemical appears to pose minimal hazard to mammalian species (LD_{50}’s greater than 1000 mg/kg) while being extremely toxic to the target species (LD_{50} for starlings <10 mg/kg). To date, no definitive assessment of the mode of action has been performed. Previously published research demonstrated that CPTH is eliminated from exposed birds by a two-compartment model, with very rapid elimination occurring between time zero and 4 hours and a much slower elimination phase occurring after that. The exact nature of these residues had not been determined. To investigate the nature of the residues, ring-labeled ^{14}C-3-chloro-4-methylaniline hydrochloride was delivered to 3 red-winged blackbirds (Agelaius phoeniceus) and 2 dark-eyed juncos (Junco hyemalis) via oral gavage. The birds were euthanized 1 hour after dosing and the tissues subjected to sequential extraction with organic solvents, acid digestion, and finally combustion of bound residues. Direct measurement of radioactivity as well as measurement following combustion was accomplished using a liquid scintillation counter. Tightly bound residues accounted for 8.5% of the recovered radioactivity in juncos, while 20% was bound to blackbird tissues. The majority (74%) of the bound radioactivity was found in the GI tract of juncos. In the more sensitive blackbird species, 50% of the radioactivity was tightly bound to kidney tissues, suggesting that CPTH is acting as a nephrotoxin in sensitive target species.

37. HPLC determination of Nicarbazin in avian whole blood, blood solids, and plasma fractions

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Nicarbazin is currently being evaluated as an infertility agent in waterfowl by researchers at the USDA/APHIS/WS/National Wildlife Research Center. Blood samples were drawn from a mixed (age/gender) population of mallards ducks fed a 500 µg/g Nicarbazin fortified corn bait. The blood samples were subdivided as plasma, blood solids, and whole blood fractions and subsequently analyzed by high performance liquid chromatography. Details of the method developed for the analysis of the whole blood and blood solids fractions are presented. Concentrations of Nicarbazin in the whole blood samples were highly correlated with the concentrations determined in the separated plasma and blood solids fractions using linear regression analysis. The whole blood method was developed to support field work where blood sample storage and processing issues preclude the preparation of plasma.

38. Award Address. Metabolism and effects of organophosphorus insecticides

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The primary biochemical lesion of the organophosphorus insecticides (OP's) is the persistent inhibition of brain cholinesterase. This persistent phosphorylation of brain cholinesterase by the oxons induces compensatory reactions in the neurochemistry. The metabolism of phosphorothionate insecticides is complex, involving important activations and detoxications by cytochromes P450 and important detoxications of the active metabolites, the oxons, by carboxylesterases (stoichiometric) and A-esterase (paraoxonase) (catalytic). The rates and/or effectiveness of these several metabolic pathways vary substantially among various compounds, and are important biochemical determinants of the acute toxicity levels. The various efficiencies of these routes of metabolism affect the detoxication of OP's when they are present in mixtures, and subsequently the amount of brain cholinesterase inhibition observed *in vivo*. Knowledge of *in vitro* parameters and interactions allows prediction of many *in vivo* observations. (Supported by NIH R01 ES11287, NIH R01 ES10386 and American Chemistry Council CRAM 2a-99).

39. One source of genetic variability affecting the detoxication of chlorpyrifos and diazinon

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The observation that a reaction observed in vitro results in the hydrolysis of a specific organophosphorus compound (OP) does not indicate that the reaction plays a physiologically significant role in the detoxication of that OP. Chambers and coworkers had predicted, based on rates of hydrolysis of low concentrations of paraoxon and chlorpyrifos oxon, that the plasma enzyme paraoxonase 1 (PON1) would be important in the detoxication of chlorpyrifos oxon, but not paraoxon. The development by Lusis and coworkers of PON1 null mice and transgenic mice expressing the high-activity paraoxonase alloform (PON1R192) and the low-activity paraoxonase alloform (PON1Q192) on the PON1 null background has allowed this question to be addressed more directly. PON1 null mice exhibited dramatically increased sensitivity to exposure to chlorpyrifos oxon or diazoxon, but not to paraoxon, confirming Chamber's prediction that PON1 plays an insignificant in vivo role in the detoxication of paraoxon.

40. *In vitro* studies using human tissues as a tool to identify inter- and intra-species differences in pesticide metabolism

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Most modern synthetic pesticides are lipophilic compounds and require extensive metabolism to be excreted after absorbed in body. Metabolism has been suggested to be one of the major factors determining the toxicity of pesticides. However, metabolic studies performed in laboratory animals resulted in many uncertainties when extrapolated to human health. Data from in vitro human studies can provide useful information to reduce or redefine those uncertainties. In vitro human metabolism of chlorpyrifos, carbaryl, and fipronil has been studied using human and rat liver microsomes and human recombinant cytochrome P450 (CYP). Rat liver microsomes displayed higher activities than pooled human liver microsomes toward these three pesticides in their major metabolic pathways. CYP3A4, 2B6, 2C19, and 1A1/2 were identified to be the major CYP isoforms responsible for metabolizing these pesticides. The difference in metabolic activity toward these pesticides can be as great as 40 times in the human population. The results of these studies can be used to address the uncertainties of inter- and intra-species extrapolations in metabolism.

41. Metabolic interactions of agrochemicals in humans

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Agrochemicals and other xenobiotics are metabolized by xenobiotic-metabolizing enzymes (XMEs) to products that may be more or less toxic than the parent chemical. In this regard, phase I XMEs such as cytochrome P450s (CYPs), are of primary importance. Interactions at the level of metabolism may take place via either inhibition or induction of XMEs. Such interactions have often been investigated, in vitro, in experimental animals, using subcellular fractions such as liver microsomes, but seldom in humans or at the level of individual XME isoforms. We have been investigating the metabolism of a number of agrochemicals by human liver microsomes and recombinant CYP isoforms and have recently embarked on studies of the induction of XMEs in human hepatocytes. The insecticides chlorpyrifos, carbaryl, carbofuran and fipronil, as well as the repellant DEET, are all extensively metabolized by human liver microsomes and, although a number of CYP isoforms may be involved, CYP2B6 and CYP3A4, are usually the most important. Permethrin is hydrolyzed by esterase(s) present in both human liver microsomes and cytosol. A number of metabolic interactions have been observed. Chlorpyrifos and other phosphorothioates are potent inhibitors of the CYP-dependent metabolism of both endogenous substrates, such as testosterone and estradiol, and exogenous substrates, such as carbaryl, presumably as a result of the interaction of highly reactive sulfur, released during the oxidative desulfuration reaction, with the heme iron of CYP. The hydrolysis of permethrin in human liver can be inhibited by chlorpyrifos oxon and by carbaryl. Fipronil can inhibit testosterone metabolism by CYP3A4 and is an effective inducer of CYP isoforms in human hepatocytes.

42. Key questions when addressing the efficacy, environmental behavior and side effects of chiral pesticides

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The last years have seen the successful replacement of a series of racemic pesticide active ingredients with enantiopure or enantioenriched ones (“chiral switches”), thus offering various advantages: reduced amount of pesticide to be synthesized and formulated, higher specific activity in the field and reduced deployment of inactive pesticides into the environment. A closer look at the advantages of using enantiopure pesticides often reveals open questions and analytical and environmental-chemical challenges to be answered. A comprehensive understanding of the stereochemistry of the active ingredient molecule, including the exact composition of the technical material, as well as the role and stability of possible conformers, rotamers, etc., forms the basis of all further considerations. As the generation of data on efficacy toxicology or environmental behavior of individual stereoisomers is not required by the relevant guidelines in most countries, these data are often not available upon the first registration of a new pesticide. In many cases, when such data are generated over time and particularly when a compound is successful in a competitive market, a chiral switch may become beneficial both from a commercial and from an environmental point of view. In our presentation we discuss important aspects of environmental behavior and fate, ecotoxicology, and residue formation on food and in the environment, of chiral compounds using selected case histories from the field of modern pesticides such as MCPP, propiconazole, metolachlor and others.

43. Chiral switch from metalaxyl to metalaxyl-M: Lessons learned from a registration authority perspective

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Chiral pesticides often undergo enantio-/stereoselective degradation in soils. In the case of the metalaxyl, an important fungicide used to control pathogens such as Phytophthora, the fungicidally active R-enantiomer degraded faster in soil than the inactive distomer, with no detectable racemization. Though already the racemic metalaxyl was judged to be an environmentally friendly compound, the introduction of metalaxyl-M, the enantiopure R-metalaxyl, to the market, was considered to lead to further reduced exposure of soil and non-target species. Results published later showed that the stereoselectivity of metalaxyl degradation may be different in different soils. Therefore, we investigated the enantioselective degradation of R- and S-metalaxyl in twenty different soils, selected to cover a wide range of soil properties (e.g., acidic/alkaline soils, aerobic/anaerobic), rather than to consider soils of agricultural importance. Racemic metalaxyl was incubated in these soils under laboratory conditions and the degradation of the enantiomers as well as the enantioselective formation/degradation of the primary major metabolite, metalaxyl acid, was followed over time, using enantioselective GC-MS after ethylation with diazoethane. Our results confirmed that the enantioselectivity varies strongly between soils and apparently correlates with the soil pH. In alkaline to slightly acidic soils, the R-isomer is degraded faster, whereas in acidic soils (pH < 4), the S-isomer is degraded faster. Reevaluation of published kinetic data for the herbicides dichlorprop and mecoprop indicated a similar correlation between enantioselectivity and soil pH as for metalaxyl. These results clearly show that for a comprehensive understanding of stereoselective degradation in soil, studies are required in different soils, covering a wide range of soil properties.

44. Modern chiral pesticides: Chirality and its significance in some currently used chiral herbicides in Nigeria

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Pesticides can be described as any substance or mixture of substances used to kill, repel or otherwise control a pest. Many pesticide molecules are chiral (asymmetric) and thus have a non-superimposable mirror image or enantiomer. Chiral pesticides constitute about one quarter of all pesticides in the market while the rest are sold as 1:1 mixture of two enantiomers (racemates). Chirality occurs widely in synthetic pyrethroids and organophosphates which are the mainstay of modern pesticides. Enantiomers of single chiral pesticides can differ significantly among each other in their biological activity, environmental persistence and other important properties. This paper tends to review the environmental risks and significance of chirality in some currently used chiral herbicides in Nigeria.

45. Bioaccumulation and enantioselective biotransformation of fipronil and selected conazole fungicides

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Presently, there is a lack of understanding about the accumulation of currently used chiral pesticides and their enantiomers in aquatic biota due to their susceptibility to biotransformation. Because biological processes such as metabolism are stereospecific, selective elimination or biotransformation of one enantiomer may occur. In this research, bioaccumulation and enantioselective biotransformation data were determined for rainbow trout (Oncorhynchus mykiss) exposed separately to the phenylpyrazole insecticide fipronil and to a series of selected conazole fungicides. Preliminary results indicate the rapid elimination of fipronil in fish ($t_{1/2} = 0.5$ d), corresponding to preferential metabolism of the (+) enantiomer as indicated by non-racemic residues. The results of this study indicate that chiral analysis may serve as a tracer for biotransformation in fish, which are considered to have limited metabolic capability. Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

46. Chirality in currently used insecticides and its environmental implications

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Chirality occurs widely in several insecticide classes that have heavy current use. These include synthetic pyrethroids and some organophosphate compounds. Compared to other compound classes (e.g., organochlorine insecticides and some herbicides), our knowledge about enantioselective behaviors of these chiral insecticides is quite limited. Here we will provide an overview of our research results on this topic since 2001. So far we have considered four pyrethroid insecticides, bifenthrin, permethrin, cypermethrin, and cyfluthrin, and three chiral organophosphate compounds, fonofos, profenofos, and trichloronate. We will summarize progresses related to development of analytical methods for resolving enantiomers on chiral HPLC or GC columns, and evaluation of enantioselectivity in aquatic toxicity and during biodegradation in soil and sediment. At the end we will outline future research needs and interests.

47. Degradation of Indoxacarb and its R-enantiomer in soil, sediment and water

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Indoxacarb ((S)-methyl 7-chloro-2,5-dihydro-2-[[(methoxycarbonyl)[4-(trifluoro methoxy)phenyl]amino]carbonyl]indeno[1,2-e][1,3,4]oxadiazine-4a(3*H*)-carboxylate) is a chiral insecticide developed by E.I. du Pont de Nemours and Company. The manufacturing process used to produce indoxacarb can also form the insecticidally-inactive R-enantiomer. Mixtures of indoxacarb and its R-enantiomer have been registered in many countries for the control of lepidopteran pests in various crops. The route of degradation of mixtures of indoxacarb and its R-enantiomer has been studied in soils and aquatic (water and sediment) systems. Chiral HPLC methods have been used to measure the concentrations of indoxacarb and its R-enantiomer over time and to measure any changes in the enantiomeric ratio in these environmental matrices. A change in the enantiomeric ratio would suggest differential degradation of the two enantiomers. The data shows no change in enantiomeric ratio over time; therefore, there is no differential degradation of indoxacarb and its R-enantiomer in soil, sediment and water.

48. Degradation of Indoxacarb and its R-enantiomer in rats, livestock and fish

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Indoxacarb ((S)-methyl 7-chloro-2,5-dihydro-2-[[(methoxycarbonyl)[4-(trifluoro methoxy)phenyl]amino]carbonyl]indeno[1,2-e][1,3,4]oxadiazine-4a(3H)-carboxylate) is a chiral insecticide developed by E.I. du Pont de Nemours and Company. Current production of indoxacarb also forms the insecticidally-inactive R-enantiomer. Mixtures of indoxacarb and its R-enantiomer have been registered in many countries for the control of lepidopteran pests in crops. The route of degradation of mixtures of indoxacarb and its R-enantiomer has been studied in plants, rats, cows, hens and fish. Chiral HPLC methods have been used to measure the concentrations of indoxacarb and its R-enantiomer in crops and tissues. The data revealed some differences in the absorption, distribution and/or metabolism of indoxacarb and its R-enantiomer.

49. Human carboxylesterases and their role in pyrethroid metabolism

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The carboxylesterases (CEs) are an important family of xenobiotic-detoxifying enzymes found in the mammalian liver. These promiscuous enzymes catalyze the hydrolysis of several drugs and pollutants, including pyrethroid and organophosphate insecticides. Pyrethroids rank second only to organophosphates in terms of total insecticide usage in U.S. agricultural practices. Thus, human populations are widely exposed to these compounds; however, a role for pyrethroids in the etiology of human disease has not been elucidated. The identities of the human carboxylesterases responsible for pyrethroid detoxication are still incompletely defined. Two human hepatic CE enzymes (hCE1 and hCE2) have recently been cloned and recombinantly expressed (Morton and Potter, 2000). We have used these enzymes to study the hydrolysis of model pyrethroid compounds and examine the substrate specificity of these enzymes. We have also compared the levels of hCE1 protein in 11 human livers (determined by immunoblotting) with the inter-individual variability of hydrolysis rates toward trans-permethrin. The pure hCEs exhibit markedly different kinetic parameters toward pyrethroid substrates. For example, the catalytic efficiency (k_{cat}/K_m) of hCE1 was 5.2-fold greater than for hCE2 with respect to the hydrolysis of trans-permethrin. Furthermore, 1*R*, trans-resmethrin was efficiently hydrolyzed by hCE1, but hCE2 had no catalytic activity. Individual human liver microsomes demonstrated >4-fold variability in their trans-permethrin hydrolysis rates and immunoinhibition experiments using anti-hCE1 antibody blocked up to 80% of the trans-permethrin hydrolysis activity in human liver microsomes. Despite these findings, hCE1 protein levels did not correlate with trans-permethrin V_{max} values in the human samples. Thus, we are currently exploring the possibility that the glycosylation state of the hCE1 protein may influence pyrethroid hydrolytic activity. (Supported by NIH P20RR017661)

50. Exactly the same but different: Analysis and implications of the promiscuity of ligand-dependent activation of the Ah receptor signaling pathway

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The aryl hydrocarbon receptor (AhR) is a ligand-dependent transcription factor that mediates many of the biological and toxicological actions of structurally related halogenated and polycyclic aromatic hydrocarbons, including that of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD, dioxin). Observations that the AhR can also bind and be activated by structurally diverse synthetic and naturally-occurring chemicals and classes of chemicals suggest that our current ideas regarding AhR ligand structure are too simplistic. To further define the actual spectrum of AhR ligand structure, we used several recombinant AhR-dependent high-throughput screening bioassays to identify and characterize novel AhR activators and inhibitors present in large collections of chemicals (both synthetic and natural). While these studies have resulted in the identification of many new exogenous and endogenous AhR ligands (agonists and antagonists), the majority of which are relatively weak, they clearly demonstrate a significant degree of structural diversity in AhR ligand binding specificity and suggest that many more AhR ligands remain to be identified. The presence of AhR ligands/agonists/antagonists in crude extracts of various different vegetables, fruits and herbs as well as numerous commercial and consumer products support this conclusion. The identities of the responsible chemicals in these extracts are being assessed. The structural diversity of AhR ligands also suggests that the AhR contains a very promiscuous ligand binding pocket, however, the absence of an actual 3D structure of the AhR ligand binding site has hindered detailed analysis of the structural basis for ligand binding and signaling specificity. We have used a 3D homology model of the AhR ligand binding domain based on the crystal structures of homologous PAS amily members to analyze and characterization residues involved in ligand (TCDD) binding. This analysis will provide insights into the mechanisms by which structurally diverse ligands can bind to and activate the AhR and AhR-dependent toxic and biological effects.

51. Predictive xenobiotic metabolomics: Integrating biochemical toxicology with computer modeling

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The recent emphasis on the application of “systems biology” to biomedical research invariably traces its origin to “cybernetics,” as advanced by Norbert Wiener in the mid 20th century. In those early days, the integration of “computing machines” and biology was advocated by a handful of visionaries. Our research group, in the past 15 years, has attempted such a systems biology approach towards the advancement of chemical mixture toxicology. Specifically, we aim to integrate computational modeling with in vitro and in vivo experimentation to address the question “How does one deal with the potentially astronomical number of combination of chemicals and other possible stressors in the context of cumulative risk assessment?” Our answer is to first focus on the fundamental biological and toxicological processes occurring in the normal system. The idea is that once we have sufficient understanding of normal biological processes, all stimuli and insults from external stressors can be treated as perturbations to these processes. The next step is to capture the essence of these processes into modeling frameworks by integrating recent advances in computational technology and modern biology. In the case of complex chemical mixtures and their interactions, the computer-assisted approach of Biochemical Reaction Network Modeling offers a ray of hope. The possible linkage between this novel computational methodology and physiologically-based pharmacokinetic (PBPK) modeling could result in a multi-scale computer simulation platform capable of predicting complex pathway interactions and metabolite concentrations at the molecular level up to tissue and organ concentrations and exposures at the organism level.

52. Comparative detoxication of organophosphates by serum and liver esterases of neonatal, juvenile and adult rats

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Detoxication of 12 organophosphates (OP's) by esterases was studied in tissues from neonatal, juvenile and adult rats. Carboxylesterases in homogenates of adult liver detoxified all OP's tested except methyl coumaphos oxon, but, in general, diethyl OP's were detoxified to a greater extent than dimethyl OP's. None of the dimethyl OP's were detoxified by carboxylesterases of neonatal or juvenile liver or of juvenile or adult serum. Liver and serum A-esterase (paraoxonase) showed significant detoxication of only 4 of the 12 OP's. Activities of the carboxylesterases and A-esterase were higher in liver than in serum, and were highest in adults and lowest in neonates. Lower esterase activity in young animals is likely to be responsible, at least in part, for the greater sensitivity of young animals to some OP's. Supported by NIH R01 ES11287.

53. Multi-step model for the molecular mechanism of organophosphates binding with acetylcholinesterase

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It is well established that the primary toxicity of organophosphates comes from their inhibition of the enzyme acetylcholinesterase (AChE). Specifically, the organophosphate irreversibly phosphorylates the active-site serine of AChE. What is not well understood is the chemical mechanism that leads to this phosphorylation. To address this question we have run a series of molecular dynamics simulations of mouse AChE interacting with the organophosphate metabolite paraoxon. These simulations suggest that the paraoxon initially forms a non-covalently bound complex, where the oxon sits in the entrance channel of the AChE. The next step involves the relaxation of the protein structure to accommodate the oxon into the protein's active site. The final step is the actual phosphorylation reaction. This mechanism is in contrast to the reaction of acetylcholine with AChE, where the only intermediate is with the substrate already in the active site of the protein.

54. Mechanism of selective toxicity of insecticides in mammals and insects

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Whereas the mechanism of selective toxicity of various insecticides in mammals and insects varies considerably, it is becoming abundantly clear that for certain insecticides the selectivity is due to differential sensitivity of target receptors to the insecticides. In some cases, a sensitive insecticide target receptor is found in insects but not in mammals. We will provide a few such examples from our recent studies. Fipronil blocks the GABA receptors much more potently in cockroaches than in rats. Furthermore, fipronil potently blocks the glutamate-activated chloride channels that are present in invertebrate including cockroaches but not in mammals including rats. These differences clearly explain the selective toxicity. Indoxacarb blocks the cockroach sodium channels more potently than the rat sodium channels; this also contributes to the selective toxicity. The major action of pyrethroids is to prolong the opening of the sodium channels thereby causing hyperexcitation. Large differences in sodium channel sensitivity to pyrethroids have been demonstrated between cockroaches and rats. The molecular mechanism that underlies these differential sensitivities remains to be seen, yet it is most likely to be due to some differences in the amino acid compositions of the target receptors/channels between mammals and insects.

55. Mathematical manipulations of enantiomeric data

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The measurement of enantiomeric parameters such as enantiomeric ratio (ER) and enantiomer fraction (EF) are subject to mathematical and statistical pitfalls. Typical integrators give poor results for low responding compounds or peaks that are not baseline resolved, leaving the analyst no choice but manual integration. Researchers often calculate the average of a group of samples and then compare it to literature values. Because of the properties of ratio functions, using an arithmetic mean can be misleading. Converting average ERs to the EF scale can lead to discrepancies in the true value. This work describes some powerful alternatives to problematic mathematics. Peak fitting can provide error estimate data in addition to area, and minimizes analyst bias. Statistical problems can be avoided through the use of nonparametric statistics. Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

56. Investigating the enantioselective toxicity of conazole fungicides in rainbow trout through the use of NMR-based metabonomics

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The conazole fungicides represent a large group of compounds widely used agriculturally for the protection of crops and pharmaceutically in the treatment of topical and systemic infections. Almost all conazoles possess at least one chiral center and thus exist as a pair of enantiomers with differing biological properties. The determination of any enantioselective toxicity is essential to accurate risk assessment. In support of the Environmental Protection Agency's Computational Toxicology Program, metabonomics, the quantitative measurement of a broad spectrum of metabolic responses of living systems in response to disease onset or genetic modification, is being employed to enable rapid identification of mechanisms of toxicity for compounds of environmental concern. Recently, we have begun to investigate the potential for this new technology to differentiate the toxicities of the enantiomers of triadimefon and other conazoles in rainbow trout using nuclear magnetic resonance (NMR) spectroscopy. Preliminary NMR data show a significant metabolic response to racemic triadimefon, fed to the trout through gavage, as indicated by differences in the endogenous metabolite pattern from that of a control. Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

57. *In vitro* phase I metabolism of the triazole fungicide bromuconazole and its four enantiomers

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Triazole and imidazole containing chemicals are frequently used as antifungal agents due to their ability to inhibit fungal sterol synthesis. In nearly all cases, these fungicides are chiral, with most containing multiple chiral centers. The triazole fungicide bromuconazole contains two chiral centers and exists as two diastereomers, each with two enantiomers. It has been widely used as a mixture of its diastereomers on food products. Here we report on the in vitro metabolism of the individual and combined diastereomers and enantiomers of bromuconazole. Although the enantiomers have tentatively been shown to produce the same phase I metabolism products (i.e., hydroxylation of the dichlorophenyl ring), the rates of bromuconazole depletion and product formation differ dramatically. Docking studies with cytochrome P450 3A4 are being planned in an attempt to explain these differences. Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

58. Determination of metolachlor ethanesulfonic acid (ESA) enantiomers in water by chiral LC/MS/MS

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The chloroacetanilide herbicide, metolachlor, was introduced into the marketplace in 1976 as a racemic mixture of two pairs of diastereomers, 1'S (aS,1'S/aR,1'S) and 1'R (aR,1'R / aS,1'R). In 1997, S-metolachlor, consisting of an 88:12 ratio of 1'S:1'R isomers was registered as a reduced risk herbicide which allowed the reduction of the application rate and environmental loading by 35%. A primary environmental degradate, metolachlor ethanesulfonic acid (MOC-ESA), (2-[(2-ethyl-6-methylphenyl)-(2-methoxy-1-methylethyl) amino]-2-oxo (R)(S) exhibits the same chirality as metolachlor (2 stereogenic centers). To aid in the environmental monitoring of the degradates from the two different metolachlor formulations, an enantioselective method was developed to separate the diastereomers of MOC-ESA in both ground and surface water. Samples are analyzed using reversed-phase (C18) solid-phase extraction and chiral HPLC with mass spectrometric detection (LC/MS/MS). Electrospray ionization in the negative mode is utilized to achieve an analyte limit of quantitation (LOQ) of 1.0 ppb.

59. Determination of the ratio of the 1'S and 1'R diastereomers of metolachlor and S-metolachlor in soil and water by stereoselective immunoassays

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S-metolachlor is a reduced risk herbicide registered under the EPA's Reduced Risk Initiative. S-metolachlor contains an 88:12 ratio of the 1'S to 1'R diastereomers in contrast to the 50:50 ratio in metolachlor. Stereoselective immunoassays for 1'S and 1'R were developed to quantitate the diastereomers in soil and water samples. Soil samples collected as part of an S-metolachlor field dissipation study in Georgia were found to maintain the 88:12 ratio of 1'S to 1'R up to 540 days post-application. Half of the metolachlor residues in ground and surface water samples collected in eleven states prior to the introduction of S-metolachlor were determined to be 1'R, reflective of the 50:50 ratio of metolachlor. Ground and surface water samples collected subsequent to the registration of S-metolachlor were found to contain a gradient of residues increasingly enriched in 1'S. Based on these data, the profile of 1'S and 1'R residues in environmental samples is consistent with the applied formulation. Stereospecific degradation of either diastereomer was not observed.

60. Selectivity in aquatic toxicity and biodegradation of the herbicide Metolachlor

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Racemic metolachlor contains two R-enantiomers and two S-enantiomers. S-metolachlor is used increasingly in place of rac-metolachlor, for the two S enantiomers have about 90% of the herbicidal activity. We compared the acute and chronic toxicity of rac- and S-metolachlor to Daphnia magna (D. magna) and measured their biodegradation in soil. The acute 24-h LC50 for rac- and S-metolachlor to D. magna was 69.4 and 51.2 mg/L, respectively, indicating that the acute toxicity of S-metolachlor is slightly higher. In chronic toxicity tests, the LOEC, NOEC, days to first brood, length, longevity, number of broods per female, number of young per female and intrinsic rate of natural increase (r) were determined. The results indicated that rac-metolachlor possessed significantly ($P < 0.05$) more chronic toxicity than S-metolachlor to D. magna. In soil, S-metolachlor degraded faster than rac-metolachlor; after 42-days incubation, 73.4% of rac-metolachlor and 90.0% of S-metolachlor were degraded. Degradation in sterilized soil showed no selectivity, confirming that degradation in the natural soil was biologically mediated. Selectivity in toxicity and degradation should be considered when the environmental behavior of metolachlor products is assessed. *The research was supported by the National Key Project for Basic Research (2002CB410800).

61. Repellency of catnip and Osage orange essential oils to two mosquito species

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Recent research has focused on the repellent properties of extracts from the catnip plant (*Nepeta cataria*) and the Osage orange (*Maclura pomifera*) fruit. This study evaluated catnip and Osage orange essential oils, and a sesquiterpene found in Osage orange, elemol, for repellency to the northern house mosquito (*Culex pipiens*) and the yellow fever mosquito (*Aedes aegypti*). Treatments were compared to commercial standard mosquito repellents, N,N-diethyl-*m*-toluamide (DEET) and citronellal. Short-term and residual repellency was evaluated in a static-air bioassay and mosquito distribution was observed over 180-minutes. Tests conducted with *A. aegypti* were observed for an extended 360-minute period. Mosquito repellency data was analyzed as percentage and contact repellency. Individuals responded with high percentage repellency to surfaces treated with catnip essential oil. In the residual repellency study, the high initial repellency to catnip oil significantly decreased over the 180-minute period. Elemol and DEET treatments did not show a negative relationship between percentage repellency and time. Bioassays conducted with *A. aegypti* showed similar trends in repellency with DEET and elemol-treated surfaces. Surfaces treated with elemol or DEET exhibited greater significance in contact repellency compared to catnip essential oil.

62. Effects of dietary conjugated linoleic acid on the European corn borer

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Conjugated linoleic acid (CLA) has been shown to adversely affect the rate of egg production and body weight gain in hens when fed a 5% CLA diet. The proportions of fatty acids in the egg yolk lipids were also shown to be significantly altered. Several studies have shown decreased unsaturated fatty acids in tissues after feeding a CLA-incorporated diet. Little is known of the effects of a CLA-enriched diet on insects. Our hypothesis is that insects may react similarly to hens in their response to dietary CLA; they may demonstrate decreased egg production, altered lipid profiles of the egg, and growth inhibition. Thus, CLA may have potential for insect control. Our objectives in this study were to examine the effects of CLA on the survival, development, and egg production of the European corn borer (ECB), Ostrinia nubilalis. ECBs were fed artificial diet optimized for ECB with various amounts of CLA or linoleic acid (0.005 to 5.0% of the diet) and reared to maturity in individual diet cups in an incubator set at 80 o F, 70-75% humidity, and constant lighting. Pupal mass was measured, and maturation rate was monitored by measuring time to pupation and adult emergence. After emergence, adults will be kept for breeding trials to study dietary CLA effects on egg production and lipid composition. Males from the CLA-treatment groups will be bred with both CLA-treated and untreated females; untreated males will also be bred with both CLA-treated and untreated females. Egg masses will be collected and the lipid profiles determined.

63. A brain detoxifying enzyme for organophosphorus nerve poisons

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Organophosphorus (OP) insecticides and chemical warfare agents act primarily by inhibiting acetylcholinesterase. There are many secondary targets for OP toxicants as observed for example with the major insecticide chlorpyrifos and its bioactivated metabolite chlorpyrifos oxon (CPO). It was therefore surprising that the predominant mouse brain protein labeled in vitro by [3H-ethyl]CPO (1 nM) (designated CPO binding protein or CPO-BP) is not one of these known OP toxicant targets. CPO-BP is a 50-kDa membrane-bound serine hydrolase measured by derivatization with [3H]CPO and SDS/PAGE or filtration binding assay. It appears to undergo rapid diethylphosphorylation by [3H]CPO followed by either dephosphorylation and reactivation or aging on loss of an ethyl group. CPO and several other OP toxicants potently inhibit CPO-BP in vivo (i.p., 2 h) (50% inhibition at 2-25 mg/kg) and in vitro (50% inhibition at 8-68 nM). Using three chemical labeling reagents, i.e. [3H]CPO and the activity-based proteomic probes fluorophosphonate-biotin and fluorophosphonate-rhodamine, mouse brain CPO-BP is identified as serine hydrolase KIAA1363 of unknown function. Brains from KIAA1363-/- mice show greatly reduced levels of CPO labeling and hydrolytic metabolism compared to brains from wild-type mice. KIAA1363 therefore is the principal enzyme for metabolizing low levels of CPO in brain and may play a more general role in detoxification of OP nerve poisons.

64. AEI: Mechanistic interpretation of molecular interactions of tetracycline with clay and organic matter using nuclear magnetic resonance, mass spectrometry, and attenuated total reflectance Fourier transform infrared spectroscopy

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Tetracycline-class of antibiotics is licensed as growth promoters for livestock in United States. This has also led to increased emergence of resistant strains of pathogenic bacteria that could potentially impact human health. Tetracycline input to the soil and aquatic environments due to the use of manure and sewage sludge in agriculture as soil conditioners requires the knowledge on their fate, transport and factors that affect their mobility in soil. To determine the factors that might affect the mobility of these antibiotics in soil, the mechanisms of interaction of oxytetracycline with model clay adsorbents and organic matter were investigated as a function of suspension pH. The adsorbents used were native montmorillonite (SWy-2), Na-montmorillonite (Na-SWy-2), and hexadecyl trimethyl ammonium-montmorillonite (HDTMA-montmorillonite) and natural organic matter. Attenuated Total Reflectance Fourier Transform Infrared (ATR/FT-IR) showed that tetracycline hydrogen bonds with inter-layer water molecules in montmorillonite, Na-montmorillonite, and humic acid-montmorillonite at lower pH values whereas it directly co-ordinates with HDTMA cation in HDTMA-montmorillonite at alkaline pH values. Nuclear Magnetic Resonance (NMR) parameters such as spin-spin, spin-lattice relaxation and subtle chemical shifts of ^{1}H, ^{13}C, ^{15}N nuclei also provide molecular information on the predominant sites and the interaction mechanisms between tetracycline pollutants and environmental matrices. Mass Spectrometry analyses confirmed the formation of new products as a result of cross coupling between tetracycline and organic matter surrogate.

65. Anaerobic bacterial degradation of agrochemicals in laboratory microcosms

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Chlorinated organic pesticides such as DDT and toxaphene used in the 1970s and 1980s may have been responsible for a number of adverse environmental effects around Lake Apopka, FL, including the death of hundreds of white pelicans in 1999. The overall objective of this study was to identify those electron donating processes leading to the efficient microbial degradation of toxaphene in Lake Apopka soils. To optimize extraction of toxaphene from soils, accelerated solvent extraction (ASE) was compared with the traditional soxhlet extraction and showed higher efficiency of extracting toxaphene and DDT from both highly and moderately contaminated soils from around Lake Apopka. A series of laboratory microcosms was established to identify anaerobic processes leading to the decomposition of the recalcitrant pesticides. Lactate, butyrate, H_2, formate, acetate, and propionate were tested as electron donors to stimulate different groups of anaerobic bacteria responsible for degradation. After a two-month incubation, microcosms with lactate, butyrate, and H_2 showed the greatest losses of the target compounds. Based on these results, indigenous bacteria with the capability to dechlorinate toxaphene were enriched using lactate as the electron donor in the presence of 20ppm toxaphene. After five transfers, release of Cl^- was measured by ion chromatography with time. A rapid and significant rise in concentrations of Cl^- was observed in all replicates relative to controls, indicating biological dechlorination of toxaphene. DNA was isolated from these enrichments, from which 16S rRNA genes were amplified, cloned, and sequenced. Sequence analysis revealed the presence of three strains, and sequences similar to Citrobacter were most abundant in the clone libraries. Efforts are currently underway to isolate the three strains and determine if Citrobacter alone is required to degrade toxaphene, or if the consortium of three strains is required.

66. Bioavailability of tylosin in environmental matrices

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Tylosin is a veterinary antibiotic commonly used as a feed additive in livestock production for growth promotion and disease prevention. Tylosin is excreted by the livestock in urine and feces, and enters the environment via manure application. Little is known about the fate of tylosin in terrestrial and aquatic ecosystems. Understanding the bioavailability of pharmaceuticals in environmental matrices is particularly important considering they are often in an active form. In this study, the bioavailability of tylosin in soil and water was evaluated using Empore SDB-RPS ™ extraction disks. Incubation systems consisted of 100 ml of autoclaved pond water or 40 g agronomic soil, each spiked with tylosin to achieve a range of concentrations of tylosin (0.01 to 100 ppm). Empore disks were conditioned and added to treatment vessels for 24 hours. Disks were then extracted with 98:2 acetonitrile:glacial acetic acid, and water was extracted using Waters Oasis HLB ™ solid phase extraction cartridges. Soil was extracted with 85:15 acetonitrile:phosphate buffer pH 2.3 and concentrated under nitrogen flow. Determination of tylosin factors and metabolites was achieved using LC/MS/MS. Data suggest that tylosins remain tightly bound to soil particles, thus decreasing their bioavailability. In an aquatic system, sediments would likely become the sink for the tylosin residues, which would have implications for benthic organisms.

67. Development and characterization of improved extraction methods for transgenic Bt proteins from soil and sediment

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Transgenic crops containing *Bacillus thuringiensis* (Bt) insecticidal proteins were introduced in 1996. Despite increasing worldwide usage, relatively little is known regarding Bt protein fate in the environment. Development of a more accurate analytical method for Bt proteins is crucial for the investigation of their environmental fate, but current methods are lacking and extraction efficiency from soil and sediment is low (30-60%). Enzyme-linked immunoassay (ELISA) has proven to be a sensitive quantification method and was used in this study to evaluate the extraction efficiency of two buffer systems. Previous work in this laboratory appears to show improved extraction efficiency of Bt protein from soil using a high-salt/high-pH buffer with 5 mg/mL trypsin. However, it is unknown if cleavage of the protein is occurring, resulting in multiple detections and a false increased recovery of the protein. The objective of the first study was to determine if the trypsinated buffers used were cleaving the protein. Cry1F protein was treated with a high-salt/high-pH buffer with 0.5, 5.0, and 10.0 mg/mL trypsin. A Western blot was conducted and the banding pattern was compared to that of Cry1F standard. Evidence from collaborators indicates that the addition of surfactants to a buffer will also improve the extraction efficiency of Bt proteins. Therefore, the objective of the second study was to evaluate the effectiveness of the addition of sodium taurocholate to the high-salt/high-pH trypsinated buffer. Soil and sediment samples were spiked with Cry1F protein. Fresh and aged samples were extracted with a high-salt/high-pH buffer containing 5 mg/mL trypsin and 1, 3, or 5% (w/v) sodium taurocholate. The extracts were analyzed by ELISA.

68. Enantiomeric sulfoxidation of the organophosphate pesticide fenthion in fish

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The objective of this study is to examine the enantioselective sulfoxidation of fenthion, in liver microsomes of various fish species (rainbow trout, hybrid striped bass, tilapia). Microsomes from striped bass, trout, and tilapia primarily formed (-) sulfoxides in approximately 65% enantiomeric excess. Enzyme inhibitors lubrol (cytochrome P450) and methimazole (Flavin Monooxygenases) were used to determine sulfoxide relative contributions from each enzyme system. In striped bass microsomes, P450 was responsible for 74% of sulfoxide formation. Co-incubation with methimazole or lubrol in trout liver microsomes enhanced sulfoxide formation. Salt water treatments which typically induce FMOs, did not significantly alter enantioselectivity or rates of fenthion sulfoxidation, even though toxicity tests indicated saline environments enhanced the toxicity of fenthion in trout. These results indicated either the formation of additional metabolites of fenthion or the contribution of additional oxygenases to S-oxidation. There was no significant difference in tilapia toxicity between fresh and salt water environments.

69. Environmental fate of tylosin and analysis of immunological cross-reactivity among tylosin isomers

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Tylosin is a widely used antibiotic for the treatment of disease and the promotion of growth in swine, beef cattle and poultry production. Tylosin consists of 4 isomers (A, B, C, D) in its parent formulation. Through the application of organic fertilizers to farmland, tylosin enters into the environment, and its degradation products may form to some extent. The objective of this study was to develop an analytical method suitable for detection of tylosin isomers, and to investigate their fate in the environment. HPLC conditions for determination of tylosin isomers were established, and tylosin isomers were identified by HPLC/MS. Tylosin isomers were purified and tested for their cross-reactivity to ELISA method. The dissipation of tylosin in water was monitored by ELISA and HPLC methods and the results were compared. The dissipation of tylosin in pond water and sterilized pond water was conducted to evaluate the contribution of biotic degradation compared to the physical/chemical degradation.

70. Evaluation of the transport of selected contaminants in recycled water in tropical soil

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The purpose of this study is to evaluate the leaching properties of selected wastewater contaminants such as lindane, atrazine, octylphenol, nonylphenol and N-nitrosodimethylamine (NDMA) in a tropical soil. Both batch sorption and column studies were conducted to investigate the transport mechanism of these contaminants in soil. Batch sorption experiments were conducted to evaluate the effect of the controlling parameters which include pH, ionic strength, and organic carbon on the sorption. Breakthrough curves of these contaminants were obtained by conducting leaching experiments through columns packed with topsoil (an Oxisol) and subsoil (Saprolite). BTCs of these hydrophobic contaminants were relatively fast in saprolite compared to topsoil. NDMA was found to move like tracer in soil. Atrazine and lindane moderately adsorbed to the soils. Both phenolic compounds showed significant adsorption on these soils. Transport parameters of these compounds were estimated by inverse modeling using HYDRUS 1-D software.

71. Modeling the variability in aerial concentrations of atrazine, endosulfan and chlorothalonil at a rural location on the Delmarva Peninsula

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Weekly air samples (n=129, 2000-2003) were collected at a rural location on the Delmarva Peninsula, to investigate temporal trends in the atmospheric concentrations of current use pesticides in this predominantly agricultural region. Atrazine was detected in 80% of the samples followed by α-endosulfan and chlorothalonil in 97% each. Pesticide concentrations exhibited a log-normal distribution, and the median concentrations ranged from 75 pg/m3 for α-endosulfan to 700 pg/m3 for chlorothalonil. A multiple linear regression model that incorporates temperature and time explains 32-43% of the variability in concentrations. The addition of an agricultural cycle (approximated by a Lorentzian function) to the model improved predictions by up to 7%, especially for α-endosulfan. Wind speed and wind direction did not have a statistically significant influence on concentrations at our site. The model shows that the agricultural cycle is centered in April for atrazine and July for the other two pesticides, which is commensurate with local practices. The calculated heats of phase transition (atrazine: 29±9.6 kJ/mol, α-endosulfan: 43±15 kJ/mol and chlorothalonil: 46±12 kJ/mol) are much lower than the heats of vaporization for these compounds. This suggests that vaporization from soil surfaces is not the controlling factor in their atmospheric presence. The relative persistence of the pesticides is reflected in their atmospheric half-lives. Atrazine has the shortest half life (1.2±0.2 yr) followed by α-endosulfan (1.4±0.2 yr). Chlorothalonil concentrations did not show a statistically significant dependence on time. Results indicate that temperature and application cycle are the main drivers for the occurrence of current use pesticides in the atmosphere of the Delmarva Peninsula. The study highlights the importance of incorporating the agricultural cycle while interpreting data for pesticides, especially for rural locations.

72. Responses of juvenile salmon to aquatic herbicides

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Herbicides are frequently used to control exotic or nuisance aquatic plants. However, use has been hampered by concerns directed at non-target effects, particularly in light of new State permitting processes in response to a recent Federal Court ruling requiring western states to issue National Pollutant Discharge Elimination System permits for the use of pesticides and adjuvants in aquatic systems. Unfortunately, data on non-target toxicity of aquatic herbicides are lacking, threatening the permitting process. Recent declines in several species/stocks of salmon and emphasis to restore these populations heighten concerns in the Pacific Northwest. Behavioral responses such as avoidance can alter the exposure of fish to pesticides and such behavior has been suggested as important in mitigating hazards aquatic herbicides pose to juvenile salmonids provided suitable uncontaminated habitat is accessible. The aquatic herbicides we selected for study, Sonar®AS (fluridone), REWARD® (diquat), and RENOVATE® 3 (triclopyr), are permitted for use in Washington State. Our objective was to determine if juvenile Chinook salmon (*Oncorhynchus tshawytscha*) avoid these herbicides. The maximum application rate and ten times the maximum application rate were tested as well as a positive control. We used five replicate uni-directional flow chambers adapted for juvenile Chinook and photographed the position of fish (n=10/chamber) for 15 min (1-min intervals) before chemical exposure, during chemical exposure, and after clean water was re-introduced into the chambers. One water sample from each concentration tested was chemically analyzed. Responses were quantified using a novel method comparing mean position and slopes of lines generated by mean position in the test chambers over time. Juvenile Chinook were neither attracted to nor avoided maximum rates of the herbicides, but were attracted to 10x maximum rates of RENOVATE and REWARD. Research in 2005 will focus on effects on olfactory performance; preliminary results will be presented.

73. Overview of permitted and prohibited listing approaches for new and emerging invasive plants

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Traditionally, most federal and state plant regulatory agencies have used a prohibited list approach for regulating the introduction and spread of designated noxious weeds into and through a state or country. Under this approach, which is exemplified by the Federal Noxious Weed Act of 1974 (now superseded by the Plant Protection Act of 2000), a species must be officially listed to be denied entry, unless otherwise restricted under other rules or regulations. To date, about 100 taxa have been listed as Federal Noxious Weeds by USDA APHIS. A second approach to listing is the permitted list approach, that was originally pioneered by Australia and New Zealand in the 1990s. Under this approach, all new species proposed for importation, must be assessed to determine their potential for harm. Proposed species that are approved for entry are placed on the official permitted list by the authorized agency. Proposed species that are not approved for entry are placed on the prohibited list of regulated noxious weeds. A third approach to listing, the mandatory prohibited list approach, would continue to use a prohibited list as the primary regulatory tool, but would require that all new species proposed for importation be formally assessed to determine if they should be regulated. Under this new approach, “approved” species would be maintained on an informal (non-regulated) permitted list. A non-regulatory approach to listing is the Weed Ranking System that was developed by NatureServe, in cooperation with the Nature Conservancy. Under this system, species of concern are scored for invasiveness using a standardized ranking process. This permits comparison of new species to other species of concern within a designated area such as an eco-region or geo-political land unit. Each of these forms of listing provides a valuable mechanism for identifying and addressing new and emerging invasive species.

74. Proposed revisions to U.S. Department of Agriculture's Animal and Plant Health Inspection Service Quarantine on Plants for Planting

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The regulation of Federal Noxious Weeds by the U.S. Department of Agriculture's Animal and Plant Health Inspection Service is done by regulation based on risk assessment. Various stakeholder groups have encouraged APHIS to broadly expand the number of regulated species. The Plant Protection Act of 2000 officially recognized the use of stakeholder petitions to request regulation or deregulation of taxa. APHIS is, in addition, considering substantial revisions to the regulations known collectively as Quarantine 37 (7 CFR Part 319.37). The regulations are also known as the quarantine on Plants for planting; aka Q-37. Changes in patterns of transportation and world-wide production and marketing have exposed problems with the current regulatory scheme. Proposed changes include: 1) establishment of programs to reduce risk of entry and establishment of plant pests (e.g. a clean stock program); 2) establishing a new import entry category of plant taxa to be excluded from import pending risk evaluation; 3) improved data collection to determine taxa imported, origin, and volume; 4) reevaluation of taxa currently prohibited; and 5) consolidation of all plants for planting into one regulation. The proposed changes were the subject of an ANPR (advanced notice of proposed rulemaking) published Dec 10, 2004 as “Nursery Stock Regulations”, Docket No. 03-069-1.

75. Developing a U.S. national invasive plant list

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To date, despite many policies and programs focused on non-native species, there is no broad agreement on which non-native plants are considered the most invasive in the United States. In January 2004, NatureServe implemented our newest standardized methodology - the “Invasive Species Assessment Protocol” - to assess and categorize the estimated 3,500 non-native vascular plants that have escaped from cultivation in the United States. The assessments yield an Invasive Species Impact Rank (I-Rank) for each species which can be used to develop a prioritized list of species based on their impact to biodiversity. The information developed from this process should greatly benefit the work of land managers, as well as gardeners, landscapers, the nursery industry, private landowners, and conservation organizations. The information can focus management, research and prevention programs; influence land-management decisions; create consensus about the most problematic species; and increase public awareness about invasive species.

76. Regulatory and cooperative responses to noxious and invasive exotic plants by the Maryland Department of Agriculture

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Three types of noxious weeds (thistles, shattercane and Johnsongrass) have been regulated for over 40 years, primarily in agriculture, with Right of Way also receiving attention in cooperation with the MD Dept. of Transportation. In 2005, an interagency cooperative project was initiated to address the growing problem of invasive exotic plants IEP in forest habitats, especially on public lands. A Steering Committee was assembled to oversee all aspects of the project. First, a multidisciplinary approach was taken to assign a priority ranking to sites which may be vulnerable to impacts of IEP. A site inventory and assessment protocol is being developed to rate current impacts of IEP at each site. Sites will be prioritized for management by formally considering site priority rank, rating of IEP impact, potential for increasing impact, and difficulty of management. Subsequent to approval, custom integrated management actions will be undertaken at the next appropriate opportunity.

77. Probabilistic risk assessment for identifying acceptable methods to control invasive species

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Introduced species can negatively impact native ecosystems. In many areas, broadcast application of pesticide formulations are successfully used to control invasive pest species. While chemical pesticides offer many potential benefits to agriculture and ecosystem restoration efforts, potential risks to non-target wildlife must be considered before wide scale application programs should be initiated. Widely used worst case deterministic risk assessment approaches often over-estimate risk to non-target species. This may result in the elimination of plausible invasive species control options and continued damage to native ecosystems. Probabilistic risk assessment methodology generally leads to more accurate predictions of risk to non-target species. This probabilistic based approach will likely identify a greater range of acceptable control methods for control of invasive species.

78. Invasive species challenges and perceptions in the horticultural industry: Regulative and legislative

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The perceived impact of invasive species and the control thereof translate into operational challenges for the nursery operator. From production to sales, from propagation to marketing, each step of a the process is, as of this writing, not well defined, leading to future predictive models, which are not synchronized with actual business needs. The paradigm for deciding which plants are suitable for commerce, in which region, is still under development; the choices for control are steadily eroding under environmental pressures. The environmental concerns are related philosophically to the political understandings, which are attempting to limit plant selection in the horticultural industry.

79. Registration of aquatic herbicides: A new model

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Only nine herbicides have national (Section 3) labels for aquatic sites in the US, and from 1971 (the year the USEPA was established) until 2002 only two, glyphosate (1977) and fluridone (1986), received aquatic registrations. Yet, during this same period invasive aquatic weeds increased dramatically, and the awareness and need to control these weeds has never been greater. The cause for this conundrum was driven by a number of factors. Cost of registration was estimated at $10-40 million and total annual sales in the aquatic market were estimated at $100-150 million, a minor share of the overall pesticide market. Major changes in regulatory requirements, such as re-registration and the Food Quality Protection Act, have complicated and slowed the entire process. State regulatory and permitting processes, National Pollution Discharge Elimination System permits, risk cup issues, and public perception of pesticides have placed added complexity and burdens on registrations. Also, patent life of a molecule, combined with the specter of generics, discouraged development of proprietary products. The combination of these factors resulted in an increased risk of a low potential return on investment for registrants. In addition, critical interactions among the research community, the registrants, and the regulatory community, were greatly diminished. All three groups had lost in-house technical expertise, been downsized due to reduced budgets/resources, and had lost the interactive communication required to secure an aquatic label. Recently, a public-private-academic partnership has emerged that is changing the aquatic registration landscape. Cooperators include Federal and state agencies, selected research institutions, and non-profit research organizations. Through this partnership, three new aquatic registrations have been secured since 2002: triclopyr, imazapyr, and carfentrazone-ethyl. Operational success of this partnership will be discussed and this collaboration may well represent the future of aquatic herbicide registrations.

80. Inclusion of noxious weed management in the reform of the Endangered Species Act

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The Endangered Species Act (ESA) of 1973 was designed to support the “continued existence” of species determined to be endangered or threatened. The ESA strives to “conserve” and “prevent further decline” of species and critical habitat through: □Cooperation among and between Federal and State agencies. □Monitoring □Federal land acquisition from private or state landowners □Prevention of destruction or adverse modification of critical habitat □Disallow taking of endangered and threatened species □Penalties and enforcement. No action strives towards species recovery. Science has consistently shown an expansion of critical habitat as a component to the increase of a diminished species population. There is only one provision in the ESA for expanding critical habitat. However, it is associated with granting approval of an agency activity (typically development) that could lead to harm of existing critical habitat. “Exemption” to approve a project with an acceptable plan of reasonable mitigation and enhancement measures includes habitat improvement, but only to the degree to sustain the present endangered and threatened species population (Sec. 7.(g)(5)(C)). The 1973 ESA has no action to encourage species recovery. The number of species gone extinct can measure failure of the act. The number of species that remain on the list is the only measure of success. The ESA would be more effective if it supported provisions for species recovery. Recovery can be achieved through habitat rehabilitation, such as, noxious weed management. Management options should include those that may result in endangered and threatened species collateral damage, but will ultimately provide greater habitat leading to greater likelihood of species recovery. There are numerous examples where management of noxious weeds has and would lead to increased numbers of a declining species.

81. Research on the fate of pesticides applied to turfgrass: A perspective by a scientist, administrator and emeritus

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During the final two decades of the last century there appeared to be increasing concern for the potential movement of chemicals from intensively managed turfgrass. Funding opportunities appeared and numerous research programs were initiated across the U.S. Results of a research program, conducted at UGA (1992-1997), indicated that very small fractions, of certain pesticides, were transported through lysimeters underlying turfgrass maintained as golf course greens. Additionally, small quantities of certain pesticides were transported, in the surface-runoff water, from treated mini-plots simulating golf course fairways and home lawns. It was concluded that certain pesticides can be applied to turfgrass with minimum risk. Other research programs, conducted during the 1990's, obtained similar results with similar conclusions. Did these publicized conclusions result in apathy toward risk assessment research on turfgrass management? It appears that the importance of risk assessment studies, on turfgrass management strategies, has lessened during the past five years. Special funding (eg. grants and gifts) has been reduced considerably. Reduced state and federal budgets have impacted the formula funding at Land Grant Universities (LGU's). Currently in LGU's, use of formula funding for this research suffers compared to other disciplines (eg. genomics, proteomics, and metabolomics). The clientele of these universities demand research programs for improved production profitability. Administrators in LGU's are faced with tough decisions. The lack of funding sources, the absence of clientele support, and the apparent non-use of the data by regulatory agencies places a dilemma, on administrators of LGU's, when it comes to utilizing the limited funding for risk assessment programs. These research programs need organizations (eg. regulatory agencies) that command their data; a clientele base that depends on the data for the profit margin; and funding agencies. Probably, the pendulum will swing back and hopefully it does not take a catastrophic event to reverse the swing.

82. Farmer's perspective on modern turf farming

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Successful turf farming as a business depends on many factors: land utilization, seed and variety research, Retail/wholesale sales, transportation/preservation, Irrigation, crop protection, harvest pressures, labor force management, and of course the weather. Real life experiences from a family turf farm on Long Island, NY will add insight and perspective on the challenges, pressures, and demands placed on the Northeast US turf farming community.

83. Impact of lawn care practices on aquatic ecosystems in suburban watersheds: EPA STAR grant research findings

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In this project funded through the US EPA's Science to Achieve Results (STAR) program an integrated science approach pooling scientific expertise within the physical, biological and social sciences was used to assess the natural and anthropogenic processes governing the quality of water resources in human dominated systems. Major finds from this project were: 1) Concentrations of pesticides detected appeared to be related to watershed size, with streams draining larger areas having higher concentrations. 2) Concentrations of ammonium nitrogen and phosphorous were correlated at the two high income sites indicating lawn-fertilizer runoff in these watersheds. 3) The three biological assessment methods used in this investigation yielded mixed results indicating that multiple biological assessment methods may be necessary to measure impacts of contaminants on aquatic biota, considering not all organismal responses are sensitive to all chemical exposures. 4) Types and concentrations of pesticides detected in the streams were not related to the socioeconomic status of the neighborhood. However, the majority of biological effects were observed at the two high property values sites indicating potential stress from additional contaminants or factors not measured in this investigation. 5) Homeowners identified pride of ownership, respect for neighbors and pride of place as the primary motivations for maintaining their residential landscapes. The concept of the ideal lawn was consistent among residents within neighborhoods but was different among neighborhoods. Owners of the high-property value homes preferred the highly manicured lawns while those in the lower property value area preferred more natural looking lawns. 6) Residents have a diverse set of labor and expenditure patterns toward their lawns. Activities with the potential for environmental damage are widely but not universally practiced. Professional applicators and maintenance companies are prevalent, but household labor is also a very significant part of the pattern in applying insecticides, herbicides, and fertilizer.

84. Effects of lawn-care chemicals on macroinvertebrate communities

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To determine the potential impacts of lawn-care pesticides on aquatic ecosystems, the macroinvertebrate communities of six streams were assessed using a multimetric approach. Four streams flowed through residential neighborhoods of Peachtree City, GA, USA, with differing mean property values and two reference streams were outside the city limits. A series of correlation analyses were conducted comparing stream rank from water quality and physical stream parameters, habitat assessments, benthic macroinvertebrate metric, pesticide toxicity and metal toxicity data to determine relationships among these parameters. Significant correlations were detected between individual analyses of stream rank for pesticide toxicity, specific conductance, turbidity, temperature and dissolved oxygen with benthic macroinvertebrate metrics. An upstream/downstream assessment was also conducted on a stream flowing through a golf course in Alpharetta, GA, USA, using similar sampling protocols and metric analysis. Of the nine metrics used to assess the macroinvertebrate community, four were statistically different between the upstream and downstream sites. However, the habitat quality of the downstream site was poor for macroinvertebrates compared to the upstream site. Thus, the absence of many macroinvertebrate taxa is likely related to physical constraints of the habitat rather than chemical impacts considering high pesticide concentrations were detected at the upstream site. In addition to the field assessments, three of the most common lawn-care insecticides detected in urban watersheds were evaluated in the laboratory to determine their toxicity to an aquatic insect species Simulium vittatum IS-7. Results showed chlorpyrifos to be the most toxic to black fly larvae followed by carbaryl, and malathion. These insecticides were also tested as binary and ternary mixtures using the toxic unit (TU) approach. Toxicity was shown to be greater than additive for the ternary mixture of chlorpyrifos-carbaryl-malathion, and the binary mixtures of chlorpyrifos-malathion, and carbaryl-malathion. The binary combination of chlorpyrifos and carbaryl was shown to be additive.

85. Missing links in ecological risk assessment: Use of biomarkers in freshwater bivalves to establish causal relationships between pesticide exposures from turfgrass runoff and effects on stream ecosystems

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Impacts of turfgrass pesticide runoff on stream ecosystems are difficult to assess because in urban landscapes any pesticide-induced stress occurs concomitantly with stressors from a multitude of other sources. Biomarkers are cellular and physiological stress responses that provide important mechanistic information, and such responses may be particularly valuable when combined with more ecologically relevant endpoints in risk assessments. Our research evaluated oxidative stress responses in freshwater clams (Corbicula fluminea) deployed in streams receiving pesticide runoff from residential lawns and a golf course. Clams accumulated a variety of persistent metals and pesticides in their tissues, and concentrations were typically highest in clams from streams that drained lawns within high property value neighborhoods during times of heavy rain and in a stream that drained a golf course. Clams exposed in situ to turf contaminants exhibited signs of oxidative stress, and controlled laboratory studies confirmed that the turf contaminants were important contributors to the etiology of stress observed in clams exposed in urban streams. These data when combined with other ecologically relevant endpoints may help to identify what factors (chemical, hydrological, geomorphological) are impacting suburban and urban streams.

86. Aesthetics and practice of maintaining the ideal lawn in Peachtree City, GA

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People prefer and find more beautiful landscapes that give an overall impression of moderate to high complexity yet retain legibility and an element of mystery. To achieve this aesthetic in residential neighborhoods requires numerous homeowner decisions about lawn care. How do homeowner beliefs, values, and socioeconomic status determine loads and ecological impacts on turf care chemicals in aquatic ecosystems in suburbanized watersheds? Peachtree City homeowners identified pride of ownership and respect for neighbors as the primary motivations for maintaining their residential lawns. A lawn's consistency with its surroundings and its place in the overall flow and balance of the landscape in a neighborhood are the basis for evaluating its maintenance. Within-neighborhood participants were highly consistent in their overall ranking of landscapes, but differences

between neighborhoods were significant. The average Peachtree City household spent 20 hours and $103 per year applying herbicides, pesticides and synthetic fertilizers. Of the 48% of households applying non-zero amounts of these products, the average was 36 hours and $215. Biological pest controls of low-toxicity insecticides were used by 23% of Peachtree City households for an average of six hours at a cost of $44 vs. two hours and $51 on the use of biological pest controls. Peachtree City residents expend labor and money in varied ways on their lawns, although the activities with the potential for environmental damage were not universally practiced. Professional applicators and maintenance companies are prevalent, but household labor remains significant in the application of insecticides, herbicides, and fertilizers. Programmatic interventions that target "average" behavior and ignore the scaling of social-biophysical interaction can easily overlook the exceptional behaviors disproportionately driving system outputs. Who adopts particular practices or why they adopt them may ultimately be less important in suburban landscapes than understanding where and when certain behaviors occur.

87. Lessons learned from invasive species management in the National Wildlife Refuge System

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The National Wildlife Refuge System (NWRS) manages 545 refuges and 3,000 waterfowl production areas encompassing 96 million acres. These lands span a wide range of ecotypes and provide habitat for 25% of the nation's threatened and endangered species. Invasive species have been ranked as the number one threat to the ecological health of the NWRS. Successful management of invasive species in natural areas requires recognition of the problem, planning, infrastructure development, prioritization of treatments, working with partners, standardization of information and most importantly, results in the field. To meet these challenges, the NWRS has developed several innovative approaches such as Strike Teams to focus on Early Detection and Rapid Response to new invasions, partnering with the US Geological Survey to develop invasion modeling and using citizen volunteers to map and manage weed infestations.

88. National Park Service exotic plant management teams: An innovative model for wildland weed control

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Today, invasive plants infest approximately 2.6 million acres in the national park system, reducing the natural diversity of these places. In order to address, this invasion the National Park Service has established rapid response Exotic Plant Management Teams (EPMTs) to control invasive plants. Modeled after the approach used in wildland fire fighting, EPMTs provide highly trained, mobile strike forces of plant management specialists who assist parks in the control of exotic plants. Each EPMT serves multiple parks within a broad geographic area. They work through steering committees to identify, conduct, and evaluate exotic species removal projects and undertake appropriate restoration efforts. Each of the 17 established teams has developed site-specific strategies in partnership with other entities for combating exotic plants that reflect the needs and resources of the more than 219 parks they serve. This paper will describe the history, operation, successes, challenges and partnerships associated with this innovative model.

89. Overview of NEPA requirements for federal invasive species management

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Overview of NEPA Requirements for Federal Invasive Species Management Programs - Noxious and Invasive Weeds. In this session, participants will gain a working knowledge of the National Environmental Policy Act (NEPA) the law and how it applies to federal invasive species management programs. They will understand the differences between Categorical Exclusions, Environmental Assessments and Environmental Impact Statements. They will understand why there are differences in the application of NEPA by the various federal agencies. They will also learn about the parts of an EIS or EA and get some insights on how invasive species can be effectively addressed under the act.

90. USDA Forest Service national strategy and implementation plan for invasive species management

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The Chief of the Forest Service has identified invasive species as one of the top 4 threats to our Nation's forest and rangeland ecosystems. In response, the agency is taking a leadership role to "raise the bar" for increased action against this national and global threat, beginning by taking a strategic approach with one focused goal: "To reduce, minimize, or eliminate the potential for introduction, establishment, spread, and impact of invasive species across all landscapes and ownerships". The release of the USDA Forest Service National Strategy and Implementation Plan for Invasive Species Management takes a major step forward to reach this goal and will guide the agency as it builds capacity to strategically and effectively meet the invasive species challenge collaboratively with partners. The National Strategy and Implementation Plan is built around 4 Program Elements: Prevention, Early detection and rapid response, Control and management, Rehabilitation and restoration. Each program element includes a description of success, achievable accountability measures, and prioritized strategic actions that are specific and achievable steps to reach the stated goal. Also, the Strategy contains guidance related to 4 Common Themes, relevant to all Program Elements: Partnerships and collaboration, Science based—including scientific information, assessment and monitoring, and prioritization, Communication and education, Organizing for success—incorporating the themes of improving capacity, procedural streamlining, and funding flexibility with long-term commitment.

91. Overview of the Giant Hogweed eradication project in Pennsylvania

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The Federal Noxious Weed Giant hogweed (*Heracleum mantegazzianum* Sommier & Levier) is known to be naturalized in some settings in the northeastern United States, and a few isolated finds in the Pacific Northwest. Currently a survey and eradication program is underway in western Pennsylvania. Survey is underway in several other states. APHIS is encouraging the development of a Northeast regional survey/eradication project. A Memorandum of Understanding is currently being circulated for signature by the states of the Eastern Plant Board regarding a coordinated regional Hogweed eradication program. The plant, a biennial or short-lived perennial herb, is up to 5 m tall; with a taproot and hollow stems. Lower leaves are up to 2.5m long, with flowering heads comprised of several loose compound umbels; often up to 75cm wide. The sap is a skin photosensitizer, resulting in large painful blisters in sensitive people. It grows in areas of human habitation and in such un-cultivated or waste areas as edges of woods or clearings, and riparian zones. Most infestations are initiated as ornamental plantings. The mericarps or whole fruits are also used as a spice in Iranian cooking and are thus frequently intercepted in baggage by during border clearance of passengers entering the United States.

92. The Department of Defense Invasive Species Management Program

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The Department of Defense (DoD) has a multi-faceted program. Executive Order 13112 Invasive Species, initiated the formal development of instructional guidance on invasive species Prevention, Control, and Restoration. Long before many pests had acquired the umbrella term of invasive species the DoD was like many other agencies already fighting these pest problems. DoD has many Federal, State, local and non-government organizations as partners that we work with in our fight to control these pests. I will briefly outline some of the programs and problems we are engaged in controlling. In addition I will note some of the successes we have achieved.

93. National Invasive Species Council update

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The National Invasive Species Council (NISC) was established by the Executive Order 13112. NISC works to ensure that federal invasive species activities are coordinated and complementary. NISC is co-chaired by the Secretaries of Agriculture, Interior, and Commerce and includes the Secretaries of Transportation, DHS, State, Defense, Treasury, HHS, the Administrator of the EPA, the Director of the USAID, U.S. Trade Representative, and other federal members. Invasive species cause immense harm to the economy, the environment, animal and human health. They can be found in habitats ranging from home to the open ocean. Some species such has Asian longhorn beetle, emerald ash borer, sudden oat death, hemlock wooly Adelgid, Chestnut Blight together have the potential to destroy entire ecosystems. Invasive species are the second leading cause, after habitat loss, of species being listed as endangered or threatened with extinction. Harm caused by invasive plants, like yellow star thistle, tamarisk, leafy spurge, hydrilla, and others have lead to legislation and other responses. The coordination task of NISC is large and diverse. NISC coordinates the efforts of about 40 federal agencies that in FY04 spent collectively $1.1 billion on invasive species. NISC staff has some level of engagement with over 1,800 individuals and has identified over 290 programs, 160 organizations, and 130 groups that have a role in invasive species. NISC invasive species management plan contains 57 action items that call for 170 identifiable efforts. About 100 of the 170 require an on-going coordination effort.

94. Development of an early detection and rapid response system for the Pink Hibiscus Mealybug through education, training, and implementation of Integrated Pest Management

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The pink hibiscus mealybug (PHM), Maconellicoccus hirsutus (Green), is an exotic pest species that invaded California in 1999 and Florida in 2002. Worldwide, PHM has been recorded from over 300 host plant species, including citrus, ornamentals, and vegetables. Despite federal (USDA-APHIS) and state (FDACS-DPI) efforts to regulate and control the spread of PHM to other susceptible states, a nursery in Homestead, FL, accidentally shipped 900,000 hibiscus plants from potentially infested stock to 36 states in the U.S. from January through July 2004. According to USDA-APHIS personnel, 11 of the states that received plant shipments are climatically suitable for establishment of the mealybug. Of these plant shipments, which went to retail outlets in the 36 states, PHM was confirmed from plant material in Kansas, Louisiana, and North Carolina. In order to ensure effective coordination of this effort, a Pink Hibiscus Mealybug Steering Committee will be formed, comprised of representatives from the Regional IPM Centers, National Plant Diagnostic Networks, LGU's, Federal Agencies (USDA-APHIS, USDA-ARS, USDA-CSREES), and other entities. Successful management of PHM will require monitoring, detection, correct identification, and the implementation of management strategies (including natural enemy releases/monitoring of natural enemy impact, sanitation, chemical control, and other approaches). If PHM is able to gain a foothold in a number of climatically suitable states in the U.S., it is anticipated that potentially severe economic damage could follow unless an early detection and rapid response system is established. Dr. Robert M. Nowierski, National Program Leader for Bio-Based Pest Management, USDA-CSREES, is helping to facilitate the development of such a system for the pink hibiscus mealybug with help from the Regional IPM Centers, National Plant Diagnostic Networks, Land Grant Universities, federal and non-federal entities.

95. Achieving the goal that invasive plant removal is standard in natural areas

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Non-native invasive species such as English Ivy, Japanese Stiltgrass and Kudzu are covering our natural areas that we in the conservation movement have worked hard to protect from habitat destruction, erosion and water pollution. Just as we are making progress on wetlands, stream bank stabilization, and endangered species, these plants from other parts of the world have covered 30-90% of the surface area of our forests, streams and meadows. Many of us feel demoralized and powerless to combat these invaders that have few natural herbivores or other controls. The Anacostia Watershed Society is establishing a program to empower local groups and land owners with several models to draw upon in the region. We are assisting in developing a major work effort at each site for about 3 to 5 years to remove massive populations of about a dozen species. Regular stewardship projects are conducted in all seasons including Winter, early Spring, late Spring, Summer, and late Summer. This high intensity program is followed by a low intensity annual maintenance program for plants we have missed, plants emerging from the seed bank, and occasional plants migrating in from neighboring areas.

96. Progress on development of a National Early Detection and Rapid Response System for Invasive Plants in the United States

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To minimize the establishment and spread of new invasive plants in the United States, the U.S. Geological Survey, Biological Resources Discipline (USGS), in cooperation with the Federal Interagency Committee for the Management of Noxious and Exotic Weeds (FICMNEW), is leading a national effort to develop a National Early Detection and Rapid Response System for Invasive Plants in the United States. To achieve this goal, a coordinated framework of new and established public and private partner groups at the local, state, regional, and national levels is being organized to: detect and report suspected new plants to appropriate officials (volunteer groups and active surveys); identify and voucher submitted specimens (designated botanists); verify suspected new plant records (state interagency weed teams and FICMNEW); archive new records in designated regional and plant databases (e.g., the Invasive Plant Atlas of New England (IPANE), and the USDA PLANTS Database); rapidly assess confirmed new records (federal and state weed scientists); and rapidly respond to confirmed new invaders (through actions by land owners/managers and cooperative weed management areas). In 2003, phase one of the project, a Conceptual Design Plan for the proposed system, was finalized and published. In phase two of the project, USGS is cooperating with a number of state and regional groups to develop and field test components of the system that were identified in the conceptual design. Once implemented nationwide as a component of a National All Taxa EDRR effort, the new system will provide an important second line of defense against invasive plants and complement federal efforts to prevent further introductions of foreign invaders at U.S. ports of entry. With both exclusion and early warning systems in place, the nation will be better able to defend against future economic and environmental losses due to 'plants out of place'.

97. Determination of transferable residues of carbaryl from turf

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In support of the USEPA registration of SEVIN 2G applied to residential turf, Bayer CropScience performed a study to determine the specific transferable residues of carbaryl from turf following one application of SEVIN 2G at the maximum proposed label rate of 0.18 lb ai / 1000 square feet. Trials were performed on established turf stands in Florida (St. Augustine grass), Kansas (Fescue), and California (Bermuda grass) where Cloth Dosimeter samples were collected, using the Modified California Roller Technique, from both irrigated and non-irrigated plots at various times following application of SEVIN 2G. Additionally, the transferability of residue from turf to hands was measured in the Kansas test using dry and moist hand wipes. This paper will discuss the design parameters and experimental results from those tests.

98. Surface drinking water assessment and monitoring for oxadiazon herbicide on golf courses

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Modeling studies and drinking water monitoring were conducted to determine potential dietary exposure to oxadiazon as a result of its use on golf courses. As part of their Reregistration Eligibility Decision the USEPA performed a worst case exposure estimation using the PRZM/EXAMS Index Reservoir model, assuming a maximum application rate of 8 lb a.i./A applied through ground spray resulting in an acute exposure of 181 ppb and a long term mean of annual concentrations in drinking water of up to 56 ppb. A refined drinking water exposure assessment was conducted by the authors using the same modeling tools, but adopting more realistic assumptions. For example, 90% of the product is used as a granular formulation with typical use rates of 6 lb a.i./A. In addition, a GIS evaluation of land use in Florida determined that golf courses represent a maximum of 6% of the surface area in watersheds where surface water is abstracted for drinking. Taking into account these and other refinements resulted in reductions in the estimated concentrations of over two orders of magnitude. To confirm the refined exposure assessments, a three-year surface water monitoring program has been established in Florida and North Carolina to measure the potential of oxadiazon reaching surface drinking water source in three community water systems with the highest use of oxadiazon. Residues were detected in raw water in two of the three community water systems and in finished water in one. However the maximum observed concentrations were more than three orders of magnitude lower than the acute drinking water concentration originally estimated and about 25 times lower than the refined assessment. The monitoring program also demonstrates that oxadiazon can be removed in drinking water treatment systems.

99. Monitoring residues from use of an agrochemical product on golf courses at the watershed scale

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Plant-protection compounds are often necessary to maintain the value and aesthetics of turf including those of golf courses. However, plant protection products can enter aquatic systems either by direct or indirect application. In order to better understand the possible frequency and magnitude of exposure, golf courses were identified within watersheds that have been historically treated with vinclozolin fungicide. Golf courses selected in this work were chosen based on their geographic distribution, representation of the products use area, and course position in a watershed relative to a surface water intake(s). Additionally, wells were identified adjacent to courses treated with vinclozolin so that the extent of possible exposure to ground water could also be determined. Analytical results from the study were then compared to three exposure models, Sci-Grow, FIRST and PRZM/EXAMS following EPA methodology to evaluate the ability of the methodology to predict concentrations found in drinking water when compared to actual monitoring data. Results from this examination indicate the exposure from the models can over predict concentrations found in water by several orders of magnitude.

100. Differential application of fluorobenzoic acids to evaluate surface runoff from turfgrass

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Potassium bromide and fluorobenzoic acids, traditional and alternative conservative-tracers, have been utilized as valuable hydrologic tools for characterizing water movement through soil. In this study, three fluorobenzoic acids (2,6-difluorobenzoic acid, 2-trifluoromethylbenzoic acid, and pentafluorobenzoic acid) and potassium bromide were applied to selected locations of fairway creeping bentgrass turf to evaluate water movement and the influence of placement of the chemical to transport with surface runoff. Use of conservative water-soluble tracers represents a worst-case scenario for off-site movement of pesticides and fertilizers with runoff, and can identify areas of high impact that contribute the most to chemical transport. This data can be utilized in model simulations to assess potential environmental impacts as well as provide information to determine cultural practices or application strategies to reduce off-site transport of applied chemicals, increasing their efficacy at intended sites of application and minimizing adverse impacts to surrounding sensitive non-target areas.

101. Cyazofamid Turfgrass dissipation studies with modifications to measure loss from clipping removal

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Traditionally the fate of pesticides applied to turf has been measured by a 120-day dissipation study to satisfy EPA data requirements. Primary concerns have been the rate of degradation of the active ingredient and its degradates as well as the potential for leaching of each of these compounds into the soil. Historically all grass clippings were left on the plot to recycle the residues. Recently concern has also been raised about the loss of residues from the treated area via removal of the grass clippings during the mowing process. The fate of cyazofamid, a cyanoimidazole fungicide, used for Pythium control in turf was investigated with and without removal of clippings at sites in North Carolina and Virginia. Comparison of loss of cyazofamid by clipping removal to other mechanisms of dissipation indicates that for a pesticide such as cyazofamid, which has very short half-lives both on plant surfaces and in soil, and which does not leach, the loss due to removal in the clippings is minimal (0.7-2.2%). Even with application rates of 1 lb a.i./A, dissipation of cyazofamid from turf was rapid (half-lives of 8 to 19 days). There was very little movement of either cyazofamid or its degradates into the soil. By 120 days after the last of three applications, 94-98.8 % of the applied cyazofamid had degraded to form bound residues.

102. Reducing pesticide residues in finished compost resulting from urban applications onto turfgrass

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Clopyralid is a highly effective broadleaf herbicide used in agricultural and until recently, urban settings. In 2001, clopyralid residues were detected in finished compost leaving a municipal composting facility at Spokane, WA. Clopyralid mass was believed to be entering in the compost feed stream via residues on grass clippings from urban treatments to turf. This work assembles pertinent clopyralid degradation research, market share analysis, proposed Best Management Practices

(BMPs), and expert opinion to quantify the likelihood of reducing clopyralid residue levels in finished compost to below threshold levels for hyper-susceptible plants. The entire process from the urban application of clopyralid to turf through the composting process is modeled as a series of interconnected, mass conserving, physical processes. Variability in input is stochastically represented using probability density functions and the system of material balance equations is evaluated using Monte Carlo techniques for input parameter uncertainty. Simulation results are validated against several experimental observation scenarios with good success. Predictive results suggest realizable BMPs can lead to end-user compost residue levels below 5 ppb at the 95th percentile. Product stewardship decisions to withdraw clopyralid from the urban market were made before the results of this modeling effort were available.

103. Overview of a project to improve pesticide runoff estimation from turfgrass

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An estimated 50 million acres of managed turf are grown in the U.S., rivaling the land area dedicated to wheat and greatly surpassing that of cotton and rice. With increased urbanization, turf acreages are expected to steadily increase across the country. Yet, our ability to accurately model pesticide runoff from turf often lags that of major agronomic crops due to a lack of understanding hydrological and other factors controlling pesticide behavior in turf. A cooperative project was recently begun to address this issue in a comprehensive manner. Central to this effort was the development of standardized field procedures that are followed at four research locations across the nation. Three pesticides having a range of physicochemical properties are applied simultaneously to turf plots as part of the protocol. An overview of the project and findings to date will be presented.

104. Award Address. Grand challenges and opportunities in the environmental sciences: The importance of basic research and technology

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Contributions in basic research have immensely enhanced the quality of our environment. This paper focuses on recent breakthroughs in the environmental sciences, with particular emphasis on the Critical Zone, “the heterogeneous, near surface environment in which complex interactions involving rock, soil, water, air, and living organisms regulate the natural habitat and determine the availability of life sustaining resources” (NRC, 2001). Additionally, the paper will delineate frontiers for the present decade and beyond, and stress the need for increased funding for basic research in the environmental sciences. Frontiers will undoubtedly involve multiple spatial and temporal scale investigations, elucidation of reactions at biological, chemical, and physical interfaces, and the use of advanced in situ technologies in combination with interdisciplinary research efforts to unlock important information on: speciation of contaminants in soils; cycling of trace elements and nutrients and impacts on global climate change; development of field scale hydrologic and geochemical models to accurately predict the rate, fate, and transport of contaminants in the Critical Zone; elucidation of mechanisms for microbial transformations of contaminants; and enhanced understanding of rhizosphere chemistry in various environmental settings.

105. Modeling approaches to address turf and golf course scenarios

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The U.S. Environmental Protection Agency (EPA) has used the modeling tools PRZM (Pesticide Root Zone Model) and EXAMS (Exposure Analysis Modeling System) to predict the estimated environmental concentrations (EEC) of pesticides for aquatic exposure assessments and the estimated drinking water concentrations (EDWC) of pesticides for human exposure assessments. To address turf chemicals, EPA has developed specific scenarios for PRZM-EXAMS that estimate runoff of pesticides from managed turf grass. This presentation will discuss these turf scenarios and propose adjustment factors to the modeling outputs specifically for golf courses. This abstract has been subjected to review by EPA's Office of Pesticide Programs and was approved for submission. Approval does not signify the contents reflect the views of EPA, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

106. New thatch and subsurface drainage components in PRZM

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To improve applicability of PRZM for the niche use on highly managed and controlled turf systems, both tile drainage and thatch modeling components were added as optional selections in PRZM. Comparisons and modeling results will be presented for these new components including comparisons to DRAINMOD, results for edge of field turf runoff scenarios, and model programming challenges.

107. The development of a standard turf scenario

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The use of agricultural field scale runoff models to predict pesticide runoff losses from turf poses some unique modeling challenges. There are a number of aspects of turf grass culture which differ significantly from agriculture in how they affect runoff processes. In particular generally high plant and leaf density reduces exposure of the soil surface to direct impact of rain and the associated potential for chemical runoff; the potential for development of increased surface organic matter levels, in varying stages of decomposition and incorporation into the soil matrix - ‘thatch', should be taken into account; highly managed turf grass areas susceptible to runoff are generally smaller than the typical field size for agricultural crops; the potential for erosion of soil is generally much reduced under turf compared to row crops. EPA evaluated a published small plot study to develop a standard turf scenario that is now in use. Published data on mecoprop, dicamba, dithiopyr and 2,4-D was re-evaluated with additional more detailed unpublished data from the study files. In addition chlorpyrifos, a more strongly sorbed compound, was included. Model performance using the key features of the standard turf scenario was generally good for the weakly sorbed compounds. Performance for the strongly sorbed compounds was poor due to over prediction of adsorbed chemical losses in eroded soil. Adjustments to soil erosion parameters and consideration of scale effects resulted in improved predictions.

108. Modeling 2,4-D transport in turfgrass thatch and soil

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In a rapidly draining porous media such as an organically rich turfgrass thatch, pesticide sorption equilibrium is rarely achieved; hence solute transport models which consider non-equilibrium or two-site sorption processes may offer better predictions of pesticide transport. The transport of 2,4-D [(2,4-dichlorophenoxy) acetic acid] was measured for replicated soil columns containing a surface layer of Southshore creeping bentgrass (Agrostis palustris Huds.) or Meyer Zoysiagrass (Zoysia japonica Steud.) and for soil columns devoid of thatch. Following the application of bromide to determine transport parameters, 1.12 kg 2,4-D ha-1 was surface-applied to undisturbed columns under steady state unsaturated conditions. Linear equilibrium (LEM), two-site non-equilibrium (2SNE) and one-site kinetic non-equilibrium (1SNE) models were curve-fitted to experimentally determined breakthrough curves. Pesticide degradation rate constants were independently measured using mass-balance techniques. 2,4-D leaching for columns with bentgrass thatch layers was ca. 60% less than soil columns devoid of thatch. Twenty-seven to 58% of the 2,4-D remaining in columns at the conclusion of the leaching event was tightly bound to the thatch and soil and unlikely to move with additional leaching. Modeling of bromide transport did not present strong evidence of significant two domain flow. All models provided reasonable estimates of 2,4-D transport with slightly improved fits from the 2SNE model through soil columns and the thatch plus soil columns when the retardation factor was a fitting parameter. When retardation factors based on laboratory measured adsorption coefficients were used, significantly improved fits from the 2SNE model were obtained in comparison to the LEM and 1SNE models, suggesting the occurrence of both instantaneous and kinetically driven adsorption. Parameter estimations of 2,4-D retardation factors based solely on curve-fitting techniques may result in inappropriate model selection although excellent curve fit solutions during model calibration may have been previously obtained.

109. Development and testing of a comprehensive model of pesticide losses from turf

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Turf systems have been identified as contributors of pesticides to the environment, and may affect both human and ecological health. While monitoring and field studies provide valuable information they are costly and time consuming to implement. Mathematical models are viable alternatives for studying pesticide fate and transport from turf. To date, few models have been developed specifically for turf. Current literature shows that most modeling efforts of turf systems involve adapting soil chemistry models to account for a thatch layer, and many require extensive calibration to obtain credible predictions. Also, many models have numerous input parameters, which makes their widespread application difficult. A model is presented that is capable of predicting pesticide losses via volatilization, runoff and leaching specifically from turf. The model is based on previously tested runoff and volatilization models. A pesticide-leaching component has been developed and tested. The development of this component, its integration with the runoff and volatilization models, procedures for testing the complete model and the test results are presented. Major advantages of this model are that it requires few input parameters (which can be easily obtained from existing climatic, pesticide and soil databases), and that it performs well without calibration. We envision that the model may be used to provide information for environmental and human health risk analysis assessment, total maximum daily load (TMDL) studies, comparison of turf management scenarios (including inter-media tradeoffs) and development of best management practices for turf systems.

110. Regional analyses of pesticide runoff from turf

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Pesticide runoff loads from turf can be expected to vary dramatically with chemical properties and application regime, geographic location, irrigation rates and turf surface. Given the limited availability of field data, it is extremely difficult to realistically consider the range of these variations in exposure assessments. The TurfPQ pesticide runoff model has been combined with several other models and data bases to provide a general framework for efficient estimation of turf pesticide runoff loads on both a yearly and daily basis. The modeling process involves selection of a U.S. location and associated growing season based on freeze/frost probabilities. Weather data is then generated by the ARS weather model USCLIMATE. These data are input to an irrigation model which determines required turf irrigation based on daily evapotranspiration, and produces a new weather file which includes both daily precipitation and irrigation. Chemical information is selected from a data base of 29 commonly used turf pesticides differentiated for home lawns and golf greens and fairways. Weather and pesticide data are input to TurfPQ, which estimates daily runoff mass loads for each of the selected pesticides. The process is used to investigate differences in bensulide, MCPP, iprodione and carbaryl runoff from fairways for four U.S. locations with widely differing climatic regions, plant hardiness zones, and growing seasons. Among the factors which accounted for the observed differences were pesticide properties and application frequencies, irrigation applications and growing season runoff. The simulations indicated that runoff loads of a particular pesticide could vary by as much as an order of magnitude between the locations.

111. Biopesticides meet the marketplace: Opportunities for eco-products in agriculture and communities

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A rapidly growing market has emerged for products and services produced or delivered in ways that reduce impacts on health and the environment. An example is the organic marketplace, with 2004 sales exceeding $26 billion worldwide. Less known is the market for non-organic, eco-certified products and services, with 2004 worldwide sales exceeding $1 billion annually. Certified products and services include food and fiber products, and structural pest management and landscape maintenance services. Similar to organic, these eco-certification programs apply performance standards based on environmental and health impacts, and often verify performance with independent, third-party audits. A number of these programs have detailed criteria for approved pesticides, analogous to the National List of approved and prohibited substances under the Organic Foods Production Act. A review of these programs indicates a wide variety of criteria and decision-makers for selecting approved pesticides and an opportunity for biopesticides as generally “reduced-risk” options.

112. Nematode-antagonistic natural products

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The inexorable decrease in the number of available nematicides for control of plant-parasitic nematodes has resulted in enhanced efforts to isolate and identify nematode-antagonistic natural products. A diverse spectrum of active compounds has been discovered from a wide range of organisms, including vascular plants, mosses, algae, fungi, bacteria and sponges. We examined culture filtrates of 253 fungi obtained from soybean cyst nematode (SCN) eggs; many inhibited hatching of eggs of SCN or root-knot nematodes (RKN). A few of the filtrates stimulated hatching. From one of these fungi, *Fusarium equiseti*, we isolated and identified two compounds inhibiting RKN hatching and mobility: 4,15-diacetylnivalenol and diacetoxyscirpenol. The phenolic flavipin, isolated from *Chaetomium globosum*, exhibited similar nematode antagonism.

We have also discovered that two cyclic hydroxamic acids occurring in rye inhibit RKN egg hatching and juvenile mobility.

113. Plant volatiles: From compounds to metabolic pathways and their regulation

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Volatile compounds released from leaves, flowers, and fruits play important roles in plant life as attractants, repellents, and signal molecules. While floral volatiles play a vital role in the plant reproductive cycle by attracting pollinators to flowers, volatiles emitted from vegetative tissues during pathogen or herbivore attack are important for plant survival. The majority of herbivore induced volatiles is represented by terpenoid compounds, which could operate as direct defense agents by repelling microbes or animals or indirectly protect the plant via tritrophic interactions by attracting natural predators of attacking herbivores. Terpenoids originate through the condensation of the universal five-carbon building blocks, isopentenyl diphosphate (IPP) and dimethylallyl diphosphate (DMAPP) in a reaction catalyzed by geranyl diphosphate synthase (GPPS). Using functional genomic and biochemical approaches, we have identified and characterized several genes responsible for the formation of plant volatile terpenoids. Snapdragon flowers which emit several monterpenes including myrcene, (E)-B-ocimene and linalool, and a sesquiterpene, nerolidol, in a single scent bouquet were used as a model system to study the flux through the metabolic pathway(s) in situ. Presented results will show how the integration of metabolic profiling, a functional genomic approach, targeted metabolic engineering with metabolic flux analysis and modeling can provide a comprehensive understanding of the regulation of flux through the metabolic networks.

114. Insect semiochemicals and their applications in pest management

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Semiochemicals or infochemicals are the substances used in chemical communication among organisms. Included among the semiochemicals are pheromones which act as vectors of communication between individuals of the same species, as well as kairomones (beneficial to receivers in different species, but maladaptive to the emitter), allomones (beneficial to emitters in different species), and synomones (beneficial to receivers and emitters in different species). From a pest management view, the highly specialized sense of smell of insects can be utilized to control pests that are in direct competition with human beings for agricultural products. These semiochemicals combine advantages of the high activity, specificity, non-toxicity, low residues and, consequently, minimal environmental pollution and are being extensively used in integrated pest management for population monitoring, mass trapping, and mating disruption. Several methods for identifying these activities are described.

115. Detection of genetically modified plant material: Analytical methods

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Plant-Incorporated Protectants (PIPs), a class of genetically modified organisms, express pesticidal gene products. PIPs include both the pesticidal protein produced by the modified plants and the genetic material necessary for the plant to produce that substance. Under Public Laws, the EPA regulates the protein and its genetic material, but the plant itself is not regulated. How can enforcement officials identify PIPs, if necessary? Because a plant expressing a pesticidal protein does not look any different than its conventional counterpart, detection methods may target either protein or DNA that is unique to the PIP plant material. Methods differ in their level of sensitivity, specificity, equipment requirements, time for reaction, and observation techniques. Some methods are suitable for screening in the field while others are more time-consuming and require controlled laboratory conditions and skilled personnel. The OPP Microbiology Laboratory validates the detection methods submitted with registration applications for PIPs before they are accepted for registration purposes. The framework for laboratory validations and an update on the program using gene amplification techniques will be presented.

116. Regulatory issues with the development of biological pesticides

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Biological pesticides are defined as agents derived from natural sources that usually work by a non-toxic mode-of-action and generally pose fewer risks than conventional (chemical) pesicides. Biological pesticides include microbials (e.g., bacteria, fungi, viruses) and biochemicals (e.g., pheromones, plant extracts, oils). In recognition of the unique issues posed by biological pesticides, the Biopesticides and Pollution Prevention Division (BPPD) was created within the Office of Pesticide Programs to facilitate regulatory for these substances. As is done for all pesticides under FIFRA, FQPA, and PRIA, BPPD evaluates biological pesticides in four major areas: composition and analysis data, residue data (i.e., tolerance), toxicity to humans, and effects on non-target organisms and the environment. Pesticide producers are responsible for producing these safety data, which involve standardized testing procedures and indicator species. Since many biological pesticides are novel approaches to pest control, BPPD also focuses on risk issues specific for each case. For example, with microbial pesticides, BPPD determines any possible pathogenicity of the active ingredient as well as the potential for production batches to be contaminated by other microorganisms. Additional information of the regulation of biological pesticides can be found at the following web site: www.epa.gov/pesticides/biopesticides.

117. Strategies for incorporation of biopestides into IPM programs

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Demonstration grants, research and information about biopesticides can influence growers to incorporate biopesticides into IPM programs. A cooperative demonstration program which funds on-farm research to evaluate the utilization of biopesticides as part of a pest management strategy is sponsored by the USDA IR-4 Project and the US EPA Biopesticides and Pollution Prevention Division. Results of some projects involving microbial pesticides as protectants against pathogenic fungi and other diseases of fruits, vegetables and turf are discussed. Other strategies for implementation of biopesticides in IPM include research. After several years of experimenting with Aspergillus flavus AF36, researchers demonstrated to growers that biocontrol of aflatoxin contamination in cotton was a viable option. Other researchers used small scale plots to investigate the use of Aspergillus flavus NRRL 21882 to control aflatoxin in peanuts. Equally important are strategies used to generate needed information for integrated pest management programs. In looking to future strategies, IR-4 with support from EPA Region 2 is developing informational resources for growers, and extension personnel. consultants and other practitioners of IPM programs. By entering crop, pest and regional information, growers can obtain specific reports with biopesticide labels, worker protection information, pre-harvest intervals, organic status and supplier contact information. Such information, provided in a timely manner, can be invaluable to growers who are using crop protection strategies, such as those developed by participants in the Pesticide Environmental Stewardship Program.

118. The application of green chemistry to crop protection

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$26.5 billion of synthetic chemical pesticides are used annually to control pests and plant diseases on crops in homes and gardens. While chemical pesticides are often inexpensive and highly effective, there are issues of ground water contamination, acute toxicity, non-target effects, residues, and pest resistance development. This talk will provide an overview of the global pesticide market, examples of green chemistry for crop protection and discuss the potential for utilization of microbial natural products as green chemistry alternatives to chemical pesticides, describing the process of discovery, development and marketing of successful products.

119. The future of natural products in pest management

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Natural products offer a rich source of chemical structures with evolved biological activities, some of which can be useful to humankind. Natural products were the original basis of the pharmaceutical industry, and several major products and classes for products of the pesticide industry have been bsed on naturally-occurring compounds of biotic origin (e.g., pyrethroids, strobilurins, triketone herbicides, and glufosinate). The major players in the pesticide market are still using natural products as leads for the development of new pest management products. Smaller companies are generating natural product pesticides for small markets (e.g., pelargonic acid for weed management in turf). Since biological compounds are produced by enzymes encoded by genes, transgenic technology offers the opportunity to introduce new or increase existing natural pesticides in crops. The most successful example of this is the introduction of Bt toxins into crops. An alternative is to improve the performance of biological control organisms through genetically engineering certain natural compounds into them. The advantages, disadvantages, and potntial for future use of each of these approaches, with examples, will be discussed.

120. A comparison of two turf modeling approaches

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Existing agricultural runoff models have been adapted to suit highly managed turf grass. The Environmental Protection Agency has developed scenarios for turf grass for use with the Pesticide Root Zone Model (PRZM). An alternative approach using only those processes directly relevant to turf grass has been adopted in the TurfPQ model. These two models were compared using the experimental data from a small plot study originally used in the development of the EPA turf scenario. TurfPQ generally over predicted measured chemical runoff: by an average factor of 2.3 for the weakly sorbed dicamba, mecoprop and 2,4-D and an average factor of 11 for the more strongly sorbed dithiopyr and chlorpyrifos. PRZM results bracketed the observed values but not uniformly: chemical runoff for weakly sorbed compounds was under predicted by a factor of 1.8 and for the strongly sorbed compounds over predicted by a factor of 2.8. TurfPQ predictions of chemical runoff were particularly sensitive to K_{oc} at low values ($K_{oc} <$ 100 ml/g), driven by the assumption that all leaching occurs before any runoff.

121. Modeling offsite transport of turf-applied pesticides: model and data needs

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Offsite transport of pesticides (leaching and runoff) is measured in field and watershed-scale monitoring studies as well as in controlled test plot studies. It often is projected to other points in time and space with the use of numerical and analytical solution models such as PRZM, SWAT, and GLEAMS. However, most of these models - with the notable exception of the TURFPQ regression model (Haith, 2001, 2002) - were developed for agricultural systems. Large discrepancies between measured and predicted values indicate that different processes may exist in determining pesticide behavior in agricultural and turf systems. For agricultural systems, raindrops interact with surface soil, extract chemical, and carry it with washoff chemical into surface runoff. Most agricultural models have been developed based on these processes. For a typical turfgrass system, the dense vegetation of turfgrass foliage and thatch prevents direct interactions between raindrops and surface soil. Rather, raindrops interact more with dense turf vegetation (verdure) and thatch and less with soil. Thus pesticide loads and concentrations in vegetation and thatch are more important for determining pesticide runoff and leachate relative to soil. Over 20 years of turf modeling experience lead us to identify the following model and data needs that distinguish turf from typical agricultural crops. Model needs/deficiencies: the ability to simulate frequent mowing, which affects the leaf area index, water uptake, and ET; the representation of the surface and root zone hydrology during turf's dormant stages; the determination of whether it is valid to simulate the thatch layer as a soil layer with peculiar properties, or whether a special subroutine is appropriate. Special data needs: the bulk density and effective organic carbon content of thatch; enhanced degradation rate constants in the bioactive root zone; ET input in relation to dormant periods; and possible enhanced volatilization in turf relative to row crops.

122. Bioavailability of phytotoxins in multisolute systems as influenced by soil competitive sorption properties

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Soil sorption influences the allelochemical properties by altering their biotic availability, bioactive concentration, persistence and fate in rhizosphere. We hypothesize that in a multisolute system such as root exudates, the preferential sorption of one component could increase the soil solution concentration of the companion component. This is important in ecological perspective, as plant secondary metabolites could exhibit concerted physical phytotoxic effects. Sorption study was conducted in a clay loam soil with 6% organic matter using four phenolic acids viz. hydroxybenzoic, vanillic, p-coumaric, and ferulic acids, as they are ubiquitous in plant root exudates. The sorption and competitive sorption were analyzed based on Freundlich isotherm. Freundlich's exponents were between 0.71 and 0.81 for all phenolic acids except hydroxybenzoic acid which was 1.07. Nonlinearity of isotherms indicates site specific sorption to be a major mechanism of sorption of these chemicals in soil, which in turn could result in competition for sorption sites in multisolute systems. Preferential sorption of vanillic acid over hydroxybenzoic acid was observed in a binary mixture. The sorption affinity of hydroxybenzoic acid, described by Freundlich coefficient KF, decreased ten folds in the presence of vanillic acid in the system. Competitive sorption was much higher at lower concentration of the primary sorbate and decreased as its concentration progressed towards the concentration of competing sorbate. Competitive sorption data of other phenolic acid mixtures will be discussed. Our results show that competitive sorption of plant secondary metabolites in multisolute mixtures could alter the bioavailable concentration of its individual components, and thus could alter the phytotoxic behavior of mixtures.

123. Multiple-inlet irrigation plus intermittent flooding reduces NPS runoff in rice production

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Research was conducted in 2004 to determine the potential for water savings and reduced non-point source runoff using multiple-inlet irrigation plus intermittent flooding as compared to continuously flooded rice. Experiments were conducted at five farms ranging from the southern-most Mississippi Delta to the northeast corner of Arkansas. Each location consisted of two adjacent fields averaging 16 ha each. The two fields only differed in water management practice. The control field at each location was continuously flooded using the grower's traditional practices. The experimental field used multiple-inlet irrigation plus intermittent flooding, whereby the flood was established at the appropriate time using 38-cm diameter plastic pipe to deliver water to each paddy simultaneously. After two weeks of continuous flooding, the experimental field was allowed to dry until about half of each paddy had exposed soil. At this point, the 8 to 10 cm flood was reestablished. This cycle was repeated every 5- to 9-days throughout the growing season. All water inputs and flood depths were recorded. Water samples were collected on a weekly basis for nutrient and pesticide analysis. Intermittent flooding did not affect pest pressure, plant-nutrient content, or rice yield. However, intermittently flooded rice used 56 cm water per ha compared to 81 cm per ha with continuously flooded rice, representing a 30% savings in irrigation inputs. This savings was due to increased rainfall-holding capacity, and reduced over-pumping and subsequent tailwater runoff. Based on 25-year historical rainfall data, our model predicts an average increase in rainfall capture of 67% and a 60% reduction in tailwater runoff for the intermittent flood as compared to the conventional flood system. Water samples are currently being analyzed for pesticide and nutrient concentrations and will be used to estimate surface water loadings from each irrigation treatment.

124. Predicting soil fumigant acute, sub-chronic, and chronic air concentrations under diverse agronomic practices

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Soil fumigants are used by farmers to control nematodes and other soil dwelling agricultural pests. However, volatility losses from treated fields can create the potential for bystander inhalation exposure. Fumigant air concentrations for entire agricultural regions are calculated using multiple transient source terms (treated fields), GIS information, agronomic specific variables, user specified buffer zones and field re-entry intervals. A modified version of the USEPA Industrial Source Complex Short Term model (ISCST3) is used for air dispersion calculations. Field observed fumigant flux profiles from soil are used as transient source terms for both shank injection and drip-irrigation applications. Reference flux observations are scaled based upon depth of incorporation and the time of year in an attempt to map the complete flux response surface from select field observations. Weather information, field size, application date, application rate, application type, depth, pesticide degradation rates in air, tarp presence, ag-capable land, field retreatment, buffer setbacks, and other sensitive parameters are varied stochastically using Monte Carlo techniques to mimic region and crop specific agronomic practices. Sub-regions of agricultural areas up to 19,000 mi^2 can be simulated for temporal periods ranging from 1 day to more than 70 years for the purpose of assessing acute, sub-chronic, or chronic risk. Multi-year simulations are conducted using random field placement in all agricultural capable areas as well by selectively placing fields in historical or prospective use areas. Regional land cover, elevation, and population information can be used to refine source placement (treated fields), dispersion calculations, and exposure assessments. Algorithms used to refine exposure predictions and manage acute, sub-chronic, and chronic risk associated with the use of soil fumigants on a local or regional basis are presented.

125. Managing 1,3-D exposure and risk in the high use regions of Merced and Ventura California: Results of SOFEA(C) modeling

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Soil fumigants are effective for nematode control, however, there is the potential for inhalation exposure for any soil fumigant following treatment if the fumigant volatilizes at the soil-air interface. The use of 1,3-Dichloropropene (1,3-D) as a soil fumigant is increasing in part since it is a replacement for Methyl Bromide in many markets. Chronic exposures for the fumigant 1,3-dichloropropene (1,3-D) are managed in part by constraining the annual amount that can be used within a given area (eg. township allocations in California). A stochastic/mechanistic numerical system (SOFEA©) which uses the USEPA air dispersion model ISCST3 with links to Geographic Information Systems was constructed and used to calculate chronic and acute air shed concentrations arising from volatility losses from treated agricultural fields as township allocations are varied. SOFEA© uses field measured flux profiles for fumigant volatility from soil as transient area-source terms. Chronic exposure and risk to individuals residing in Merced and Ventura counties of California is determined for residents who are reside for 30 years within a single township (6 mi x 6 mi) or a 9 township block (18 mi x 18 mi). Weather year, application date, application rate, field size and pesticide degradation rates in air were varied stochastically using Monte Carlo techniques to mimic typical physical and agronomic practices for specific regions of California. Simulation results indicate that even with a block of 25 contiguous townships all treated at the maximum observed use levels from 1999-2004, and at projected use up to 1.5x higher than the historical township allocation in key high demand townships, the level of chronic lifetime risk to residents is acceptable.

126. Improving Day Zero recoveries in field soil dissipation studies

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Field dissipation studies for the crop protection chemicals are one of the most important and expensive portion of the environmental fate work conducted for registration of agrochemicals. One of the requirements of an acceptable field dissipation study from the regulators perspective is the verification of the amount of chemical applied. According to the results obtained by various companies (ACS Symposium Series 842, Terrestrial Field Dissipation Studies), the residues are measured in soil immediately (termed as day zero) after application often average in 50-70% range of the nominal amounts. Such an observation creates the perception that the right amount was not actually applied, or there were gross errors in the chemicals' application process. This issue was identified as a significant shortcoming in all dissipation studies in the EPA's rejection rate analysis (published by the EPA in 1992), and it has been the subject of symposia at various agrochemical scientific conferences. We investigated a few different sampling devices to see if the recoveries are dependent on soil sampling methods. With a modified sampling system, day zero recoveries have been improved to average of 80-85%. Results of our on-going investigation will be discussed

127. Pesticidal activity of phytochemicals produced by arid land flora

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Crude extracts of 21 different species of wild flora of the Sahara desert, known to be resistant to wide range of pests, were evaluated for their antimicrobial, insecticidal, nematicidal, herbicidal, and fungicidal activity. Steam distillates were performed on the fresh leaves. Organic extracts were prepared using methylene chloride/methanol mixture, and aqueous extracts were obtained from the pre-extracted materials that remained after organic extractions. All extracted materials were bioassayed for their pesticidal activity. The following plants were studied: Ruta tubereculata, Tamarix nilotica, Artemisia judaica, Artemisia monosperma, Clerodendrum acerbianum, Rosmarinus officinalis, Cymbopogon citratus, Achillea millifolium, Lantana camara, Kochia indica, Geranium cicutarium, Cassia acutifolia, Matricaria chanomilla, Thymus vulgaris, Artemisia indica, Adhatoda viscum, Alpina officinalis, Zygophyllum album, Eugina aromatica, Colligonum comosum, and Peganum harmala,. Crude extracts were further fractionated to isolate and identify the chemical(s) responsible for the activity. High Performance Liquid Chromatography (HPLC) was used to fractionate the crude extract to its individual components. Chromatographic fractionation and isolation of the active ingredient(s) was guided by the bioassay; the most effective column fraction was purified further to obtain purified compounds. Chemical purity was confirmed by gas chromatography/mass/infrared spectrometry. The chemical structures of the active ingredients were identified or partially identified based on IR, NMR and mass spectroscopy. Supported by NASA / TSU-URC # NCC165-9 and RCMI # R003045-17

128. Photolysis of [14C] furfural in aqueous solutions and indentification of photoproducts by HPLC/RAM and LC/MS

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Furfural is ubiquitous in nature and widely found as a natural component in raw and processed foods. It is Generally Recognized as Safe (GRAS) as a food flavoring agent and has also been used with significant environmental benefits as a new and effective crop protection agent to control nematodes, fungi and weeds. The present study investigated the photolytic degradation of furfural in water. Furfural readily photolyzed in aqueous solutions when exposed for 30 days to indoor artificial light with a half-life of 6.72, 6.00 and 6.69 days at pH's 5, 7 and 9 respectively. Furfural photodegradates at ≥10% of applied dose were tentatively identified and quantified by HPLC/RAM and confirmed by LC/MS. Following photolytic breakage of the 5-membered furan ring, evidence shows that furfural was converted via 2-ketoglutaric at pH 5 to succinic acid or directly to succinic acid at pH 7 or 9. Succinic acid, the major photodegradate identified at 31 to 55% of the initial dose, was converted to malonic acid at pH 7or 9; that in turn was further converted to either propionic acid at pH 9 or to formic acid at pH 7. Although tentatively identified by HPLC/RAM neither propionic nor formic acid could be confirmed by LC/MS due to instrument sensitivity problems. Details of the photodegradation pathway for furfural will be discussed. As a result of agricultural applications, residues of furfural entering natural water bodies are therefore expected to photodegrade readily to low molecular weight compounds commonly found in nature.

129. Enzymatical hydrolysis of chiral dichlorprop-methyl effecting by beta-cyclodextrins

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The effect of β-cyclodextrins (β-CDs) on the enzymatical hydrolysis of chiral dichlorprop-methyl (DCPPM) has been specifically studied. Four kinds of β-cyclodextrins (β-cyclodextrin, partly methylated-CD (PM-β-CD), hydroxypropyl-cyclodextrin (HP-β-CD) and carboxymethyl-cyclodextrin (CM-β-CD) were used. Compared with 100% DCPPM in the absence of β-cyclodextrins, the activity of lipase decreased with the increase of β-cyclodextrin and PM-□-cyclodextrin. However, CM-β-cyclodextrin stimulated the lipase activity. The inhibition effect of β-cyclodextrin and PM-β-cyclodextrin on the hydrolysis of DCPPM is affected by many factors other than degree of the methylation blocking the active site of lipase. UV-Vis and Fourier transform infrared (FTIR) spectroscopy studies of the complexation of aqueous DCPPM with β-CDs provide fresh insight into the molecular structure of the complex and explain the effects of β-CDs on enzymatical hydrolysis of chiral DCPPM. Data showed that inclusion complexes had formed by complexation of the CM-β-CD with DCPPM and the solubility of DCPPM was increased in water, which leaded to the increased lipase activity. The research was supported by the National Key Project for Basic Research (2002CB410800).

130. Quantitative structure activity relationship of antifungal terpenoids

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In the Environmental Chemistry and Toxicology Laboratory of Texas Southern University, we are interested in finding novel uses for natural products, particularly as they relate to pest management. Terpenoids with tremendous diversity of chemical structures were found to exhibit antifungal properties against a wide range of fungal species. It was also observed that certain terpenoids having apparently different molecular structures and functional groups show similarities in their effect on fungal growth. Farnesol analogs were found to mimic the quorum signaling chemicals produced by fungus to initiate biofilm formation. With the great diversity in chemical structures, the mode of action of antifungal terpenoids also varied greatly. Differences include disruption of the fungus membrane and inhibiting biosynthesis fungal sterol from blocking the formation of the fungal cell wall. Terpenoids were grouped according to their antifungal mode of action/chemical structures and compiled into a molecular spreadsheet. Quantitative Structure Activity Relationship of select terpenes was investigated using SYBYL 7.0, modeling software of Tripos, Inc. Several types of molecular descriptors including structural, conformational, and geometrical properties were used to derive a quantitative relationship between antifungal activity and structural properties. Comparative molecular field analysis (CoMFA), a method of three-dimensional quantitative structure-activity relationship (3D-QSAR) analysis and other SYBYL7.0 tools were used to determine the binding site and structural requirements essential for optimum fungicidal activity. This work is funded by NASA Grant # NCC165-9

131. Estimation of the ADME characteristics for putative insecticides using time/dose/response relationships

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During the development of a novel insecticide, data is required that can be used to assess its absorption into the insect and subsequent distribution, metabolism, elimination and toxicity (ADMET). The usual approach is to undertake in vivo and in vitro pharmacokinetic studies, which are both expensive and time-consuming. An alternative approach is to estimate these parameters, the penetration rate constant (kp), the distribution constant (l), the elimination rate constant (ke) and the toxicity (endpoint LD50), from time-dose-response curves that can be readily obtained using standard, inexpensive bioassay procedures. The presentation describes the possibility of constructing a time/dose/response relationship based on the notion that, for a response to occur, the internal exposure of the organism to an insecticide must achieve some critical value. The estimated parameters (kp, ke l, the lag time and the endpoint ED50) comprise a set of y-block response variables for use in QSAR.

132. Estimation of tissue:blood partition coefficients of carbamates and organophosphorous (OP) pesticides using relative lipid content and Log P as the mechanistic determinants

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PBPK/PD models were developed for carbamate and OP pesticides to aid in human risk assessments. Tissue:plasma ($P_{t:p}$) partition coefficients (PCs) are important pesticide specific input parameters. The experimental determination of $P_{t:p}$ requires steady-state conditions and may be confounded by metabolism in plasma. Hence there has been considerable interest in predicting $P_{t:p}$ based on tissue composition and measures of lipophilicity, such as the *n*-octanol:water PC ($K_{o:w}$) or the oil:water PC ($K_{ov:w}$). We employed the tissue-composition based algorithm of Haddad (2000) and $K_{o:w}$ or $K_{ov:w}$ to estimate adipose tissue:blood PC ($PC_{at:b}$) for 10 carbamates and two OP pesticides. The $K_{o:w}$ and $K_{ov:w}$ were determined for the pesticides of interest using SMILES notations and Accord for Excel™

$$PC_{at:b} = \frac{[PC_{o:w} \times F_{neat}] + F_{weat}}{[PC_{o:w} \times F_{neb}] + F_{web}}$$

where neat, neb are neutral lipid equivalents and weat and web are water-equivalents. In evaluating OPs and carbamates, the predictions ranged from being nearly identical for oxamyl (0.233 vs. 0.52) to over 10-fold different for propoxur (2.33 vs. 30.7). This work suggests that constituitive measures of lipophilicity may describe chemical partitioning in more complex matrices, however, the divergent results require further investigation. Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

133. Molecular transformations as a way of finding and exploiting consistent local QSAR

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The idea of a “transformation”, i.e., making a small change to a chemical structure such as removing or replacing a substituent, is familiar to chemists. We suggest two ways of representing a transformation (either as a descriptor difference vector or as the set of atoms remaining once a maximum common substructure is eliminated) such that transformations can be filtered and clustered sensibly and enable easy comparison between transformations. These representations have two applications. First, we can use these methods to automatically organize and display sets of closely related compounds such that any consistent local QSAR in a dataset can be easily seen. Second, we can suggest to a chemist how to change a probe molecule of interest to a more active one based on local QSAR for that activity. Both applications will be discussed.

134. Putting the "Structure" in (Q)SAR into context

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The development of biologically active small molecules for agrochemical applications entails exploration of a wide range of quantitative and qualitative structure/activity relationships (SARs). It is tempting to take a "one structure fits all" approach to deriving the descriptors upon which such analyses are based, but the diversity of analyses puts the validity of such an assumption in doubt. Besides bioavailabilty issues that parallel those arising in pharmaceutical development, there may be regulatory concerns about environmental dispersion (e.g., leachability) and toxicity. In addition, complex commercial considerations such as selectivity between target and non-target species, and amenability to formulation come into play. Even production cost can enter into agrochemical development in ways that rarely arise for pharmaceuticals. This talk will explore how different analyses may require different structural representations.

135. A new software-aided approach to agrochemical structure optimization

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Biological activity and environmental endpoints for compounds, such as absorption in soil and leaching, are often a function of the compound's physiochemical properties (logP, pK_a, vapor pressure, melting point, etc.). After library screening, it is often desirable to optimize the properties of selected lead compounds by making small chemical changes to them. While rules of thumb are generally applied, these synthetic modifications are often carried out without precise endpoint expectations. By combining physicochemical property predictors and a critically evaluated database of biologically-acceptable substituents (with Hammett parameters), the agrochemical chemist can reduce the number of derivative compounds that need to be synthesized to achieve optimal agrochemical-like properties. A structure design software approach, which suggests structural modifications leading to desired property and environmental endpoints—without introducing unwanted toxicity effects—will be described.

136. Organism-based QSAR models for various toxicological outcomes

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The use of QSAR models to predict various toxicological endpoints has been a part of biocompatibility investigations for some time. Unfortunately, many of the commonly accepted assays involve interactions of the analyte with living organisms. Such biologically-based data often has wide variations for the same material and the effects of other interactions between the analyte and organism cloud the results. In this paper, we will describe three quantum mechanically-based QSAR (QMQSAR) models developed in our laboratory that estimate the outcomes of the MTT/neutral red assay for cytotoxicity, the TA100 Ames assay for mutagenicity, and the local lymph node assay (LLNA) for skin sensitization. The general approach that we have taken is to CLASSIFY molecules into general toxicity categories rather than predict specific response values. Methods and procedures will be illustrated and developed.

137. Evaluation of water balance components and nitrate-N losses from a Southeastern Coastal Plain Field using the Root Zone Water Quality model

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The USDA-ARS Root Zone Water Quality Model (RZWQM) is a comprehensive agricultural model used as a research tool for investigating the effects of agricultural management on crop production and environmental quality. It combines crop growth, soil nutrient cycling, soil microbiology and hydrology to simulate the movement and fate of agrochemicals in the soil. We tested predictions from RZWQM with data from a two-year experimental data set in which corn and millet crops were grown each year on a 0.34-ha, Southeastern Coastal Plain sandy loam field. Water balance components and nitrate-N concentrations were measured in the soil profile, and in the surface and subsurface flow. For simulations, differences in soil properties between crop beds and wheel-tracks were evaluated. A measured wheel-track Ks (saturated hydraulic conductivity) was used and a soil crust was assumed for the crop beds with a calibrated Ks. The model described event runoff flows well and indicated that the wheel-tracks, which occupy about 27% of the field area, contributed about half of the runoff water. However, nitrate-N losses were over-predicted by a factor of six, indicating some process is immobilizing nitrate-N that is unaccounted for. The study suggested that by accounting for the significant differences in hydrology between wheel-tracks and crop beds, potential BMP designs are possible that would not be indicated in a uniform field simulation.

138. Tebuconazole ozonation in water: By-products and dissipation kinetics

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Oxidative destruction of pesticides with ozone has significant potential as a treatment technology. Complete removal and or substantial reduction of pesticide residues in raw drinking water, wastewater, soil, and on surfaces of fruits and vegetables have been reported; however, predicting the extent and efficacy of treatment remains difficult. Reaction rates with ozone and by-product formation have been reported for only a small fraction of the hundreds of pesticide active ingredients in use. We examined the reaction kinetics of the triazole fungicide tebuconazole with ozone by monitoring dissipation of the parent and accumulation and decay of reaction by-products in distilled-deionized water and well water by HPLC-APCI-MS^n. Dissipation data were well described by pseudo-first order kinetics (r^2=0.977 to 0.999) with the reaction rate constant in distilled water increasing about 10X as the pH was increased from 3 to 9. Fourteen by-products were identified whose structures suggested two degradation pathways; initial cleavage of the compound's t-butyl group or oxidation of its chlorophenyl ring. The later was predominant. The principal by-product accounting >50% of all products was presumably derived by complete oxidation of the chlorophenyl group to yield a γ-hydroxy acid that subsequently cyclized to produce a γ-lactone. This is the same product that was recently described as the principal product of tebuconazole aerobic soil metabolism. Results show that ozonation may effectively remove tebuconazole from water inadvertently contaminated by tebuconazole. However relatively stable by-products were formed. Their complete destruction requires further investigation.

139. Evaluation of the evaporation potential of components of agricultural products

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The purpose of this study was to compare methods of estimating the evaporation rate of chemicals used as formulants in pesticide products from plant surfaces for a range of ingredients ranging from 2 to >30,000 Pa in vapor pressure. Two methods utilized were the ASTM Shell Evaporometer test and the Woodrow et al. (2001) vapor pressure correlation methodology. Additional data from a third study by Roth et al. (2004) was utilized to validate the results of the ASTM and Woodrow methods. The ASTM method or the Woodrow correlation method can be used to determine the evaporation rate from plant surfaces for co-formulants and active ingredients exhibiting a wide range of vapor pressure. The study showed that all 3 independent datasets provide similar regressions between the natural log (Ln) of Vapor Pressure and Ln (Evaporation Rate). A new regression which utilized the evaporation and vapor pressure data from all 3 datasets was developed. The data suggests that many co-formulants will fully evaporate from plant surfaces within several hours of application under normal agricultural application conditions. Rapid evaporative losses from plant surfaces suggest that the potential for dietary residues (food-related) should be minimal.

140. Kinetic model and optimization of DEET degradation by flow-though anodic Fenton treatment (FAFT)

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Based on the previously developed batch anodic Fenton treatment (AFT) technology, a flow-through AFT system (FAFT) was systematically studied in order to bring this technology into practical general use in the field. A kinetic model (the FAFT model) has been developed to accurately describe the degradation of DEET, an insect repellent, in FAFT under various operating conditions. Systems with higher flow rate (shorter retention time), higher initial concentration of DEET, or lower delivery rate of Fenton reagent were found to have higher treatment efficiency; while the optimum H_2O_2:Fe^{2+} ratio was believed to be around 10:1. Analyses and/or evaluation of the concentrations and average lives of Fe^{2+}, H_2O_2, and the hydroxyl radical in FAFT under different flow rates and ratios of H_2O_2:Fe^{2+} revealed that only the HO• concentration could explain the change in the treatment efficiency and the existence of the optimum H_2O_2:Fe^{2+} ratio.

141. Statistically-based method for establishing NAFTA-harmonized tolerances

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Current pesticide tolerance-setting methodology in the US and Canada is based on identifying the highest residue from a set of field trial data and then “rounding up.” There is little guidance regarding how much higher the tolerance should be than the highest field trial residue, and different reviewers from different agencies/governments can have different viewpoints on the level at which tolerances should be set. Beginning in earnest in March 2004, a NAFTA workgroup was tasked to develop and propose a statistically-based methodology which could be used as a standard basis for establishing tolerances. The workgroup agreed that any proposed methodology should establish tolerances at a level which balance the probability associated with wrongly seizing a legally treated crop and the probability of being incapable with a reasonable degree of surety of detecting illegal use. In addition, any developed methodology should be reasonably simple to use by non-statisticians (requiring only calculators or spreadsheets), should aim to be reasonably well-accepted, and should be based – as far as possible – on accepted statistical principles and methods. The ultimate goal of the project was to formulate a standard methodology that can be used by the US and Canada as part of the joint review program such that the same or similar datasets will result in the same recommendation for

tolerance levels. The methodology is incorporated into an automated Microsoft Excel workbook, which can be provided upon request. This presentation will cover the history behind the project, the statistical -- and non-statistical -- principles behind the methods, and a brief description of how the method is currently being implemented in EPA's Office of Pesticide Programs.

142. Molecular interactions of Demeton S and Hg(II) by NMR

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The fate of organophosphorus pesticides (OPs) has been proven to depend strongly on the chemistry of their aquatic environment. In particular, metal ions (and metal oxide surfaces) have been known to play an important role in the hydrolytic fate of OPs. Various postulates regarding the mechanism of metal ion promoted hydrolysis of OPs have been made. However, direct spectroscopic evidence to pinpoint the hydrolytic products and the exact interaction between metal ions and organophosphorus pesticides is still lacking. We report herein the first in situ study of the interaction between an aqueous solution of Hg(II) and Demeton S using ^{1}H- and ^{31}P-NMR spectroscopy. It was found that the interactions between Hg(II), a soft Lewis acid, and Demeton S tend to be a strong function of the aqueous speciation of Hg(II), and the bonding between Hg^{2+} and Demeton S does not involve the central P=O bond, rather Hg^{2+} bonds with the two sulfur atoms in the Demeton S side chain and subsequently stabilizes the Demeton S molecule, a phenomenon not previously reported for any metal ion-OP systems studied. Overall, generalizations regarding the nature of metal ion binding even within a given class of OPs should be avoided or only made with extreme caution.

143. Organophosphate induced chronic neurotoxicity: Health, environmental and risk exposure issues in developing nations of the world

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Organophosphates (OPs) are chemical substances, originally produced by the reaction of alcohols and phosphoric acid. Organophosphate insecticides such as diazon, disulfoton, azinphosmethyl are widely used in agriculture and in household applications as pesticides. Exposures of human populations to a wide variety of organophosphates have generated profound concerns about their neurotoxic consequences. Among these concerns are their potential impacts on children and the developing nervous system, highly susceptible adult members of the population and the contribution and economic implications of such exposures to the neurodegenerative diseases associated with advancing age. This paper therefore tends to make a review of the health, environmental and other risk exposure issues of organophosphates especially in Africa and other developing nations of the world where many agents considered toxic in many parts of the world are still available and where children are still being expected to work on, or be hired out as labourers.

144. Development of a new Standard Reference Material: SRM 695 Trace Elements Multi-nutrient Fertilizer

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In the past, the fertilizer industry was responsible for validating only the nutrient content of their products. A few years ago, an imported material used to manufacture fertilizers was contaminated with Cd. The discovery of percent levels of Cd in a fertilizer material resulted in many states proposing and enacting new regulations limiting the amounts of contaminant metals in fertilizers. In response to these new and proposed regulations, this industry group and its regulatory authorities are now faced with having to develop required analytical methods and to validate these methods and results. To assist in method development and validation, NIST has been working with the agrochemical industry to develop a Standard Reference Material. SRM 695 Trace Elements in Multi-nutrient Fertilizer is a blended multi-nutrient fertilizer comprised of ammonium phosphate, different forms of urea, potassium nitrate, potash, borax, and various metal oxy-sulfates. The starting material was donated to NIST by a US agrochemical company and was jet-milled, blended and bottled at NIST. X-ray fluorescence (XRF) was used to assess material homogeneity and additional analyses (INAA, prompt gamma ray activation analysis, XRF, inductively coupled plasma atomic emission spectrometry) are underway to determine element content. Certified values are needed for the following regulated elements: As, Cd, Cr, Co, Pb, Hg, Mo, Ni, Se, and Zn. In addition, certified or reference values are desirable for the following elements that are essential for plants: B, N, P, K, Mn, Fe, and Cu.

145. Performance characteristics of urea-based polymeric controlled release fertilizers

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Economically and environmentally meeting the nitrogen requirements that maximize crop production necessitates the improved nitrogen use efficiency (NUE) of N fertilizers. This presentation encompasses the analysis and evaluation of new controlled release N fertilizers developed for improved NUE. These new controlled release fertilizer N materials are produced as a 30% N liquid, 36% N powder or 40-43% N granule at prices comparable to or more economical than similar controlled release N materials. Structural analysis reveals that the composition of the material is a blend of urea, urea-forms of various chain lengths and cyclic molecules. Studies are underway to measure: 1) the ammonia volatilization of these controlled release fertilizer N materials as compared to high (urea) and low (ammonium nitrate) materials; 2) monitor the release and movement of nitrogen through the soil by employing leaching containers buried in the ground; 3). the nitrate and ammonium release as affected by soil type, pH, time and/or carbon content; and 4) the influence of soil microbial biomass and activity on inorganic nitrogen release from these controlled release N fertilizer materials. In this presentation we will discuss the latest data from each of the aforementioned studies.

146. Review and summary of the IFA Conference on Enhanced Efficiency Fertilizers

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Impacts of nitrogen and phosphate on the environment and the need to more completely utilize fertilizer nutrients have caused increasing activity and interest within the agricultural community relating to fertilizer efficiency. As a result of this interest, the International Fertilizer Association (IFA) in coordination with The Fertilizer Institute (TFI) and others have organized a conference to examine technical aspects of "Enhanced Efficiency Fertilizers". The conference will address regulatory, environmental, and technical issues utilizing a field of invited international experts on the issues. These guests from academia, the fertilizer industry and agricultural representatives will make formal presentations on specific areas of interest including forms of slow release materials, urease and nitrification inhibitors, and other means to improve nutrient efficiency and minimize losses to the environment. Panel discussions and poster sessions will also be used to facilitate discussion regarding trends and opportunities to utilize more efficient fertilizer products in mainstream agriculture.

147. Artificial fertilizers and climate change impacts on crop yields

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The effects of different climate-rainfall situations and N-P-K, Ca and Mg artificial fertilization systems were evaluated on a Haplic Luvisol [pH (KCl) 4.7, humus 0.7%, total N 34 mg/kg, Al-P_2O_5 43 mg/kg, Al-K_2O 60 mg/kg] on yield of rye, potato, winter wheat, and triticale in a long-term field experiment set up during 1962 in Hungary lasting for 42 years. From 1962 to 1980 the experiment consisted of 2 x 16 x 4 x 4 = 512 plots and from 1980 of 32 x 4 = 128 plots in split-split-plot and factorial random block designs. The average fertilizer rates in kg ha-1 year were nitrogen 45, phosphorus 24 (P_2O_5), potassium 40 (K_2O), magnesium 7.5 (MgO) until 1980 and nitrogen 75, phosphorus 90 (P_2O_5), potassium 90 (K_2O), magnesium 140 ($MgCO_3$) after 1980. In rye the yields were greater than 3.5 t/ha in average years with good nutrient supplies (N: 90 kg/ha + NP, NK, NPK, NPKMg combinations), this was reduced by 17% in dry years and by 52% in wet years. In potato no yield-reducing effect was observed in wet and dry years at high nutrient supply levels (N: 150 kg/ha + NP, NK, NPK, NPKMg combinations). In winter wheat the yield declined even more in wet years than in the case of drought. Application of N alone or of NP and NK treatments in triticale led to yield losses of 45 and 24%, respectively, in dry and droughty years, while that of NPK, NPKCa, NPKMg or NPKCaMg caused a further 22% average drop in both wet and dry years.

148. Kinetics of radionuclides and heavy metals behavior in soils: Implications for plant growth

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The extent of metal and radionuclide contamination in the world is inmense. In soils, metals and radionuclides can be dissolved in solution,or ion exchanged in reaction, complexed with soil organics or precipitate as pure or mixed solids. Soluble contaminants are subject to migration with soilwater, uptake by plants or aquatic organisms or loss due to volatilization.Lead, chromium, zinc, arsenic and cadmium are the most frequently identified inorganic contaminants in soil and groundwater.Unlike degradable organic contaminants and ever short-lived radionuclides that can become less toxic over time, metals can be considered conservative. However, many metals, especially radio-sensitive elements such as arsenic and chromium, can undergo transformation or sorption reactions that alter both mobility and relative toxicity. This paper therefore, makes a review of these behaviours of radionuclides and heavy metals in soils, in connection to soil contamination and there effects on plant growth.

149. Agrochemical and morphological characteristics of city hard domestic wastes (HDW)

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At present the optimization of fertility and agrochemical characteristics of soil has a great importance, because the humus content and nutrients have decreased year after year. The cause of this decrease in soil fertility is the lack of organic fertilizers and lack of crop rotation including perennial leguminous grasses. However city hard domestic wastes (HDW) can be a source of organic fertilizer. In Uzbekistan, the rubbish of many cities is characterized by the high content of organic substances containing the main nutritive elements for plants (N-P-K). That is why the rubbish is a valuable raw material for composting and is valuable as an organic fertilizer. To help make the decision regarding questions about utilization and decontamination of city rubbish it is necessary to study its composition and characteristics thoroughly. According to our data, the main part of HDW is formed from paper and food wastes. On average, paper makes up 20%, food waste 34%, plastic 6%, other wastes –22% of the HDW. The presented chemical analysis shows, that the studied organic wastes differ significantly in chemical composition. The content of dry matter fluctuated in the range of 33.7-73.1% and pH- 6.0-7.5. The average ahs was 8.9%, carbon 10.9%, total nitrogen 0.26%, gross phosphorus 0.26%, and gross potassium 0.65%. The analysis of morphological and chemical composition showed, that HDWs are a very complex accumulation of all sorts of things and substances. Among those substances of organic origin prevail, that gives us the opportunity to process wastes for fertilizers.

150. The ecological consequences of application of high rates of nitrogen fertilizers in Zaravshon Walley

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The higher rates of nitrogen fertilizers are applied to obtain higher yields of field crops. Application of these amounts of fertilizers lead to a unbalance of natural biodiversity, decreasing the natural content of nutrition and is ratio in soil. A number of field experiments showed that coefficient of utilization of fertilizers depends on time, application techniques and rates of fertilization. The increase of rates of fertilizers leads to declining fertilizer usage and the nutrient content in soil. Soil pollution by nitrogen also takes place. At equalized rates of fertilizers time of application and amount of fertilizer applied over time is important. Application of nitrogen before blooming stage caused nitrogen loss and lower nitrogen use efficiency. Shifting of amounts of nitrogen from early spring to later in the season resulted in better NUE. The lower rate of fertilizer also positively resulted in its use by plants. Higher rates of fertilizers increased nitrification and denitrification and caused to nitrogen loss from fertilizers and soil, as well as humus mineralization. On the basis of long-term investigations it was possible to conclude that application of smaller amount of nitrogen fertilizers more frequently over time resulted in better NUE with less nitrogen loss and humus mineralization.

151. Effect of polyethylene film mulching on agrochemical change in Serozem soils under irrigation

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Polyethylene film is used for improving thermal, water and nutritional regimes of soil. In this context it field experiments were conducted to study the role of tobacco mulching in the Zaravshon region of Uzbekistan. The results of field experiments showed that mulching increased soil temperature and moisture content and availability of nutrients. The temperature and moisture increase also caused higher microbial activity. Higher microbial activity led to higher content of ammoniation and nitrification and availability of nitrogen in soil. The highest content of nitrogen was observed in topsoil. In subsoil horizons the differences were low. Mulching caused positive availability of phosphorus and P_2O_5 in soil due to the increase of soil temperature and moisture, as well as nitrate content. Content of P was changed both in topsoil and subsoil. Consequently, mulching with polyethylene film increased not only soil temperature and moisture, but nutrition as well. The increased content of nutrients in soil lead to higher uptake by plants. This caused higher nicotine content in the tobacco plants, as well as water-soluble hydrocarbons, proteins and shmuc number. Mulching with polyethylene film improved soil nutrition regime and quality of yield.

152. Ecological consequences of humus mineralization in Uzbekistan

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Humus mineralization takes place elsewhere in the world in addition to Uzbekistan. The mineralization of humus in the Zarafshon region has negatively impacted ecological conditions. On the basis of laboratory analysis it was shown that the higher humus positively affected soil by increasing buffer capacity, absorbency capacity and so on. The total content of microorganisms per gram of soil is higher in lower fertility soils as compared to more fertile soils, where the microbe content is low. At lower concentrations of humus were present in soils there was a negative effect from application of mineral fertilizers. In soils with lower content of humus the negative effect of water soluble salts differ, as compared to regions with higher humus content due to neutralization of these salts by humus. At lower humus content the negative effect of heavy metals was also higher. The decrease of humus content lowered the total content of microbes as well as their diversity. This led to decline of buffering capacity of the soil as well as degradation and diversification of soil. Changing the nutrition regime and water physical peculiarities of soils, leads to biocenose changes.

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