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FIFRA SCIENTIFIC ADVISORY PANEL (SAP)

OPEN MEETING

SELECTED ISSUES ASSOCIATED WITH THE RISK
ASSESSMENT PROCESS FOR PESTICIDES WITH
PERSISTENT, BIOACCUMULATIVE
AND TOXIC CHARACTERISTICS

U.S. ENVIRONMENTAL PROTECTION AGENCY
CONFERENCE CENTER- LOBBY LEVEL
ONE POTOMAC YARD (SOUTH BUILDING)

2777 South Crystal Drive
Arlington, Virginia 22202

OCTOBER 28, 2008

8:42 A.M.

FIFRA SCIENTIFIC ADVISORY PANEL

MEETING

October 28, 2008

MS. CHRISTIAN: Good morning. I am Myrta Christian and I will be serving as the designated federal official to the FIFRA Scientific Advisory Panel. I want to thank Dr. Heeringa for agreeing to serve as chair of the FIFRA Scientific Advisory Panel for this meeting. I also want to thank both the members of the panel and the public for attending this important meeting of the FIFRA SAP to consider selected issues associated with risk assessment process for pesticides with persistent, bioaccumulative, and toxic characteristics.

We appreciate the time and effort of the panel members in preparing for this meeting and taking time out of their busy schedules. The FIFRA SAP is a federal advisory committee that provides independent, scientific counsel and advice to the agency on pesticides and pesticide related issues regarding the proposed federal action on human health and environment. The FIFRA SAP only provides advice and recommendations to EPA. Decision making and implementation authority remains with the agency. As the DFO for this meeting, I serve as the liaison

1 between the panel and the agency.

2 I am also responsible for issuing
3 permission of the federal advisory committee as needed.
4 As the designated federal official for this meeting, a
5 critical responsibility is to work with the appropriate
6 agency officials to ensure that all appropriate ethics
7 regulations are satisfied. In that capacity, panel
8 members are briefed with provisions of federal conflict
9 of interest laws.

10 In addition, each participant has signed
11 a standard government financial disclosure report. I,
12 along with our deputy ethics officer for the office of
13 pesticides and toxic substances and consultation with
14 office of the general counsel have reviewed these forms
15 to ensure all ethics requirements are met.

16 For members of the public requesting
17 time to make a public comment, please limit your
18 comments to five minutes unless prior arrangements have
19 been made. For those who have not pre-registered,
20 please notify either myself or another member of the
21 SAP staff if you're interest in making a comment.

22 For presenters, panel members and public
23 commentators, please identify yourself and speak into the
24 microphone provided, since this meeting has been
25 recorded. There is a public docket for this meeting.



1 All background material, questions posed to the panel
2 by the agency and other documents related to this
3 meeting are available in the docket. Overheads will be
4 available in a few days.

5 Background documents are also available
6 on the EPA website. The agenda lists contact
7 information for such documents. At the conclusion of
8 the meeting, the SAP will prepare a report as a
9 response to questions posed by the agency, background
10 material, presentations and public comment. The report
11 serves as meeting minutes.

12 We anticipate the meeting minutes will
13 be completed in the first 90 days. Again, I wish to
14 thank the panel for their participation and I'm looking
15 forward to both a challenging and interesting
16 discussion over the next few days.

17 Finally, I just want to let you know
18 that there is a big meeting tomorrow morning at 8:30 in
19 this building. Therefore, the security line is
20 expected to be longer than normal. Please plan
21 accordingly. At this point, I would like to introduce
22 Dr. Steven Heeringa, the Chair for the FIFRA Scientific
23 Advisory Panel.

24 **DR. HEERINGA:** Thank you very much
25 Myrta. I'd like to reiterate her thanks to the members



1 of the panel, the EPA staff and to the public who've
2 assembled here this morning and potentially throughout
3 this week for a very important meeting on the topic on
4 the selected issues associated with risk assessment
5 process for pesticides with persistent bio-accumulative
6 and toxic characteristics.

7 As indicated, I'm Steve Heeringa, acting
8 chair of the FIFRA Science Advisory Panel, from the
9 University of Michigan, I'm a statistician. My main
10 role in these meetings over the next few days is to
11 facilitate the scientific discussion and coordinate the
12 exchange.

13 I'll turn now to some of the experts on
14 the panel who've been assembled and I think it's a very
15 large and diverse panel in terms of the expertise
16 that's represented here. So if they would introduce
17 themselves by name and affiliation, maybe just a short
18 description of your background. I'll begin with Dan
19 Schlenk.

20 **DR. SCHLENK:** Good morning, my name is
21 Dan Schlenk. I'm a Professor of Aquatic Ecotoxicology
22 at the University of California Riverside and my area
23 of expertise is mode of action of pesticides and
24 aquatic organisms.

25 **DR. POPE:** Good morning, my name is



1 Carey Pope. I'm a Professor of Toxicology at Oklahoma
2 State University. My area of interest is insecticide
3 toxicity.

4 **DR. PORTIER:** Good morning, my name is
5 Ken Portier. I'm Director of Statistics at the
6 American Cancer Society national home office in
7 Atlanta. I'm a bio-statistician.

8 **DR. CHAMBERS:** I'm Jan Chambers. I'm in
9 the College of Veterinary Medicine at Mississippi State
10 University and my area is pesticide toxicology. I'm a
11 member of the permanent panel.

12 **DR. BUCHER:** I'm John Bucher, I'm a
13 toxicologist at NIEHS. I'm Associate Director of the
14 National Toxicology Program and a member of the
15 permanent panel.

16 **DR. DONNELLY:** I'm Casey Donnelly, I'm a
17 Professor in the School of Rural Public Health at Texas
18 A&M University and I work with complex mixtures.

19 **DR. ORIS:** I'm Jim Oris at Miami
20 University in Ohio, a Professor of Zoology and an
21 aquatic eco-toxicologist.

22 **DR. SIMONICH:** Good morning, I'm Stacie
23 Simonich. I'm an Associate Professor at Oregon State
24 University in the Department of Chemistry and also in
25 the Department of Environmental and Molecular



1 Toxicology. My lab studies the trans-pacific and
2 regional atmospheric transport of pesticides.

3 **DR. STEENHUIS:** I'm Dr. Steenhuis, from
4 Cornell University. I'm a Professor down there in the
5 Department of Biological and Environmental Engineering
6 and I do transport experiments to see how this stuff
7 moves.

8 **DR. THIBODEAUX:** My name is Louis
9 Thibodeaux, I'm a Professor of Chemical Engineering at
10 Louisiana State University. My area of expertise is
11 chemical fate and transport in multimedia systems, with
12 exclusion of groundwater.

13 **DR. MEHTA:** I'm Dr. Mehta from the
14 University of Florida. I'm in coastal engineering and
15 I work in areas of sediment transport and coastal
16 hydrology.

17 **DR. MEADOR:** I'm James Meador from the
18 Northwest Fisheries Science Center in Seattle,
19 Washington. I'm an environmental toxicologist and my
20 area of expertise is energetics and growth in salmon
21 eggs.

22 **DR. NORSTROM:** Ross Norstrom, I'm
23 retired from the Game and Wildlife Service, Adjunct
24 Professor at Carlton University. My expertise is
25 primarily bioaccumulation in crops and wildlife.



1 **DR. MADDALENA:** Good morning, I'm Randy
2 Maddalena. I'm from Lawrence Berkeley National Lab.
3 I'm an environmental chemist, some analytical
4 chemistry, transport modeling is another area of
5 interest.

6 **DR. LICK:** I'm Willy Lick, the
7 University of California at Santa Barbara and I'm
8 interested in sediment and contaminant transport in
9 surface waters.

10 **DR. HICKIE:** My name is Brendan Hickie,
11 I'm a Professor at Trent University in Ontario, Canada
12 in the Environmental Science Program there. My area of
13 research is bioaccumulation in aquatic and marine
14 ecosystems.

15 **DR. GAN:** I'm Jay Gan from University of
16 California Riverside. I'm a Professor in Environmental
17 Chemistry. I work on transport mitigation of
18 pesticides.

19 **DR. DOUCETTE:** I'm Bill Doucette, a
20 Professor at Utah State University in the Department of
21 Civil and Environmental Engineering and I have a
22 background in environmental chemistry.

23 **DR. DELORME:** Good morning, I'm Peter
24 Delorme. I'm a Senior Advisor in the Pest Management
25 Regulatory Agency of Health Canada. My area of



1 expertise is environmental risk assessment of
2 pesticides.

3 **DR. BIDLEMAN:** Terry Bidleman from
4 Environment Canada. Adjunct Professor from University
5 of Toronto. Interested in long range transport and
6 deposition of pops and currently used pesticides.

7 **DR. ABBOTT:** Linda Abbott, I'm a
8 Regulatory Risk Analyst at USDA's Office of Risk
9 Assessment and Cost-Benefit Analysis and my area of
10 expertise is ecological modeling.

11 **DR. HEERINGA:** Thank you very much.
12 Again, panel members, I look forward to working with
13 you all over the next four days. At this point in
14 time, I'd like to begin a set of introductory remarks
15 from Frank Sanders, who is the Director at the Office
16 of Science Coordination Policy to the EPA. Good
17 morning Frank.

18 **DR. SANDERS:** Good morning, my name is
19 Frank Sanders and I am the new office Director of the
20 Science Coordination Policy. Under that office, we
21 have responsibility for the management of the
22 scientific advisory panel. Our Executive Secretary,
23 Steve Knott, who over the years has done an outstanding
24 job in working with the SAP and I'm sure we will
25 continue that sort of focus and it's important we do



1 that.

2 But I want to take a few minutes this
3 morning to welcome you and thank you for taking the
4 time to be here for this meeting. I am confident that
5 you'll find it to be very interesting and productive
6 that you'll hear from the environmental fate and
7 effects division in the office of pesticide programs
8 about this work on the assessment of ecological risk of
9 pesticides with persistent, bioaccumulative, and toxic
10 characteristics. I also want to take the time to thank
11 the director, Donald Brady, and the scientific staff of
12 EFED for all their efforts and initiatives in preparing
13 for this meeting.

14 Before becoming the OSEP director, I
15 spent most of my career in the office of pesticide
16 programs and most recently as the division director of
17 antimicrobials division. My background has been in the
18 office of pesticides programs for a long time and I
19 have witnessed some of the important decisions that
20 were made by the SAP.

21 Let me give you an idea as to some of
22 the things that I have been involved with over the
23 years. I started out as a team leader in the
24 insecticide-rodenticide branch and moved from there to
25 become a section head of the insecticide-rodenticide



1 section. And from there, I moved to become the branch
2 chief of the science review branch.

3 And from there I became branch chief of
4 the fungicide-herbicide branch and then to become the
5 director of what we had at that time, program
6 management and support division, and then to the
7 anti-microbial division director and now the director
8 of OSEP.

9 So, I've got a long history of working
10 in the office of pesticide programs and had the
11 pleasure and opportunity of dealing with many
12 scientific issues, so I really understand the relevance
13 of the decisions made by the SAP. The scientific
14 advisory panel is held in a very high regard by the
15 agency.

16 But the office of pesticides programs is
17 the main peer-review mechanism for challenging
18 scientific issues associated with pesticides. I know
19 from my personal experience in the anti-microbial
20 division how important it is to gain expert scientific
21 advice on challenging issues that directly impact our
22 ability to evaluate pesticides and ensure that they
23 present no adverse risk to human health or the
24 environment.

25 Most recently, AB brought issues related

1 to efficacy of products to inactivate anthrax exposure
2 to the SAP. In the not too distant past, we also
3 brought issues related to wood treated with CCA and
4 other preservatives to the SAP.

5 We value the SAP's advice and seriously
6 consider its recommendations as we move forward with
7 the risk assessment process undertaken before
8 registering a pesticide product for use in the United
9 States.

10 This is a very important process and to
11 me, when I was division director of the anti-microbial
12 division, one of the most important things for that
13 division is to seek advice, particularly in areas that
14 were controversial. And the advice that we received
15 was very valuable in making regulatory decisions and I
16 certainly appreciate the work that you will be doing
17 here all this week.

18 As you engage this week in the
19 discussion of PBT topics, be assured the agency is
20 looking forward to getting new expert advice and
21 recommendations to move forward with the evaluation of
22 further risk assessments of pesticides with PBT
23 characteristics.

24 Again, thank you for taking the time to
25 come to evaluate and to think seriously about the



1 issues that are going to be presented to you this week.
2 Thank you again.

3 **DR. HEERINGA:** Thank you very much,
4 Director Sanders, it's very nice to have you join us
5 here. At this point, I'll turn to Doctor Steven
6 Bradbury, who is the director of the special review and
7 re-registration division within the office of pesticide
8 programs at EPA. Good morning Steve.

9 **DR. BRADBURY:** Good morning. Good
10 morning to the panel as well. I want to also thank Dr.
11 Heeringa and the panel for your time over the next
12 several days to meet with us to discuss the issues of
13 this SAP. We really appreciate all the time and effort
14 it takes to prepare for one of these meetings as well
15 as the long hours you'll be putting in to help prepare
16 the report for us which we'll be very excited to read
17 and use that input as we move forward.

18 As you know, we have a very ambitious
19 schedule set out for ourselves and for you as we go
20 over the next several days and we'll be discussing a
21 broad range of issues including persistence and
22 bioaccumulation, sediment dynamics and how that can
23 influence bioaccumulation estimates. As well as the
24 issue of long range transport.

25 All in the context of performing



1 ecological and in some cases, human health risk
2 assessments for chemicals that have varying
3 characteristics with regard to persistence and
4 bioaccumulation and long range transport. Clearly,
5 we're not going to be able to resolve all the many
6 uncertainties and issues that face this area of
7 science.

8 But what we do hope to accomplish in
9 this SAP is to present to you, through a white paper
10 and presentations, an overview of where we're at in
11 trying to address some of these issues. And to get
12 feedback on two fronts. One area of feedback would be
13 hearing insights and advice on how one can best use
14 currently available information and currently available
15 scientific methods for decisions about pesticide
16 registrations, which I'll discuss in a bit, but how to
17 make those decisions right now.

18 With the best available information and
19 accepted scientific methods. I'm also looking forward
20 to your insights and advice as we look forward into the
21 future, in terms of what kinds of adaptations or
22 methods of development can we look forward to in the
23 future to further refine the capabilities of
24 undertaking risk assessments for chemicals that have
25 varying characteristics of persistence and long range



1 transport bioaccumulation.

2 To help put this SAP in context, I want
3 to spend a few minutes just describing some of the
4 statutes in the United States that guide us as we do
5 pesticide evaluations and make regulatory decisions
6 with regard to pesticides. The two major statutes that
7 oversee or drive out work- one is the federal
8 insecticide, fungicide and rodenticide act, or FIFRA.

9 The other is the federal food, drug and
10 cosmetic act, or FSDCA. FIFRA is the real over-arching
11 statute, the driver in terms of how we lay out the work
12 we do in the pesticide program.

13 And in the context of FIFRA, we're
14 looking at dietary risks, we're looking at ecological
15 risks, residential risks, occupational risks, as we
16 make decisions about pesticide registrations. Now, in
17 the case of dietary and drinking water exposure and
18 residential risk, that's a risk-only standard.

19 And so we just take a look at the risk
20 to make sure the risks do not exceed our reasonable
21 certainty of no harm standard. In terms of ecological
22 risk and occupational risk, it's a risk benefit
23 decision that we make.

24 So we're looking at the risks associated
25 with uses and we're looking at the benefits of those



1 uses and our decision is ensuring that the risks don't
2 exceed the benefits of the product. And so those are
3 the FIFRA sorts of things, the over-arching statute.
4 FSDCA is a statute that we followed in terms of setting
5 tolerances for pesticides that can be in the dietary
6 food chain for humans, and or in drinking water.

7 And so that aggregation is what drives
8 FSDCA in looking at tolerances in food. And that
9 aspect of our pesticide regulations does, in some ways,
10 factor into some of the discussion today in terms of
11 the potential for pesticides to get into dietary
12 sources in the environment.

13 Maybe some fish or other components of
14 the human diet. So we have these two statutes then
15 that drive both the decisions we make on registering
16 new insecticides and pesticides as well as a process to
17 re-evaluate pesticides that are currently on the
18 market.

19 Another act that was passed in the
20 mid-90's is the food quality protection act which sort
21 of helped integrate these two acts and put some things
22 in context and added some more stringent risk
23 assessment and risk management perspectives to the work
24 we undertake.

25 The acts also lay out a strategy not

1 only towards proceedings on new chemicals, but also a
2 process for looking at listed chemicals. Through
3 FIFRA, we're required every fifteen years to
4 re-evaluate pesticides that are on the market. So a
5 process that's dealing with decisions about new
6 pesticides that can come on the market as well as
7 processes that are evaluating chemicals that are
8 already on the market to ensure, over time, that our
9 decisions are meeting current scientific and regulatory
10 policies.

11 Of course, that evolves over time. I
12 think another important backdrop to the work we do has
13 to do with the throughput of work we do in a time
14 frame in which those actions have to be undertaken. In
15 the mid 2000's, 2004, and there was an update a couple
16 of years later, congress passed the Pesticide
17 Registration Improvement Act, PRIA.

18 And that act not only sets up schedules
19 for fees that the registrants supply EPA to help do all
20 this work, but it also sets up time frames in which
21 decisions need to be made. So for example, a new
22 pesticide, the EPA needs to make a decision in
23 approximately 18-24 months from submission of the
24 information to EPA. So we have a throughput that's set
25 up and time frames that have to be addressed.



1 And we typically are evaluating 10-12
2 new active ingredients per year and many more chemicals
3 are being evaluated in the context of new uses being
4 added to existing registrations. Which also requires a
5 human health and ecological risk assessment.

6 PRIA also sets a schedule for that 15
7 year cycle in terms of re-evaluating existing
8 chemicals. About 2 or 3 weeks ago, we finished our
9 first round of re-evaluation of pesticides and what we
10 accomplished a couple of weeks ago was the
11 re-evaluation of approximately 600 active ingredients
12 that had been registered prior to 1984.

13 A year or so ago, we embarked on our
14 second round of the re-evaluation program, which would
15 turn registration review, now require that all the
16 active ingredients be re-evaluated by 2022. Which
17 translates to about 70 decisions per year to meet that
18 schedule.

19 So you get a sense of the throughput
20 that's associated with the activity we take. When you
21 strive to ensure that as we make those risk assessments
22 and form our risk management decisions, that we are, as
23 best we can, taking advantage of currently accepted
24 scientific methods and high quality data as we go
25 forward.



1 As many members of the panel know, the
2 underlying scientific basis of all these decisions has
3 been greatly enhanced and enriched by meetings with the
4 SAP over the years and years and years of the
5 development of this program.

6 So insights, in terms of everything from
7 what kind of bioassays are critical to interpret the
8 potential risks of the pesticides to what kinds of
9 tests are important to understand the fate and
10 transport of chemicals and that influences the type of
11 data the pesticide registrant generate to submit to the
12 agency to support the decisions about registering a
13 pesticide.

14 As well as getting feedback from the SAP
15 on the various models and methods that the agency uses
16 to evaluate this information and integrate that
17 information into established estimates of exposure,
18 understand potential effects and then put it together
19 and make a risk assessment. Then any of the risk
20 managers are making the ultimate regulatory decision
21 about the product.

22 When we look back at where we've been
23 and where we're going forward in this risk assessment,
24 issues we're going to be talking about over the next
25 few days, many of the scientific methods and bioassay



1 techniques and the methods we use to integrate the
2 information which was aided to a great degree from SAP
3 input over the years, they tend to be based on
4 chemicals whose half-lives may be in the range of hours
5 to days.

6 So they typically tend to be chemicals
7 that don't have a potential to bio-accumulate in
8 aquatic food chains and food webs or terrestrial food
9 webs. In general, they don't have a potential for long
10 range transport.

11 So in essence, the problem formulation
12 that typically drives an ecological risk assessment is
13 based on chemicals with really short half-lives that
14 degrade relatively quickly, don't have a long range
15 transport potential, don't seem to have a potential to
16 bio-accumulate.

17 Not surprising then, the underlying
18 bioassays, for example, and some of the underlying
19 methods in the models are built for time scales that
20 say a field season or a bit beyond the field season in
21 terms of the potential direct effect of the pesticide.
22 Spatial scale tends to be at the scale of the field
23 where the pesticide is applied and some off-field from
24 spray drift or runoff that's affecting the habitat
25 around the field.



1 But generally not focused, either the
2 risk assessment or the risk management decision, on the
3 spatial scale that could be miles and miles and miles
4 from the site of application.

5 So where we've been has been risk
6 management decisions supporting risk assessment
7 decisions that are based on short lived chemicals, time
8 scales of a year or so, spatial scales of an
9 agricultural field and the surrounding habitat.

10 Recently though, in both the
11 registration process, which is a process in which we
12 evaluate new chemicals coming on the market, as well as
13 some situations where we're doing our re-evaluation
14 exercise, evaluations and looking at chemicals that are
15 currently on the market, we've started to see some
16 situations where we're looking at chemicals that in
17 fact don't have short persistence and the fact
18 persistence can be in the range of months to up to a
19 year.

20 The same chemicals whose bioaccumulation
21 potential is such that we would expect them to
22 potentially bio-accumulate in aquatic food webs and
23 terrestrial food webs. Also seeing chemicals with some
24 characteristics that would suggest they do have the
25 potential for long range transport.



1 And clearly, as chemicals with these
2 kinds of characteristics come to bear, not only does
3 that influence the kinds of tools and techniques that
4 we use to undertake those risk assessments, it also
5 changes the risk management framework, in terms of
6 chemical scale and spatial scale we begin to start
7 looking at things a bit differently and as risk
8 managers, looking towards how that science will evolve
9 to help support a risk management framework that's now
10 somewhat different from the typical scenario that we're
11 dealing with.

12 So as we go forward over the next
13 several days, we'll be looking forward to your insight
14 on these issues and again, in two contexts. One is
15 through the white paper that you'll hear from the
16 scientists in E-FED and the discussion you all will
17 have, is to give us feedback on today's currently
18 available methods and models.

19 Because as I have indicated before, we
20 have many decisions to make every year and the statutes
21 require those decisions to be made in a time sensitive
22 manner.

23 So it's important to get some insights
24 on what can we use today, what's the status of today's
25 science and tools. In addition to getting feedback on



1 what advances can we look for in the future, so that we
2 can all use our resources and our talents effectively
3 and efficiently in focusing on first-order,
4 second-order, third-order challenges and uncertainties
5 as we go into the future.

6 So again, I want to thank you all for
7 the preparation before you got here and all the hard
8 work you'll be doing while you're here. We certainly
9 look forward to the feedback and the discussions over
10 the next several days. Dr. Heeringa, I'll turn it back
11 to you.

12 **DR. HEERINGA:** Thank you, Dr. Bradbury.
13 Speaking for the panel, we look forward to engaging
14 with the scientific staff, the EPA, in the discussion
15 over the next few days. I appreciate your opening
16 remarks. At this point in time, I'd like to turn to
17 Dr. Donald Brady, who is the division director of the
18 environmental fate and effects division, OPP, EPA.

19 **DR. BRADY:** Thank you very much. I'd
20 also like to express my appreciation to the members of
21 the panel for the work you're about to undertake and
22 also right up front, to express my appreciation to the
23 members of the E-FED scientific team who will,
24 following me, begin to make the detailed presentations
25 that pose the issues and the questions we've got set up



1 here for you today.

2 So, just briefly from the standpoint of
3 the ecological risk assessment process, EPA's pesticide
4 ecological risk assessment process, which as been
5 reviewed and supported by SAP's in the past, has been
6 effective in assessing risks of pesticides to
7 non-target organisms and the environment.

8 However, pesticides with combined
9 persistent bio-accumulative and toxic characteristics
10 have presented particular challenges because the
11 methods, tools and data used in our current risk
12 assessment process have some limitations in addressing
13 pesticides with the characteristics.

14 In these situations, the office of
15 pesticides programs has made the best use of available
16 tools and methods from other parts of the agency and/or
17 the scientific community.

18 So as you heard a minute ago, one of the
19 reasons we're here today is to seek input from this
20 panel on whether we've made the best use of the
21 available data and methods for addressing those risk
22 assessment issues in past assessments.

23 We're also seeking input on how best to
24 proceed for future assessments involving pesticides
25 with these characteristics.



1 In our white paper, we used case studies
2 with four example generic pesticides to describe the
3 analyses used. The evolving tools, methods and data
4 being considered, and the issues that have arisen with
5 older pesticides and new pesticides with these
6 characteristics.

7 We have focused on methods and tools for
8 addressing a number of the risk assessment
9 uncertainties and have presented the program's
10 approaches to refine the risk assessments and to
11 highlight remaining challenges.

12 In this SAP, we also pose some questions
13 related to long range transport. Some of those will
14 also be addressed in a later SAP and Mr. Safkin will
15 describe in his more detailed presentation exactly how
16 those issues will fall out.

17 So in terms of the scientific challenges
18 that we've raised before the panel today, one of the
19 primary challenges we face concerns environmental
20 persistence. For this topic area, we're seeking advice
21 on how to quantify long term exposure to chemicals in
22 soil, sediment and pore water. And how to quantify
23 exposure to the combination of parent and degradation
24 products.

25 Another challenge area concerns sediment



1 dynamics, which has the potential to influence
2 bioaccumulation. For this area, we are seeking advice
3 on the appropriate methods and tools for identifying
4 and quantifying the principle processes related to
5 sediment dynamics. In the area of bioaccumulation, we
6 are seeking comments on quantifying pesticide exposure
7 in aquatic food webs and on assessing bioaccumulation
8 potential in terrestrial based food webs.

9 One of the primary issues involved in
10 long range transport is associated with establishing
11 relationships between near field pesticide loadings and
12 far field pesticide concentration.

13 So, we are looking forward to your
14 advice on how to best to approach the problem
15 formulation page on pesticides with some or all of
16 these characteristics as well as how to best use
17 today's available methods and models in characterizing
18 risk in these situations.

19 In addition, we are interested in your
20 thoughts on options for advancing current methods and
21 models from the existing foundation of approaches
22 developed by the EPA and the broader scientific
23 community. So again, I'd like to thank you very much
24 and that's it.

25 **DR. HEERINGA:** Thank you very much, Dr.



1 Brady. At this point we're going to begin a sequence
2 of presentations by the EPA Scientific Staff from EFED
3 who has contributed to the white paper and addressing a
4 number of topics that were covered in that paper.
5 These will be a series of presentations in which has
6 about 30 minutes set aside for each of them including
7 discussion.

8 I can tell you from experience there is
9 a trend at the start of these sessions for the initial
10 presentations, the discussions to go on longer. I
11 don't want to cut things off, but we'll try to stay to
12 the agenda schedule more or less. But without any
13 further delay, do you want to introduce your staff.

14 **DR. BRADY:** Keith Sappington will
15 discuss background and set the stage for the following
16 presentations. So I'll let Keith do that.

17 **MR. SAPPINGTON:** Good morning. I'm
18 going to talk about the issues associated with
19 assessing ecological risks of pesticides with
20 persistent bioaccumulation and toxic characteristics
21 and I'm just going to provide a background of how we
22 address these issues in the past and how our overall
23 risk assessment process is perceived.

24 I'm going to talk about three areas.
25 One is just to give an overview of our standard



1 ecological risk assessment process. That is which
2 pesticide sources, exposure pathways and ecological
3 receptors we routinely consider.

4 As well as the typical effects and
5 exposure assessment information that we generate as
6 part of these assessments. I'm going to provide a
7 brief introduction to the PBT related ecological risk
8 assessment issues and introduce the example case
9 studies which are outlined in the white paper.

10 The ecological risk assessment process
11 that is used in the office of pesticides program
12 closely follows the agency's risk assessment frame work
13 and following risk assessment guidelines.

14 And I've provided a risk assessment
15 frame work figure here. And this process proceeds in
16 basically three steps. The first is a problem
17 formulation phase and that is a lot of what we're
18 focusing on in this SAP.

19 This is basically the planning phase of
20 the risk assessment. In relation to our topic area, it
21 is where we would first identify which PBT related
22 issues that we have to be concerned about. And also
23 the methods that are available to address these issues.

24 The problem formulation phase involves
25 constructing a conceptual model that relates the

1 sources ultimately to the risks to the organisms of
2 concern. And this includes an explicit statement of
3 the assessment endpoints which is the ecological
4 receptors of concern and the attributes of those
5 receptors.

6 Ultimately, an analysis plan is
7 formulated, which is basically the blue print for the
8 ecological risk assessment. The second step involves
9 an analysis phase and that is where the exposure
10 information is assembled. It usually proceeds in a
11 predictive fashion, with environmental modeling, but
12 also would consider monitoring data. And analysis of
13 effects, this is where the effects profile is
14 assembled.

15 Again, typically these are data that are
16 generated in the laboratory using standard methods but
17 on occasion we have information available from the
18 field or field studies. The final step is the risk
19 characterization and this is where those estimates of
20 risk are generated by integrating the exposure and
21 effects profiles and the risk estimation box that you
22 see is where the quantitative risk estimate is
23 determined.

24 Usually, this is done in a deterministic
25 fashion, but when we have sufficient information, we



1 can also do this in a probabilistic fashion using all
2 the exposure information we have as well as the effects
3 information. Such as the species sensitivity
4 distribution.

5 The risk characterization or risk
6 description step is important because that's where we
7 discuss the uncertainties and sensitivities of the risk
8 assessment to different assumptions and where we can
9 bring in sort of non-standard models to the process to
10 help inform the risk estimate.

11 And importantly, while this is presented
12 in a sort of a linear fashion, there's quite a bit of
13 iteration between these steps and there's the
14 opportunity in the pesticides program to stop and
15 request more information as part of this process.
16 Although is always competing with the rigid time lines
17 we have for making decisions.

18 Now I'm going to walk through a
19 conceptual model that is in the white papers, it's very
20 similar to the one presented there. And the point in
21 doing this is to illustrate basically three things.
22 One is what are the sources and exposure pathways we
23 routinely consider in our risk assessment.

24 And then which ones are those that are
25 not routinely considered that we address on a case by



1 case basis and which pathways and sources are
2 particularly a challenge with respect to pesticides
3 with PBT characteristics.

4 So in terms of what we're trying to
5 assess risks on, we have aquatic animals, plants, both
6 terrestrial and aquatic, as well as terrestrial
7 animals. And listed below the entities here are the
8 assessment endpoints.

9 The reduction in survival growth and
10 reproduction we're mostly concerned about. I'm going
11 to start with the aquatic pathway. In terms of
12 sources, we have pesticide spray drift, runoff and
13 erosion. And we use environmental models to route
14 these loads to a standard receiving water body, which
15 generates concentrations and we're interested in
16 pesticide uptake in aquatic plants as well as aquatic
17 animals. And this is the water only phase. For PBT
18 chemicals and sediments here, we also have to predict
19 concentrations in sediments and that's particularly
20 important based on their chemical properties.

21 We also consider leaching to groundwater
22 and right now, this is evaluated or used to evaluate
23 potential impacts on irrigated crops, when groundwater
24 is used as a source water.

25 Obviously, there's a connection between



1 the groundwater and the surface water and this is not
2 evaluated routinely in our models. In terms of
3 terrestrial plants, we evaluate the risks associated
4 with runoff and erosion potential as well as spray
5 drift and for terrestrial animals we consider direct
6 deposition on food items in the treated fields and
7 evaluate this for pesticide ingestion from the food
8 stuffs.

9 This is not bioaccumulation, it's the
10 deposition or absorption of the pesticide to the food
11 item, plants, small insects. There are other sources,
12 obviously for terrestrial animals. Drinking water, as
13 well as exposures due to soil and exposure routes
14 include ingestion and dermal uptake. We have evaluated
15 these pathways in the past, but these are not routinely
16 done. And as shown in blue here, the soil is a
17 compartment of particular concern with pesticides with
18 PBT characteristics.

19 We also consider volatilization and
20 exposure through the inhalation route. This is done
21 less commonly, but we do this where it is of a concern
22 on a case by case basis. For example, for pesticide
23 fumigants with high volatilization rates. Now for
24 pesticides with PBT characteristics, tropic transfer
25 both in a terrestrial food web and the aquatic food web



1 is a potential concern. This is not routinely
2 evaluated now.

3 We have provided examples of where we
4 have done it and that's one of the big reasons we're
5 here today is to seek your input on this topic. Also,
6 long range transport and atmospheric deposition are of
7 concern in some cases. We do evaluate long range
8 transport but it's largely from a retrospective fashion
9 by looking and considering monitoring data. I'm going
10 to talk briefly about the aquatic exposure assessment.
11 Dr. Ron Parker, who will be presenting just after
12 myself, will go into more detail.

13 But you'll see a theme with most of our
14 assessment approaches. And that is using a tiered
15 process. We have quite a number of substances due
16 every year and a short amount of time to do them. And
17 so when we can, we apply a screening process, so we can
18 identify those pathways that really deserve most
19 attention in the risk assessment.

20 And in that light, with the aquatic
21 exposure assessment, we used a tier one model that's a
22 screening model, called JANIK and that's used to screen
23 out the aquatic exposure pathway from further
24 consideration. If the pesticide fails that screen,
25 then we move on to tier 2, which is the PRZM exam



1 process, which is described more thoroughly in the white
2 paper.

3 And again, Dr. Parker will be describing
4 this. The scale of the assessment is important to
5 consider. We are looking at the field scale assessment
6 that considers spray drift, runoff, and erosion to a
7 standard pond. We evaluate these parameters on a
8 region specific basis because application, timing and
9 rates, and soil characteristics as well as weather
10 conditions vary on a regional basis.

11 So we have standard scenarios that vary
12 by region and crop. The output from pesticide
13 concentrations predicted in water, sediment, and fore
14 water over a 30 year record, and that's to attempt to
15 account for some of the inter-annual variability that
16 might be expected over time. And then from this large
17 amount of information, we distill it down into some
18 statistics, that are then used to evaluate risk and
19 these range from peak concentrations to a different
20 averaging periods with a return interval of one and ten
21 years.

22 On the terrestrial exposure assessment,
23 I'm just going to talk about the spray applications. I
24 mentioned this in the conceptual model, that we
25 evaluate exposure from pesticides that adhere to food



1 items, such a foliage, seeds, and insects. And the
2 residues are estimated based on an empirical database
3 that relates just the application rate to the residue
4 concentration. We can simulate degradation usually as
5 a first order process and exposures are expressed in
6 terms of dietary concentrations and also converted to
7 an ingested dose basis. We evaluate exposure two
8 different ways.

9 On the effects assessment, typically for
10 acute toxicity, we're looking at fresh estuarine marine
11 organisms, common test species on the fresh water side
12 are bluegill and rainbow trout for fish and daphnia and
13 shrimp for invertebrates. Typical endpoints there are
14 the LC-50 and the E.C.-50. The lethal concentration
15 that effects half of the organism and the effective
16 concentration that effects half the organism.

17 For chronic toxicity for fish, we most
18 often get early life stage tests. These vary from 28
19 days to 60 days or even longer, depending on the
20 species. For invertebrates, we receive a life cycle
21 study and the endpoint from these tests are that no
22 observed adverse effect concentrations as well as
23 lowest observed adverse effect concentrations. More
24 recently, we've been requiring sediment toxicity
25 studies and these are done and conducted on a short



1 term, ten day basis, as well as a chronic basis.

2 And the effects are indexed to bulk
3 sediment concentrations as well as concentrations in
4 fore water. Typical endpoints, I mentioned this
5 earlier, are survival, growth, reproduction and
6 development. We also consider on a case by case basis
7 other endpoints that can be strongly related to these
8 assessment endpoints. We feel these are the ones that
9 are most closely tied to population level effects.

10 And again, field studies, usually in the
11 form of mesocosm studies are occasionally available
12 and some of those are described in the white paper. In
13 terms of the assessment, usually when we distill this
14 information down, we look within each taxonomic group
15 with the most sensitive species.

16 Again, occasionally if we're in a data
17 rich situation, we can actually look at the
18 distribution of sensitivities across the species and
19 actually describe that statistically and use that
20 distribution as part of the risk estimation process.

21 For terrestrial organisms, for birds, we
22 have three taxa, upland, game, species and more
23 recently, we required a passerine species. For
24 mammals, typically what we're looking at is information
25 on a laboratory rat. Chronic toxicity, again for



1 birds, we require information on two taxa, and for
2 mammals it's usually a laboratory rat. And we're
3 looking at similar endpoints, growth, survival,
4 reproduction and development.

5 We also have information that is
6 collected and evaluated as part of the agency's program
7 on incidents that occur in the field. We have a
8 database of this so we can refer to field incident data
9 as sort of another line of evidence in the effects
10 assessment. Characterization of risk usually proceeds
11 with what is known as the risk quotient method and
12 that's where the estimated environmental concentration,
13 or EEC, is divided by the toxicity reference value to
14 give us a quotient.

15 For acute risks, we usually base the
16 exposure concentrations on peak values. For chronic,
17 it depends on the species. It's 21 day average
18 concentration for invertebrates and 60 days for fish
19 and again, these are tied to a return frequency that's
20 one in ten years.

21 We compare these risk quotient values to
22 the agency's level of concern and this is just a table
23 of the LOC values for assessing aquatic organism risk.
24 For this point in my discussion, I'm going to outline
25 the major PBT related ecological risk assessment issues



1 and I'm going to start with environmental persistence.

2 One of the issues we have with
3 addressing environmental persistence of pesticides with
4 PBT characteristics is assessing exposure to both the
5 parent and degradate products. This is not a question
6 of whether we do this, but more a question of how we do
7 it. And we have a range of methods that we can use,
8 but our ability to use the more complex methods is
9 often limited by the available information that we
10 have.

11 So we have some surrogate approaches
12 that are presented in the white paper and that we're
13 seeking feedback on. We also have questions regarding
14 interpreting the degradation kinetics that come from
15 our standard studies, like our aquatic metabolism
16 study. And some of the issues here occur when you have
17 rapid partitioning occurring at the same time as your
18 degradation rates and trying to distinguish where
19 degradation is occurring in the system, in a water
20 sediment system it can be a challenge. And
21 interpreting that information for application to the
22 exposure model. In some instances, our predicted
23 concentrations from our aquatic exposure modeling can
24 exceed the solubility limit that's generated using
25 standard laboratory tests.



1 This raises questions about the
2 bio-availability of those predicted concentrations. At
3 least the concentrations are above the solubility
4 limit. And there are a couple of methods that will be
5 presented later today that will discuss how we
6 interpret these concentrations and apply them in risk
7 assessment. Assessing long term accumulation in soil
8 and sediments is also a concern, particularly the
9 potential for pesticide carryover over time, over
10 multiple years. With regard to sediment dynamics, we
11 are interested in better understanding the role of
12 sediment dynamics on pesticide bio-availability in
13 aquatic systems.

14 This can impact multiple aspects of the
15 risk assessment. As Don mentioned, the bioaccumulation
16 estimates as well as the toxicity assumptions and risks
17 to organisms. We're interested in understanding
18 sediment dynamics in the role of our standard
19 agricultural ponds, but also in other aquatic systems
20 that we might address down the road. The available
21 methods for identifying and quantifying sediment
22 dynamics, we're interested in your feedback on those.

23 And in particular, those which we can
24 use now perhaps in the screening level sense, as well
25 as those that would be appropriate for more refined



1 assessments. Again, if we can save resources by using
2 a screening level approach to identify whether sediment
3 dynamics is important to the risk estimate, that's a
4 very useful tool for us to have. And again, providing
5 feedback, both in terms of what we can do now versus
6 the future would be very, very helpful to us.

7 With regards to bioaccumulation,
8 quantifying pesticide exposure via the aquatic food web
9 is an issue of concern to us for these types of
10 chemicals and we have presented different methods for
11 doing that in the white paper. And we're interested in
12 your feedback on how best to interpret and quantify
13 bioaccumulations from these different methods.

14 Have we adequately characterized the
15 relative strengths and limitations and have we, in the
16 example case studies, integrated these methods
17 appropriately. I will mention here that in terms of
18 where we are in the process, again we're sort of in
19 that problem formulation phase.

20 We expect to come back on some of these
21 topics with more specific information about which
22 models and which methods and sort of the exact process
23 of marching through the risk assessment. But right no,
24 we're looking for input, sort of more broadly on the
25 types of methods that were appropriate here.



1 And also, this is an area, getting back
2 to the conceptual model, I mentioned that we're not
3 evaluating bioaccumulation in the terrestrial food web
4 and there are some properties of compounds that suggest
5 that bioaccumulation in terrestrial food webs may be
6 important even when screening for aquatic
7 bioaccumulations suggest they might not be.

8 So we're particularly interested in this
9 aspect and view it as sort of an emerging area. Long
10 range transport, the biggest challenge we have is
11 relating near term pesticide loadings, sort of at the
12 field scale level, to far field concentrations. And
13 we're aware that there are methods out there for
14 screening long range transport potential.

15 So these can be used in a prospective
16 fashion, but right now the current state of the science
17 is largely using monitoring information to infer long
18 range transport. For toxicity, we're also looking at
19 the toxicity of mixtures apparent in degradate
20 compounds and toxicity resulting from multiple exposure
21 routes, not just the water pathway, which is standard.
22 In the aquatic toxicity test, anyway.

23 And I introduce the pesticide case
24 studies, and the purpose for providing these in the
25 white papers is to illustrate some of the refinements



1 we've made on a case by case basis to our methods for
2 addressing PDT related issues.

3 The focus here is on the methods, and
4 not on the chemical specific issues, and that's one of
5 the reasons why we did not name the pesticides. We're
6 really interested in the process we used for
7 determining and addressing these issues. The
8 characteristics of the 4 case studies regarding
9 hydrophobicity, there is a range of hydrophobicity
10 there. Typically log KOW from 4 to 8, depending on the
11 chemical in degradate. And they display high
12 environmental persistence through either the parent or
13 the degradate, and relatively high toxicity, and we
14 have concerns on long range transport for 2 of the case
15 studies.

16 And we brought these case studies to the
17 SAP, because based on the national and international
18 criteria that are established to classify compounds
19 according to their persistent bioaccumulative and toxic
20 characteristics, these raise flags that some of these
21 issues regarding bioaccumulations and environmental
22 persistence and toxicity would be of concern. And this
23 table just provides a road map for your reference with
24 regards to the white paper. The parent and degradate
25 exposure are illustrated for pesticide 2. Solubility



1 issues are for pesticide 3 and 4.

2 We have an example of the degradation
3 kinetic output and how we interpret that in pesticide
4 3, and long term accumulation and sediment in soils are
5 presented for pesticides 1 and 4, and these are all
6 found in Chapter 3 of the white paper. For sediment
7 dynamics we present information for how sediment
8 dynamics may effect exposure concentrations for
9 pesticide 4 as well as the bioaccumulations for
10 pesticide 3. And in the white paper we provide
11 examples, summary examples, of how we access
12 bioaccumulation, aquatic bio-cumulation for pesticides
13 1, 3 and 4.

14 I mentioned already that long range
15 transport is an issue for us with pesticide 1 and 2, as
16 well as toxicity, assessing toxicity in both the parent
17 and the degradate compounds. And then we provide an
18 approach for addressing aquatic toxicity from multiple
19 exposure out, particularly for the diet for pesticide
20 4, and that uses a tissue residue approach. And that's
21 it.

22 **DR. HEERINGA:** Thank you very much, Mr.
23 Sappington. At this point we have time for a few
24 questions of clarification on this background and
25 overview presentation. Panel members, any questions



1 that you would like to raise at this point? I'm sure
2 Keith will be here throughout the sessions if anything
3 else comes up. Yes, Dr Doucette.

4 **DR. DOUCETTE:** Just one quick question.
5 Measured versus estimated values, in certain situations
6 when you are going through the assessment you've got
7 the availability of both, ideally, you know, you've
8 always got measured, but a lot of times you may have
9 both, and if there is a conflict between the two how do
10 you weight whether you are going to use a measured
11 value or an estimated value if there is a large
12 difference between them? Do you always go measured, or
13 not?

14 **MR. SAPPINGTON:** I'll address that in the
15 context of bio-cumulation, which is my background. I
16 think it's important to understand the strengths and
17 limitations of the method that's used to generate both
18 estimates.

19 For example, you could have a
20 scientifically valid measured bioaccumulation factor in
21 the field, but if information suggests that the
22 pesticide would be accumulating over long time periods,
23 much longer than used in that study, then you could
24 bring that into play, in terms of how you interpret
25 that, and potentially weight or explain differences



1 between what a model may predict for bioaccumulation
2 versus a measured value.

3 And so I think it's really on a case by
4 case basis which ones you use, because...and I'll go
5 through this in the bio-cumulation presentation. Each
6 of the methods has their strong points and their weak
7 points, and we feel we really need to evaluate those in
8 a final selection process.

9 **DR. HEERINGA:** Dr. Maddalena.

10 **DR. MADDALENA:** Yeah, just a quick
11 question on the scope of your, I guess your problem. A
12 dozen or so new active ingredients per year, 70 some
13 new evaluations a year, of that batch, how many would
14 fall into this PBT characteristic? Just to give me a
15 sense of the workload that you are going to have in
16 this area.

17 **DR. HEERINGA:** Dr. Bradbury, do you want
18 to tackle that one?

19 **DR. BRADBURY:** Good question. With
20 regard to the new active ingredients, that's even more
21 difficult to project because we won't know what is
22 going to come in till it comes in. But I think our
23 sense in looking at some new active ingredients are
24 that group of 10 or 12 gave us some sense that for a
25 couple of chemicals at least, we had to deal with these



1 issues and we felt it would be wise to have...use these
2 two situations to expand our thinking in terms of risk
3 management and risk assessment, so that we are prepared
4 to take on anything that comes in the future with sound
5 science and good decision making. With the existing
6 chemical universe there are clearly some chemicals out
7 there that we have dealt with.

8 We dealt with Indane some years ago, and
9 went through a cancellation process for that. There
10 are other chemicals that are you, you know, in Congress
11 now that we are starting to take a look at. Some are
12 being dealt with at the international level and at the
13 national level.

14 So I wouldn't say that there is a large
15 percentage of compounds, I mean some of the experiences
16 I think...DDT, Aldrin, Dieldrin, Endorin, there was
17 movement away from the kind of characteristics that
18 lend chemicals to persist in bio-cumulation, because of
19 the issues that society faced in looking through those
20 structures.

21 But erythroids, you know, we are dealing
22 with some issues in terms of maximum bioaccumulation,
23 but what's going on in sediment...better understand
24 that, both in Canada and here in the U.S. and some of
25 the States have those issues too.



1 And again, I think it's to be prepared
2 for taking on the re-evaluation of the tools in our
3 toolbox, because we know right now as Keith described
4 and Don described, not all the tools in the toolbox are
5 quite tuned to this kind of issue. I think it's good
6 to be prepared, we are going to have to deal with some
7 of those problems.

8 **DR. HEERINGA:** Thank you. Dr. Norstrom.

9 **DR. NORSTROM:** Just a point of
10 clarification. I noticed in the generic conceptual
11 model here that you don't appear to have any direct
12 update by terrestrial plants and soils. Maybe that's
13 not relevant for PBT substances, but is that just an
14 oversight, or ... you have it for aquatic plants but
15 not for terrestrial.

16 **MR. SAPPINGTON:** You know the testing for
17 which we evaluate threshold plants are emergent studies
18 and vegetative vigor. And the product is applied as a
19 fraction of the application rate, so it uses spray
20 drift. But we also evaluate the using a screening
21 level model called Tur Plant. The effect of runoff and
22 steep runoff next to the field on plants. So maybe it
23 needs to be included in the model, in the conception
24 model.

25 **DR. NORSTROM:** Thanks.



1 **DR. HEERINGA:** Dr. Simonich, and Dr. Gan.

2 **DR. SIMONICH:** Staci Simonich, Oregon
3 State University. I actually have 2 questions, the
4 first is why isn't long range transport and atmospheric
5 deposition to bodies of water considered in the
6 conceptual model? For example, lakes and oceans.

7 **MR. SAPPINGTON:** Yeah, I think it clearly
8 is a relevant process, and I think one of the
9 challenges in putting any kind of generic conceptual
10 model together is trying to make sense out of it when
11 you are done. And that's exactly why I animated
12 walking through the model. And so we could have
13 another sort of line going over there. We tried to
14 really emphasize generically the things that we do more
15 commonly and those that we do not do more commonly.
16 So, yes, in fact, in our assessment themselves we
17 usually will have a conceptual model for terrestrial
18 and aquatics separate because of all the details and
19 the arrows running across on another...good point, I
20 don't.

21 **DR. SIMONICH:** And my second question.
22 Why would an aquatic toxicity test being conducted over
23 the aqueous solubility of the chemical be acceptable?

24 **MR. SAPPINGTON:** The aquatic studies,
25 with a number of these compounds solubility limit is



1 extremely low. And my understanding is that this could
2 present a challenge in actually conducting the study
3 for making stock solution, which have to be at higher
4 concentrations in the solution in order to expose the
5 organisms to a range of concentrations and elicit
6 effects.

7 We do have limit tests in which the
8 registrants are required to test up to some particular
9 limit, but they are expected to generate a toxicity
10 value up to that limit. If it's above the limit, I
11 think it's a hundred, I think for aquatic it's 100
12 milligrams. I'm not sure what the limit is, but we do
13 have a limit which they can then just do a screening
14 test, and not actually generate a dose response. But
15 as part of the guidelines themselves we are expected to
16 generate an actual dose response from a study.

17 **DR. HEERINGA:** I'd like to give Dr. Gann
18 a chance to pose his question, and then we'll move on.

19 **DR. GANN:** The question is do you intend
20 to address fully the sediment toxicity issues through
21 this process as well? Because these chemicals are
22 outside, the sediment toxicity would also be very
23 important, you know, I just wanted to see if you plan
24 to address this here or in the future?

25 **MR. SAPPINGTON:** Yeah, as I mentioned in



1 the presentation, we more recently have been getting or
2 acquiring sediment toxicity tests, and as part of our
3 risk assessment process. And clearly they would be the
4 compartment, major focus on sort of a mass balance
5 basis for these compounds. And the type of comparisons
6 that we would do would be comparing the direct toxicity
7 through poured water or bulk sediment to those...to the
8 end points that would come out of those toxicity tests.
9 And as Steve mentioned, this is also an issue for other
10 compounds like the pyrethroids, so yes, we are moving
11 down the process of figuring out how best to use the
12 sediment toxicity information that we have. But it is
13 a measure of direct toxicity through the sediment
14 organisms, not so much any exposure they may be getting
15 through the food web, plankton, whatever. So yes, we
16 are marching down that road.

17 **DR. HEERINGA:** Thank you very much, Mr.
18 Sappington for that presentation, and at this point I
19 would like to move on to the next presentation by Dr.
20 Ronald Parker, also of the Environmental Fate and
21 Effects Division. And panel members, if you have
22 questions that...we'll have chances throughout this to
23 get them answered, please hold them.

24 **DR. PARKER:** Thank you, and good morning.
25 I'm going to be presenting a rapid overview of our



1 current computer modeling methods that we use for
2 aquatic ecological exposure assessment.

3 As Mr. Sappington pointed out, EFED does
4 use a tiered modeling/monitoring system to assess these
5 chemicals. The tiers are use to officially allocate
6 resources to assessment efforts of varying complexities
7 and potential risks. The tiers themselves represent a
8 level of effort and therefore expense. Lower tiers
9 require less time and effort, far less input data, and
10 the higher tiers then require more time and effort and
11 more data.

12 Each higher tier is somewhat less
13 conservative than the previous tier that was completed
14 before it. The lower tiers generally use conservative
15 assumptions in lieu of site specific data, for some of
16 the model inputs, and then in upper tiers we substitute
17 more site specific data for some of those conservative
18 assumptions. It is not a pass/fail system, but a pass,
19 progress to the next higher tier system. And the
20 higher tiers then are designed to resolve uncertainties
21 that may have arisen during implementation of the lower
22 tiers.

23 I'm going to provide a description of
24 our tier 2 aquatic assessment procedure. In tier 2, we
25 use the electronically linked US EPA PRZM and EXAM



1 models. PRZM is an inter-field model, it simulates
2 pesticide in storm water runoff using the edge of a
3 pesticide treated agricultural field. EXAMS is a
4 receiving model, electronically linked to PRZM, it
5 simulates transport and fate within the water body
6 which has received pesticide coming off the edge of the
7 field from PRZM, from the runoff model.

8 This figure is a pictorial of our
9 surface water modeling configuration. We assume runoff
10 from a single pesticide treated agricultural field to a
11 single static pond. The PRZM program simulates the
12 hundred percent treated, 10 hectare field, providing
13 runoff to the 1 hectare by 2 meter deep pond, which is
14 then simulated by the exposure analysis modeling
15 system, the EXAMS program.

16 Why do we simulate a farm pond? Two
17 basic reasons, first the OPP static pond serves as a
18 simple yet conservative surrogate for all surface water
19 in the U.S.. Our assumption in that static pond is that
20 inflow from runoff is exactly equal to the outflow from
21 seepage plus evaporation. And I might add that we
22 consider there is no chemical removal in that seepage
23 from the pond. When compared with monitoring data,
24 this single static pond has been shown to be
25 appropriately conservative as a surrogate for other



1 surface water.

2 We have noted however that if we add
3 significant flow through that pond, which is an option
4 within the EXAMS program, that it is no longer as
5 useful as a conservative screen, and we do start seeing
6 many times substantial monitoring values that are
7 higher than what are predicted by our...in our pond.

8 The second major reason for using a farm
9 pond is that the U.S. does have at least 2.6 million
10 natural and constructed ponds. I've seen estimates of
11 up to 8 to 9 million ponds, and so we believe that the
12 pond itself is a significant ecological resource. They
13 are resources in their own right, for wildlife
14 conservation.

15 So, in other words, we thought this farm
16 pond is a conservative screen for rivers and streams,
17 which do receive runoff from multiple agricultural
18 fields as a result of multiple rainfall events over a
19 substantially sized watershed. PRZM has fairly simple
20 hydrology. A simple water balance, inflow is equal to
21 outflow plus any change in storage. Inflow comes from
22 precipitation, snow melt and irrigation. Irrigation in
23 many parts of the country, as you are well aware, is
24 used to bring soil moisture up to field capacity.

25 Outflow is from evaporation and



1 transpiration from the field as well as runoff to our
2 standard assessment pond, and percolation into the lake
3 ozone and or into front water. PRZM runoff assumes
4 Hortonian flow, assumes that that occurs when the
5 precipitation rate exceeds the conductivity of the soil
6 surface.

7 Runoff is typically delayed until
8 infiltration produces saturation at that soil surface.
9 The runoff estimation depends on the antecedent
10 Moisture content of the soil and on the hydro logic
11 root, on which I'll say more in a moment. And PRZM
12 does use the NRCS proof number approach to relate
13 runoff from the soil site to the soil type to land use,
14 and in farm management practices that may be put into
15 practice by the farmer or the grower.

16 PRZM is a scenario driven model. There
17 are 2 basic inputs that go into PRZM, the first is the
18 simulation data input file. That includes a wide
19 variety of inputs. The pesticide environmental fate
20 data, specific pesticide application timing, and
21 application method information, field soil properties
22 that typically a specific soil series in each of the
23 input files. Cropping data, which includes growth
24 rates, crop heights, rooting depths, fueled water body,
25 geometry and also allows the user to select the type of



1 output and units that are desired for output from the
2 model.

3 The other input file is the weather
4 data. That includes daily measured values for
5 rainfall, for high and low temperatures measured at
6 that site, for Pan evaporation. Total amount of wind,
7 in some cases we have wind direction, for looking at
8 spray drift and solar radiation. EFED uses
9 approximately 80 standard scenarios. We also have
10 additional special purpose scenarios, which are used
11 for cumulative assessments for chemicals that would
12 have a common mode of action, and sometimes for
13 endangered species assessments.

14 There are 4 basic steps that we use in
15 developing a new scenario for PRZM. First step is to
16 identify the potential national usage area for the
17 chemical that we are looking at developing. For
18 example, a scenario for corn we would be looking at the
19 central part of the United States where corn is grown,
20 would be the likely area for developing a corn
21 scenario, for obvious reasons.

22 Secondly, we select a location with high
23 runoff, and the USGS Isobars For Runoff is an excellent
24 resource for that. We can actually see where higher
25 runoff area is, so for example, going back to our corn



1 scenario, we see that if this central area of the
2 country is the area where corn is grown, we would be
3 more likely to have our scenario down in this part of
4 the country, where we do have higher runoff.

5 Next, we look at the soils, again these
6 are selected by the USDA Hydro Logic Group. USDA
7 classifies all soil series. I think there are
8 approximately 20,000 soil series in the United States,
9 divided into 4 hydro logic classes. The A hydro logic
10 group has the highest infiltration and the lowest
11 runoff rates. D soils on the other end of the spectrum
12 would have the highest runoff and lowest infiltration
13 rates. So for selecting a higher runoff soil series we
14 would typically select a C or D soil, as providing the
15 most runoff.

16 We're also wanting to select a erosion
17 soil series. We also use the hydro logic groups for
18 that. A soils are typically sandy, and for that reason
19 large soil particles are not highly erodible. D soils
20 are more "clayey", and may adhere and therefore are
21 frequently not highly erodible.

22 So for a high soil erosion we would
23 typically select a D or a C soil. So the overall
24 choice in looking at both runoff and erosion is likely
25 to be a C soil which would then maximize both the



1 runoff and the soil erosion, in order to provide a
2 conservative assessment site.

3 The fourth step is to select weather.
4 That is a fairly easy process once you have selected
5 the soil series, we select the nearest weather station.
6 We have roughly 320 weather stations for which we have
7 daily...30 years of daily weather data. So we use that
8 measured data from the National Weather Service. The
9 reason we use multiple years of weather is to simulate
10 the temporal distribution of concentrations at the
11 assessment site.

12 A year or two of data may vastly
13 underestimate or overestimate the overall amount of
14 rainfall that you might be looking at. Looking at the
15 exposure analysis modeling system, this is our farm
16 pond configuration. It is a 1 hectare farm pond,
17 10,000 square meters, 2 meters depth of water,
18 underlain by a sediment layer of 5 centimeters depth.
19 That gives us a 20 million liter assessment area in
20 which that 20 million liters obviously is then the
21 denominator in our exposure assessment calculations.

22 EXAMS is also driven by inputs that are
23 selected by EFED. Chemical specific inputs; with the
24 molecular weight and solubility, also a number of
25 degradation inputs; pH specific hydrolysis, aqueous



1 photolysis, aerobic and anaerobic aquatic metabolism.
2 Movement inputs within and around the aesthetic water
3 body. Vapor pressure, and Henry's Law Constant are
4 used to calculate volatilization, adsorption,
5 desorption, obviously are used to determine how much of
6 that pesticide is dissolved, and how much of it is
7 orbbed to the eroding soil.

8 Fixed inputs for all cropping scenarios
9 don't change typically with the chemical. There are
10 pond water chemistry inputs, pond sediment inputs. Go
11 over those, as that's sort of the focus of what we are
12 talking about today. The characteristics of a
13 suspended sediment, the sediment biota, the organic
14 carbon content of the sediment, both density and
15 percent water. Benthic Biomass, Benthic Bacteria, and
16 the population density of both, and then the dimensions
17 of that Benthic layer, and then obviously the pond
18 geometry.

19 There are site specific inputs as well.
20 Monthly water temperature at each of the sites is based
21 on the temperature in the PRZM input file. Solar
22 radiation and wind are also site specific. Cloud cover
23 on a historical basis, and latitude and longitude of
24 that particular site. And possibly the most
25 significant, or one of the most significant inputs then



1 is the storm by storm dissolved in orbed pesticide
2 masses that are predicted by the PRZM program and then
3 go into the PRZM EXAMS, go into the EXAMS file.

4 EXAMS model reports the following
5 concentrations. Ones that are specifically relevant to
6 us are the maximum peak; which is used for acute risk
7 assessment, the maximum of the 21 day running average
8 values; which is used for the invertebrate chronic risk
9 quotient, and the maximum of the 60 day average running
10 values, which is used for the chronic risk assessment.

11 This is a graph of 10,500 and sum daily
12 values coming out of EXAMS. This is 30 years of daily
13 values, you can see that the spikes typically will be
14 pesticides applied in the summer time. So every year,
15 depending on the size of the rainfall events, you do
16 have a spike.

17 What we do is to sort and rank all of
18 those values and pick out, as I said, the maximum
19 running average for each of the exposure concentration
20 exposure durations of interest. These are ranked and
21 plotted from highest to lowest, left to right on this
22 graph, and if you look on the right hand side here,
23 this 1 in 10 year line represents the value for each of
24 these exposure durations that we would use in the risk
25 assessment.



1 That was very quick, explaining a very
2 complex system, are there any clarification questions
3 that I can answer briefly at this point?

4 **DR. HEERINGA:** Thank you, Dr. Parker, I
5 think Dr. Schlenk has an opening question.

6 **DR. SCHLENK:** Yeah, thanks for the
7 presentation, very nice. I assume you are using the
8 ponds system as a conservative worst case scenario
9 approach, in terms of the type of exposure that you are
10 going to model, as far as the risk assessment. Would
11 that be correct?

12 **DR. PARKER:** Yeah, I think it isn't
13 necessarily worst case, but it is designed as a high
14 exposure scenario. We do see...once in a while you'll
15 see monitored values that are higher than this pond,
16 but typically it is a high exposure assessment.

17 **DR. SCHLENK:** My question actually deals
18 more with residential use, particularly with some of
19 the pyrethroids. We see that as actually being a
20 little bit more of a worse case scenario in certain
21 water bodies out in the west coast, at least in urban
22 settings. And what I'm wondering, is can PRZMS or
23 EXAMS be modified to implement sort of an urban runoff,
24 or a urban deposition based exposure setting?

25 **DR. PARKER:** We have spent a lot of time



1 discussing that. We have a PRZM scenario, which I
2 don't believe we've used yet for...that would divide
3 lawn areas from hard surfaces, and route them into a
4 pond. I think our general feeling is that this would
5 be somewhat simplistic for the typical urban runoff
6 scenario, where you do have multiple holding ponds and
7 multiple storm sewers.

8 And we've always had difficulty trying
9 to estimate the inputs where you have hundreds or
10 thousands of homeowners that may be applying on the day
11 that Home Depot has a sale. It's very difficult to
12 estimate whether we have no applications in a year, or
13 10. So the inputs are different or difficult. The
14 PRZM EXAM scenario is somewhat simplistic for an urban
15 situation, and that's an issue that we are looking at
16 in various ways. So it could be done. My own feeling
17 is that that's probably too simplistic for an urban
18 setting.

19 **DR. HEERINGA:** Dr. Oris.

20 **DR. ORIS:** Excuse me, Jim Oris, from
21 Miami University. Thanks for the nice overview of how
22 this works, but if you could please, could you give us
23 a very brief description of how you get from the time
24 series information for EEC's to the exceedance
25 probability graphs that you use for doing that 1 and 10



1 year return.

2 **DR. PARKER:** Okay, the EXAMS program
3 itself predicts, produces a long output file that has
4 concentration values in all of the inputs and all of
5 the outputs for each of the 30 years, so that EXAMS
6 output file has 30 sections. There is a, I think it's
7 a table 20 in that...there are 30 table 20's in that
8 output file, probably more information than you wanted.
9 That includes the maximum running average for each of
10 the durations of interest that we care about in each
11 year. So we pick out the maximum value for each year,
12 the maximum running 4 day window for each year, the
13 maximum 21 day window for each year, and reports those
14 in the file.

15 We then take those and rank them from
16 the highest to the lowest, for each of those durations
17 and then pick the 1 and 10 year, which typically is
18 about the 4th largest of those annual values, which we
19 use for risk assessment. So it isn't the highest of
20 all of those 30 years, but it is a high value. We have
21 in the past determined that that's the level at which
22 we want to regulate using this pond.

23 **DR. ORIS:** So there's no uncertainty
24 built into these exceedance probabilities? It's a
25 deterministic measure?



1 **DR. PARKER:** It's deterministic. We know
2 the highest year, and the lowest year, but we just use
3 that 1 and 10 year value. We had that debate years
4 ago; should we be looking at the 95th percentile, or
5 the 90th percentile? To be consistent with some of the
6 other offices of EPA, we chose the 90th percentile.
7 That's obviously a judgement call rather than a science
8 call.

9 **DR. HEERINGA:** Dr. Portier, then Dr.
10 Simonich.

11 **DR. PORTIER:** I just wanted to follow up
12 on that. So the thirty years of rainfall that goes
13 into the model, that's a natural 30 year sequence from
14 site? There's no taking the years and rotate, and
15 randomly..? That site hasn't observed a drought, a long
16 drought for example, in that 30 year series. That long
17 drought is not represented in the 1 and 10 year
18 calculations?

19 **DR. PARKER:** Correct. That drought year
20 would end up in the lowest concentration years, so it's
21 typically only the high, only the wettest years that
22 would be represented in that 1 and 10 year value.

23 **DR. HEERINGA:** Dr. Simonich.

24 **DR. SIMONICH:** Staci Simonich, Oregon
25 University. I'm interested as to how the dissolved



1 organic carbons in the suspended sediments and the
2 organic carbon content values were selected, and if
3 they're conservative for the ecosystem?

4 **DR. PARKER:** They were selected by our
5 Office of Research and Development, when we started
6 using the PRZM, the linked PRZM and EXAMS models back
7 in '92 or '93, we worked with the developers of the
8 models. The developers of the PRZM EXAMS models
9 looking at what we were doing, looking through
10 databases that were available at that point, and those
11 were representative of the ponds that we were
12 simulating. They're not designed specifically to be
13 extremely high, or extremely low, so they're
14 representative I guess, is the best word I can use,
15 rather than meeting any sort of policy criteria.

16 **DR. HEERINGA:** Dr. Abbott.

17 **DR. ABBOTT:** Linda Abbott, USDA. Can the
18 electronically linked PRZM and EXAMS be used to
19 simulate an application of a pesticide to an area that
20 has one curved number, perhaps one type of practice,
21 followed by over land transport to another area that
22 has a different curve number? Perhaps a different
23 practice type, a non-cropped area?

24 **DR. PARKER:** That capability is
25 available. I don't believe we have ever done that with



1 our 10hectare field. We typically represent just one
2 soil series and then that just has one curve. He have
3 the capability of putting in up to 30 curve numbers per
4 year, so if we wanted to simulate compaction of the
5 soil as a result of tillage operations, we could do
6 that, but we don't at this point.

7 **DR. ABBOTT:** Just to be clear, I don't
8 mean in different times, using a different curve number
9 or I mean two different physical areas, with one curve
10 number in overland transport to another area that may
11 be non crop before getting to the pond.

12 **DR. PARKER:** Yeah, we can do that, we've
13 played with the model a little bit in terms of
14 simulating infiltration into buffer areas, grass
15 waterways. To my knowledge, we haven't used that for a
16 risk assessment. The capability is there, if we wanted
17 to do that.

18 **DR. HEERINGA:** Dr. Maddalena, and then
19 Dr -

20 **DR. MADDALENA:** The effort that was made
21 to decide what runoff soils and types you use, has
22 there been any effort to see that just because a
23 maximum amount of soil and water are transferred to the
24 pond, that means the maximum amount of chemical will
25 also be transported to the pond? In other words, the



1 moving, the effecting media, which is the runoff soil
2 in the water, have different characteristics at
3 different sites. So they may actually carry more
4 chemical, even with less water or particles are moving.
5 Does that make sense?

6 **DR. PARKER:** Yeah.

7 **DR. MADDALENA:** Has that been looked at?
8 Like a sensitivity analysis in this modeling system?

9 **DR. PARKER:** Well, the Koc, the binding
10 coefficient of the chemical with the partition between
11 the model loading soil and the model runoff coming out
12 of the model and so the surface water concentration is
13 pretty much fixed. I mean if we went to a different
14 site and put another high exposure site the numbers
15 could be different I suppose. Is that what your what
16 you're asking?

17 **DR. MADDALENA:** Yeah, maybe I can look
18 closer into the details of the model when I get a
19 chance. I had another sort of simplistic question in
20 the conceptual model that follows up on an earlier
21 question. We keep coming back to the pond as the
22 receiving body, but what if the house was actually the
23 receiving, the end point of your assessment? What if
24 chemicals moved from your site to the house and
25 accumulated in the house, the built environment and not



1 the pond necessarily. Is there a--

2 **DR. PARKER:** Into the house?

3 **DR. MADDALENA:** Urban environments tend
4 to be moving into these agricultural regions at a
5 phenomenal pace in a lot of places, and when you apply
6 chemicals at a site I think we all agree they don't
7 stay at that site. We're assuming here in this
8 discussion that they move from the site to a pond, but
9 there may be more important receiving environments that
10 should be considered. I don't know, but is there a way
11 to look at other off-site transports mechanisms to get
12 accumulation in different environments such as a house
13 for example? Tracking into a house of dust and
14 materials. Or is that a different agency?

15 **DR. PARKER:** That's our health effects
16 division, that typically looks at that. They do look
17 at residential exposure from pesticides that would be
18 applied to a lawn, pesticides that are used for tick
19 sprays for cats and dogs; so they do that. We pretty
20 much stick to the ecological questions.

21 **DR. HEERINGA:** Dr. Hickie.

22 **DR. HICKIE:** Just a question of organic
23 carbon. If I gathered from your presentation there are
24 6 properties from the sediment in the water? Or do
25 they change over the duration of the evaluation, and 30

1 years?

2 **DR. PARKER:** The organic carbon in the
3 water bodies, in all of the water bodies, no matter
4 what country it is are fixed valued. I suppose the
5 limitation of that is that it might not always be the
6 same as you went from site to site. It does allow us
7 one thing that we are required to do and that is
8 provide a level playing field for all of the chemicals
9 that we assess, so there is one value I think of our
10 standard pond is that we are accessing all chemicals on
11 exactly the same criteria. So it is a fixed value.

12 **DR. HICKIE:** Okay, is there organic
13 carbon coming in with runoff? I'm just wondering
14 whether the model has any check for carbon subject as a
15 balance.

16 **DR. PARKER:** There isn't organic carbon
17 specifically coming in, but there is an organic carbon
18 enrichment ratio in PRZM that adds...because a chemical
19 can be preferentially absorbed to organic carbon, you
20 do get more pesticide delivered because of that organic
21 carbon content in the soil. So that it is a fixed.

22 **DR. HICKIE:** So that the pond does not
23 have the potential for organic carbon content to
24 gradually build up?

25 **DR. PARKER:** Correct.



1 **DR. HEERINGA:** Dr. Biddle man, and I
2 think then we'll move to a break.

3 **DR. BIDLEMAN:** Terry Bidleman,
4 Environment Canada. Is there an atmospheric component
5 to either PRZM or EXAMs? If not, do you have a
6 mechanism for dealing with volatilization losses?

7 **DR. PARKER:** Yes, there is volatilization
8 predicted both in PRZM and in EXAMs based largely on
9 the vapor pressure and the end result constant for both
10 of the models.

11 **DR. BIDLEMAN:** Okay.

12 **DR. HEERINGA:** One final quick question-

13 **DR. SIMONICH:** Just to clarify on Harry's
14 point. So it accounts for volatilization but not
15 atmospheric deposition?

16 **DR. PARKER:** Correct.

17 **DR. HEERINGA:** Okay, at this point in the
18 process I want to thank everybody for the pace which we
19 have able to move in our coverage. Dr. Parker, thank
20 you very much for that presentation. I'm sure if there
21 are other questions that come up we will be able to
22 come back to you. And I'll work on getting my hard and
23 soft eyes for panel members, Simonich and Bidleman,
24 Simonich and Bidleman, and see if I can manage that
25 after the break. Let's take 15 minutes. I've got just



1 short of 10:30 on my watch, so 10:45. These EPA clocks
2 are company clocks, they're about 5 minutes slow here.
3 **(WHEREUPON , a break was taken)**

4 **DR. HEERINGA:** Okay panel members, if we
5 could have a seat we'll get under way again. Welcome
6 back everybody to the second half of our morning
7 session on the EPA FIFRA Science Advisory Panel meeting
8 on the topic of selected issues associated with the
9 risk assessment process with pesticides, with
10 persistent bioaccumulative and toxic characteristics.
11 We are in the process of hearing a number of scientific
12 presentations that center on the white paper prepared
13 by the Environmental Fate and Effects division. And at
14 this point in time Dr. Mohamad Ruhman is going to do a
15 presentation on environmental persistence issues.

16 **DR. RUHMAN:** Thank you, Mr. Chairman.
17 I'm going to present the environmental persistence
18 issues. This paper was presented by me, but Dr. Hetrick
19 is here and he is also a co-author with me. The
20 presentation outline; first I'll introduce the subject,
21 secondly, I'll illustrate four major issues for risk
22 assessment challenges. For the fourth example,
23 pesticides which we are dealing with.

24 The first one is how to estimate the
25 environmental concentration for the total residue of



1 concern. Because some of these pesticides do degrade
2 into degradates, which are persistent. That's called
3 the total residue of concern. Interpreting the
4 predicted or measured environmental concentration,
5 which is above the water solubility. If we get some
6 measures above the water solubility, how we look at
7 that.

8 Second thing is interpreting the
9 degradation half lives with a compound which has a high
10 sorption to the soil, which the four pesticides which
11 we are dealing with have this characteristic.

12 And the last thing is to quantify the
13 long term residue accumulation in soil and sediment.
14 I'll come up with some conclusions through my thought.
15 For environmental fate I will transfer there, you don't
16 have it there in the hand out. It's actually a fate
17 and transport processes. Those fate and transport
18 processes close the dissipation of pesticide. We look
19 at dissipation of pesticide here as 2 things. First
20 degradation, and second is movement. For degradation,
21 the processes are hydrolysis, photolysis and metabolism
22 in different environmental compartments.

23 For movement, we look at things which
24 cause movement, like vapor pressure or movement between
25 phases, like absorption from one phase to another from



1 water into the sediment. We get studies for all these,
2 from these studies we can say that then pesticide is
3 degrading or not degrading by hydrolysis or photolysis,
4 and they are specific, like for hydrolysis, specific
5 for hydrolysis instead of all the other processes. And
6 for Photolysis is also strict for photolysis. But then
7 aerobic soil linked up with, it's actually a
8 combination of 2, metabolism and sometimes hydrolysis.

9 For our example, pesticides, we have 4
10 example pesticides that are here. Pesticide 1,
11 Pesticide 2, Pesticide 3, and Pesticide 4. Pesticide 1
12 is 2 isomers and a common degradate, and this is TROC's
13 total residue concerned. It's a degradate, isomer 1
14 and isomer 2. That's all of them together.

15 This is site 2, we have the parent and
16 the total residue of concern because the parent also
17 degrades into about 4 degradates, which is also of
18 concern to us. For pesticide 3 and 4 only the parent is
19 mainly of concern to us.

20 If you just ignore everything and look
21 at the red numbers there, you can see that for the half
22 life of these pesticides, either the isomers or the
23 degradates or the parent or the degradates or the total
24 thing is between 114 to stable in almost all systems.
25 These systems which I have, we look at the half life



1 and different environmental compartments in order. We
2 looked at the hydrolysis half life, which indicates to
3 us if it's resistant or not. So here is stable, so
4 it's resistant to hydrolysis.

5 This pesticide is resistant to
6 hydrolysis. And photolysis same. Aerobic soil...for,
7 for aerobic aquatic, look at the water ponds for the
8 water. For the soil compartment look at the aerobic
9 soil half life. For the sediment we look at the
10 anaerobic soil half life. As you can see that
11 everything is giving resistance, except there is some,
12 as you can see here, there is no resistance for isomer
13 1 or isomer 2 in hydrolysis. So that indicates that
14 the degradate is a little more persistent, although we
15 don't have any data for it.

16 We look at the photolysis. At the
17 photolysis you can see that this is side 2 and 3 and 4
18 are not persistent, but we are looking at...it's not
19 persistent, it's specific environmental compartment
20 where you have a clear water, and also very shallow
21 water. So in most environments it's all the pesticides
22 are persistent. If we look at the...in the soil the
23 aerobic soil, we can see that it's all persistent
24 except one of the isomers. But when we look at the
25 pesticide 1, we look at the total residue of concern,

1 because isomer 1 is a concern, isomer 2 is a concern,
2 degradate and also the total. And you can see that
3 it's persistent.

4 Here we can see that pesticide 2, parent
5 is not persistent in an aerobic aquatic system, but if
6 we look at it and the degradate with it, it's highly
7 persistent. So we can say that these pesticides are
8 persistent in most environmental compartments.

9 I agree on example this pesticide 1 can
10 be an example for pesticide 1 and 2. As you can see
11 here, it has, parent has 2 isomers, that's 64% and 30,
12 40, 55, 70 percent, and isomer 1 degrades very quickly,
13 as you can see here. Isomer 2 degrades rather quickly,
14 but there is a common degradate forming, and this is
15 the degradate forming, which is a common degradate from
16 both pesticide, from isomer 1 and isomer 2, and this
17 degradate when it forms, comes to a maximum and it
18 flats out, so it's highly persistent. When you look at
19 the system we look at the total there. The total
20 amount which is left is highly persistent.

21 We look at another example for another
22 pesticide, and this pesticide is pesticide 3. And you
23 can see that the degradates of all the degradates are
24 not that very highly important, not important. The
25 most important, persistent chemical is the parent and



1 you can see the parent is degrading not very quickly.
2 It's persistent, and the DT 50 for this pesticide is
3 about over 200 days.

4 Now we look at why are pesticides
5 partitioned either into the soil or sediment, and they
6 partition sometimes to the earth. That's pesticide 1
7 and 2. If we look at values on adsorption coefficient,
8 the adsorption coefficient for all the pesticides and
9 also their isomers or degradates are very high. Goes
10 from 10,600 and carries it to 1.2 million, indicating
11 that partitions into the soil and sediment, that's all
12 of our pesticide. We look at which partition into the
13 air.

14 We can see that here we look at the
15 Henry's Law Constant and here is between 10 to the
16 minus 6, 10 to the minus 5, pesticide 1, the isomers
17 and also for pesticide 2, you have 10 to the minus 5,
18 10 to the minus 6. But the other, the degradate of
19 pesticide 1 and pesticide 3 and 4 are not of concern to
20 us when they partition into the air. That's a
21 movement, a qualitative movement.

22 Now I'll go through the four major risk
23 assessment challenges. The first challenge is to
24 estimate the environmental concentration
25 of the total residue of concern. That's the parent

1 plus the degradates. Total residue of concern.

2 First I'll give you some definitions and
3 I think some of them have been already given to you.
4 Hour exposure is just by looking at the EEC or the
5 expected estimated environmental concentrations, so
6 exposure is synonymous with EECs.

7 So if you want to measure exposure using
8 your EEC, which is estimated environmental
9 concentration, we could give this estimated
10 environmental concentrations as a daily concentration,
11 which is a daily EEC, or a one in ten years EEC, that's
12 what the bar graphs told you, it's a summary of what we
13 have here which used data to get the 90th percentile.
14 This actually is the one we used in our risk
15 assessment.

16 I also use words like TROC which is the
17 total residue of concern. That means the degradates and
18 the parent that we, the parent sometimes too, like this
19 is the side one isomer on isomer 2, and a common
20 degradate. That's the total residue of concern.

21 The IROC, which is the individual
22 residue of concern, meaning either isomer 1 or isomer 2
23 or degradate. The methods we use for estimating that
24 exposure, EECs are three methods. The simulation for
25 measuring the parameters are standard gold method and



1 estimation of this, the results of that by the residue
2 summation method or the total residue method.

3 I would just go through what issues we
4 have to consider when choosing between these methods.
5 We have to ask ourselves similar questions and do some
6 analysis to our answers to see which one we could use.

7 First question is are data available to
8 conduct scientific analysis? Do we have data available
9 to do scientific analysis? Are data available for
10 individual compounds? Is there data available for
11 isomer 1 and isomer 2 and degradate, or just for all of
12 them? Do we have data that supports similar toxicity
13 or can we say that the whole isomer 1, isomer 2 and
14 the degradate are having the same toxicity or are they
15 different? So that give us, either we go this way or
16 the other or use this method or the other.

17 Can we accept assumptions because each
18 one of these has assumptions. Can we accept these
19 assumptions, given case by case situation. Is the
20 degradate from a fine application because the two
21 method, the RS method and the TR method assumes that
22 degradate forms at time of application which is not
23 actually the case all the time, but epidemiologists
24 know it takes care of the time of application, of the
25 time of formation of the degradate.



1 The methods used to partition the
2 application rate, how we do the partitioning of the
3 application rate between the degradate and the parent.
4 And the assumption of the total residue method where
5 you get a physicochemical product before three or four
6 chemicals which is an assumption in that. Is that
7 acceptable or not?

8 I go through method by method how we do
9 the execution of these methods. The first method,
10 which should be our standard gold method is the
11 formation of decline method and we estimate the
12 simultaneous decline of isomer 1 and isomer 2, this
13 is, all these three examples is for, this is side one
14 which has an isomer 1 and an isomer 2 and a common
15 degradate. So estimate the simulation of decline
16 curve for the isomer 1 and isomer 2 which forms isomer
17 common degradate 1 and isomer 2 also the common
18 degradate 1.

19 From that we get a rate constant, we get
20 the ratio between the formation rate of common
21 degradate over the degradation rate of the isomer 1 and
22 degradation rate of isomer 2. Then we execute two
23 separate parent-daughter PRZM exam model. And we do
24 modeling, we get parent to go like isomer 1 go into
25 full degradate, isomer 2 go to the common degradate.



1 We have two, two things here. Actually if we have
2 only one parent, the other we have two parents, we can
3 use only one.

4 This mother runs with parent break,
5 divided between two isomers according to the ratio in
6 the, in the material, in the pesticide and each one
7 produce daily EECs. We combine those daily EECs and
8 from that we calculate or summarize it into the one in
9 ten year EECs.

10 The second method is the RS method.
11 Here we divide the application at the application
12 timing between the three compounds, which is isomer 1,
13 isomer 2 and degradate, and we use the surrogate for
14 that is the aerobic size study, when we get how much of
15 it, of isomer 1 and how much of isomer 2 and how much
16 of the degradate and then add them up, if it comes to
17 over a hundred, we normalize into a hundred and then
18 we, we make corrections of the molecular weight so we
19 divide the application at three all three.

20 Then we exclude freons for PRZM exam,
21 which is the two isomer and the common degradate, and
22 we combine the freons to get the EECs and then we
23 summarize it, the one that's in here.

24 The last method is the TR method which
25 is a simple method. Here we obtain only one set of

1 physicochemical work. Although we have three chemicals
2 we get one set of physicochemical. We, for the half
3 lives it's probably as simple because we calculate the
4 half life. We see how much is of the added material is
5 for isomer 1 and isomer 2 and degradate, we add them up
6 and then we recalculate the half life so we have a half
7 life for the total residue of concern. And we execute
8 a PRZM exam run and we produce the EECs and the one
9 continues for only one run. Okay?

10 I want to compare these methods and I
11 look in comparing these methods is the formation
12 decline method, the residue summation method and the
13 total residue method. I use attributes here to
14 compare them.

15 First is the feasibility of using any
16 one of those. For the feasibility I have, I use the,
17 it's based on the availability of. If we have
18 scientific data and also for fate data for each one of
19 those members of the residue of concern, which is the
20 IROC, the individual residue of concern fate data then
21 I could use the FD method. If I have only the IROC
22 for the fate data only then I can use the RS method.
23 If I don't have either the scientific data nor the IRO
24 fate data for the individual degradates, then I have to
25 use the TR method.



1 The second attribute is when the method
2 is recommended and this is based on the toxicity data.
3 If we have different toxicities we use either the FD or
4 the RS method, are approximated by the RS method. If
5 we have similar toxicity, we could use the TR method.
6 For the epidemiologist it has two unique strengths
7 which doesn't have, appear in any one of those two.
8 These two unique strengths that incorporate the
9 formation of the kinetics and that accounts for timing
10 of formation. These are simpler because it doesn't do
11 that and also this is more simpler because you had only
12 one run.

13 The assumptions you have here, list
14 assumptions. The only assumption you have is that the
15 kinetics go first order, but here you have to assume
16 that the timing is okay to be at the beginning of the
17 application so you have more assumption if you go this
18 way from the epidemiological approximations.

19 And the required data and therefore we
20 have high requirement for this epidemiological method
21 and not only for that method. We could say that the RS
22 and the TR method are actually an approximation to the
23 FD method.

24 Method compare the outputs, the outputs
25 we got from the FD and R method is different from that



1 of the TR method. It's different because the FD and
2 the R, RS method generate the EECs for the individual
3 residues of concern, each one of them and also for the
4 total, the TR method only for the total. So but both
5 of them generates EECs and both of them we
6 calculate whether the 90th percentile are the
7 assimilation of the EEC or the daily EECs.

8 I give you an example of this, and you
9 can see that I'm just giving only examples for sides
10 one and two because we just said before that this is
11 side four, three and four, our concern is only the
12 parent. Here we have also degradate.

13 Daily EECs for assimilation, for this is
14 side one and this is side two. For side one we use
15 the scenario simulation, we squirted that tomato with
16 three applications per year, as, as will be labeled.
17 But on this side two, we used a simulation of
18 Pennsylvania turf one application per year. We look at
19 the output. As you can see here, the epidemiological
20 is the red line. The RS method which is an
21 approximation on the FD method is the black line and
22 the TR method is the blue line.

23 As, if we look at the peak here we can
24 see on the simulation here, I'm choosing to do for only
25 two years but it goes also for 50 years and this is the



1 concentration in parts per million. I want you to
2 notice that our gold method is somewhere in between.
3 That the TS, TR method which is the blue here is
4 overestimating and the TR, the RS method is less
5 estimating our gold standard.

6 The next thing is for, this is side two
7 and I'm looking also at daily concentrations. and I'm
8 just, I've choose to do only two years, but there's the
9 third year. Here is the time and here is the
10 concentration in EEC in parts per million.

11 We can see here in the peak, the main
12 constituent of the peak is the parent, but if you go
13 down here that the degradates become more important and
14 you can see here and then right here, right here is the
15 degradate is the main, is the one which is taking,
16 which is reducing the concentration in the pond so the
17 outlook for one in ten years EEC for pesticide one so
18 these same simulations I'm going to just talk about the
19 summary of these simulations.

20 As you can see here for, this is side
21 one is one in ten year EECs. As I told you before,
22 here is the EEC in parts per million. Here is the
23 peak concentration, the 21 day concentration, this is
24 the one in ten year concentration, 60 days
25 concentration right here. Mr. Parker has told you



1 about what this means.

2 As you can see here, you can
3 differentiate between the constituents of the residue.
4 That's the parent, that's, that was isomer 1, parent
5 isomer 2, and here is the degradate and here is the
6 degradate coming from isomer 1, and here is the small
7 one of that degradate coming from isomer 2. So it
8 actually gives you the epidemiologic method, gives you
9 also the, what is contributing to the total and you can
10 see the total. I want you to notice the total here is
11 about 40 parts per million, parts per billion.

12 Okay, next. That's the RS method. It's
13 giving the same thing but also it's less estimating.
14 As you can see here, it's about 30 parts per billion is
15 the peak and also the same goes for the annual and 60
16 day and the 21 days.

17 For the TR method, as I said before, we
18 just get only one thing which is for total. It's a
19 mixture of isomer 1, isomer 2, and common degradate.
20 Only one concentration. As you can see here, it's
21 overestimating the peak and also 21 day and the annual
22 and as I can, I showed you before for, this is side 2,
23 how the degradate is important to time. And the long
24 term degradates are important. As you can see here,
25 the peak mainly is, the contribution's coming from



1 parent, and this is the amount of degradate, there's
2 actually four degradate.

3 Going with time, the parent contribution
4 is very little because the amount of degradates are
5 important in determining. So we have to look at the
6 total residue of concern because these degradates are
7 of concern and would be of concern at the chronic time
8 and it's a long term exposure. The second thing that
9 it's interpreting, can be predicted or measured
10 environmental concentration above is also significant.

11 The ability to measure solubility for
12 the pesticides, we have, we can compare the two
13 categories, this is sides one and two and this is sides
14 three and four and there's about two, two, one to two
15 order of magnitude and that's solubility. I guess this
16 is sides one and two, between 500 and 440. This is
17 side three is between 1.75 and .15 parts per billion.
18 It's very non-significant.

19 To decide solubility in an aquatic
20 environment is uncertain. Why? Because the solubility
21 in the level of the water may not be reflective of
22 what's in the actual ambient environment. Because you
23 have temperature variation, you have pH, you have all
24 these, you have all kinds of things in the environment
25 of waters or natural waters. The possible effects of

1 formulation also might reduce, might increase the
2 solubility, and that's because you have some, what is
3 the chemical phase in there, is it solid or liquid and
4 also the additives, there's solvents and elements of
5 fires with the formula.

6 So the message here is that it's not
7 always, the limit of solubility from the lab is not
8 always the case. Solubility in the environment is
9 uncertain. Why the water solubility is an issue
10 because of the problems in experimental variables.
11 Experimental issues we have modeling issues.
12 Experimental issues is that we are not able to
13 solubilize enough material for testing and therefore it
14 needs a cross over.

15 When you add a cross over, you introduce
16 bias, you might mis-estimate the Kd and the Koc and
17 also introduce cross over, there's uncertainty in the
18 toxicity studies with the concentration I mentioned
19 above the solubility limit because we have enough
20 separation between those phases or not.

21 There's modeling issues. Our present
22 exam has no bounding. It just assumes that solubility
23 is okay, can go up, over the solubility limit of the
24 compound.

25 What we do in interpreting, these are

1 more than values, we get more than values from codon.
2 This one, this is side four, these are the
3 concentrations which is the environmental
4 concentrations which we have and you can see that's
5 different scenarios, you get different concentrations
6 and if you look at the solubility limit there, the
7 solubility limit is there for this pesticide.

8 So all of our estimated, our estimated
9 EEC's are above the solubility limit. So what we do,
10 what we do is that we constrain, we constrain the
11 predicted pesticide EEC in the water column to be
12 absent, so we just say that the results of this
13 exercise is that EECs in this compound is .15
14 micrograms per liter.

15 The second thing we get studies where you
16 have like concentrations applications, this is a MecO
17 positive study for pesticide four, you get
18 concentration measured with time. You can see these
19 are four applications. When the pesticide was applied
20 one, two, three, four times, you can see the
21 concentrations above the solubility limit. There is
22 the solubility limit. Above it's here, here, it's
23 about five days which is above the solubility limit.

24 For us when we look at an experiment
25 like this, we just consider it to be a suspect unless

1 it is validated. The validation is not to say that,
2 okay, that was no precipitate forming here or give us
3 the reason why this, all the precipitate is combined
4 here. So we have to show that the precipitate is
5 separated well from, in these, in these samples.

6 Our conceptual model for interpreting
7 this water solubility is that when the pesticides come
8 to an aquatic system which contains a sediment metrics,
9 a water column of sediment per water or sediment
10 particles. It comes through both soluble, insoluble
11 phase or adsorbed phase. It just goes into three
12 different bowls, the insoluble bowl, the soluble bowl,
13 and the adsorbed bowl with air purity in between them
14 as can be seen here and the adsorbed bowl is, we'll
15 take that capacity as adsorption capacity of the
16 sediment particles.

17 The soluble bowl should not be over the
18 solubility, because if it's over the solubility, it
19 goes into the insoluble bowl as precipitate. Right
20 here. And if the solubility go, if the concentration
21 go under the solubility here, then you get solution,
22 you get to the soluble bowl. And the pesticide has to
23 go through that to go, to be air absorbed.

24 In, in PRZM exam modeling, or EXAMS
25 modeling mainly in the front, we just look at only the



1 soluble bowl and the insoluble. We don't take care of
2 the insoluble bowl.

3 The third thing which I'm going to talk
4 about is interpreting degradation half-lives when it
5 combines with high adsorption for soil and sediment
6 constituents. Well, our example pesticides, the
7 partition from water into the sediment, and they cause
8 major concentrations to decrease in the water and
9 increase in sediment.

10 The half lives calculated for either
11 water or sediment is actually a function of two things:
12 degradation and movement. Degradation in the water and
13 sediment cannot be separated. We cannot separate how
14 much was degraded in the water, how much was degraded
15 in the sediment. But what we can do, we can know
16 exactly how much degraded in the whole system, in the
17 system as a whole.

18 I'll give you an example to that.
19 That's pesticide 3, and you can see here that when the
20 pesticide, this is the concentration first to apply and
21 here is the time. The pesticide's up right here,
22 applies to the water, it goes rather very quickly in
23 the water. This is movement. Because if you look at
24 the sediment, it's going up in this movement.

25 So it is, the process here is actually



1 movement of pesticide between the water column and the
2 sediment.

3 But the degradation if you look, that's
4 what we look at when we look at degradation.

5 Degradation is the pesticide is not degrading very
6 much. That's the amount in the total system. Okay?

7 The last thing I'm going to talk about
8 is the quantification of long term residue accumulation
9 in the sinus rhythms. Exposure assessment for our
10 examined pesticide indicate that it required reach a
11 long period for the steady state and this often exceeds
12 the duration of most levels that is usually about a
13 year. And that possible appearance of substantial long
14 term accumulation because of that. Because the
15 partition into the sediment and soil.

16 We can quantify this, the long term
17 accumulation, maybe the other end of it, is by looking
18 at results from our modeling, from PRZM and from lake
19 PRZM exam. There is an example for quantification of
20 pesticide long term accumulation pesticide 1 in soil.
21 And these are results from PRZM. That's the total,
22 here is the total concentration in kilogram per hector,
23 and here is the data. As you can see, over 5.2 years,
24 there is the accumulation, and that goes with the,
25 these are applications. So it accumulates with time.



1 These are results from PRZM only.

2 If we look at residue exam, we have
3 different scenarios, and different scenarios as Dr.
4 Parker has told you, that gives you different things,
5 depending on, on the site, which is a site specific.
6 We have New York grapes, California lettuce, and
7 Florida turf. As you can see here, that very little
8 accumulation is evident in the turf, more accumulation
9 in the California lettuce, but substantial accumulation
10 is evident in the New York grapes.

11 In conclusion, examined pesticides, as I
12 said before, either the pesticide itself or, and/or the
13 degradates, which we call the total residue of concern,
14 is considered persistent. We feel the formation of
15 decline method or one of its, we look at the RS or the
16 TR method as an approximation to the FD method. They
17 can be used to estimate exposure concentrations. This
18 we should look at it case by case. We always look to
19 get all of them at the FD method, but we have to go
20 look at case by case basis.

21 The choice will depend upon the data
22 availability, if we have fate data and toxicity data,
23 also the toxicity data and what kind of fate data and
24 toxicity data. We analyze the situation and from that
25 we can choose these methods. Observed and/or model



1 predicted concentrations are expected to be at or below
2 the limit of solubility. Therefore, if we get any
3 values over that solubility from a, from our modeling,
4 we just cap it at the solubility and if we observe
5 concentrations above that solubility which is reported
6 to us, we need validation for such results.

7 The last two things and conclusions is
8 the aquatic metabolism studies are designed to
9 differentiate degradation occurring, they are not
10 designed to do that. They're designed to get the
11 degradation in the whole system.

12 Adsorption from the water pond, because
13 this adsorption from the water pond should be
14 interpreted as, should not be interpreted as a
15 degradation process, but it's actually a movement
16 process from one phase to another. The total system
17 half life should be used in modeling, especially in
18 modeling we use Koc to account for the movement. We
19 don't want to do double account, double counting.

20 And PRZM or link PRZM exam modeling can
21 assist the long term exposure in threshold ecosystem
22 like the soil and also in benthic compartments. As I
23 show you.

24 Any questions?

25 **DR. HEERINGA:** Thank you very much, Dr.



1 Ruhman, I appreciate the way that you moved so crisply
2 through this material and hit the high points from the
3 white paper. I want to acknowledge your colleague,
4 too, Dr. James Hetrick, Dr. James Hetrick welcome too,
5 I want to make sure everybody gets acknowledged for
6 their participation as panel members. I'm sure there
7 are some questions of clarification with regard to this
8 section of the white paper and this presentation. Dr.
9 Delorme and then Dr. ...

10 **DR. DELORME:** Peter Delorme from Health
11 Canada. You made mention for photolysis that it's
12 really only important when water is shallow and clear
13 so what is your definition of shallow water, do you
14 have a specific depth or...

15 **DR. RUHMAN:** Well, it's, that's a good
16 question. For me it's more clear water. I would assume
17 something like 30 parts per million.

18 **DR. HETRICK:** I can say that in our
19 standard pond that photolysis really doesn't, is not
20 that critical of a dissipation process. I wouldn't
21 want to hesi...I don't want to hesitate and say or give
22 you any clear example what's considered shallow but a
23 two meter deep pond with the characteristics of our
24 standard farm pond, photolysis is really not that, in
25 water is not really that important.



1 **DR. DELORME:** And, and just a followup.
2 How do you guys determine what a degradative concern
3 is, is it based on toxicity, is it based on
4 persistence, is it based on both? I mean you haven't
5 provided any criteria when you would consider a
6 degradata a problem.

7 **DR. RUHMAN:** We have a process here, we
8 have a committee called the ROC committee, where we
9 just give them our degradates and they look at
10 the, the degradata structure and see structural
11 relationships and see if they...also they look at the
12 degradates which indeed help a specific division and
13 they look at also their studies which they have to see,
14 but it's not actually an ecology problem, it's more
15 like human health.

16 **DR. DELORME:** So it's, it's partly
17 driven by human health, partly driven by environmental
18 fate?

19 **DR. HETRICK:** There are many components
20 of that. We have to confer with our toxicologists to
21 insure that we're all on the same page as far as the,
22 what the toxic residues are, that's number one, and
23 that's in consultation not only with our eco
24 toxicologists but also with our human health
25 toxicologists.

1 In addition to that we look at the
2 concentration of these degradation products that are
3 formed in these metabolism studies. Generally if
4 they're greater than ten percent of the applied, we
5 consider them to be major degradation products and we
6 tend to focus on them.

7 **DR. DELORME:** Thank you.

8 **DR. RUHMAN:** But even if the
9 concentration is just ten percent and it's toxic, we
10 think, we consider it to be.

11 **DR. HEERINGA:** Dr. Bidleman?

12 **DR. BIDLEMAN:** Terry, excuse me, Terry
13 Bidleman, Environment Canada. I have a question about
14 the statement, observed concentrations above the
15 solubility limit are suspect until validated. The
16 normal way of analyzing water samples is to pass them
17 through a filter and a lot of stuff goes through the
18 filter that is not truly dissolved, it is colloidal or
19 it can be associated with dissolved humic materials and
20 so there may be good reasons why those so called
21 dissolved water concentrations are higher than the
22 solubility limit, and I have a concern that discarding
23 them may underestimate the true concentration.

24 **DR. RUHMAN:** Well, we have to, they have
25 to just prove to us that there is a good separation



1 between the two phases and concentration's not always
2 good because also these pesticides actually the
3 formulations are less than one micron.

4 And you know, if you get part of it
5 going through the filter so you have, we have, it's
6 actually it's an interesting standard where you have a
7 certain force which you have centrifuge to get the rest
8 of the precipitate that's forming to go down,
9 especially in those pesticides where especially the
10 concentration was very low.

11 **DR. HEERINGA:** Dr. Gan and then Dr.
12 Maddalena.

13 **DR. GAN:** Well, my question also is
14 similar to Terry's since in the real water samples you
15 have a lot of DOM and, you know, we have, we have some
16 model studies showing that DOM can enhance the
17 solubility of these chemicals so maybe, you know, it's
18 pretty typical I guess.

19 **DR. RUHMAN:** Well, I do, I agree with
20 you. That's why I sit there and my conclusion that the
21 solubility method which we do here, we always ask the
22 respondent to give us some solubilities in metro waters
23 but it doesn't come to us all the time but we do ask,
24 we are, and especially also for formulations if the
25 formulations can also enhance the solubility of the



1 compound.

2 **DR. GAN:** I have one more question
3 regarding degradation kinetics. You know, I, since
4 that's one question that's charged to me and I want to
5 know what's the purpose of getting these half life, is
6 that for modeling as a parameter for modeling exercises
7 or what's the use of this half life?

8 **DR. RUHMAN:** Well, the use of...you
9 mean the half lives in the different compartments of
10 the environment?

11 **DR. GAN:** That's right.

12 **DR. RUHMAN:** We use those for modeling,
13 we don't actually only have one, one value as you can
14 see there. That is, we, we have many values.
15 Hopefully it's representative. We actually looked into
16 that, it's representative of the areas where the
17 pesticide is going to be applied, and they get similar
18 soils, and from those similar soils, something, the
19 half life would be low, some high, and so on, so we get
20 the 90th percentile of that and we use it for modeling
21 and also we use it for saying that the pesticide has
22 persistence...

23 **DR. GAN:** No, I'm sorry. I was talking
24 about, you know, the distinction between movement and
25 degradation. I guess your purpose is to get a true



1 half life and is the purpose of getting that half life
2 for modeling or for some other purposes?

3 **DR. RUHMAN:** It's for modeling but for
4 describing what's happening and why would we just do
5 say that this pesticide does not stay long in the water
6 column, it just, it just partitions into the sediment.
7 So we qualify that, but for degradation which we use in
8 modeling, we just use only degradation, how far for the
9 total system because it's actually a reflection of the
10 degradation not movement and the movement is taken care
11 of by Koc which we enter into the modeling so the
12 partitioning will happen, too. There, too. So we take
13 care of that, too.

14 **DR. HEERINGA:** Dr. Maddalena, then Dr.
15 Simonich.

16 **DR. MADDALENA:** Would it be possible to
17 pull up slide, that 36 again that showed the three
18 different scenarios on pesticide four and sediment. My
19 question just to give you a heads up and this slide
20 kind of points it out, I'm not quite sure this slide
21 shows three different, I guess you would call it time
22 and steady state or overall persistence, persistence
23 overall.

24 **DR. RUHMAN:** Accumulation.

25 **DR. MADDELENA:** Well, accumulation but



1 it may also, the uptake curves tend to reach steady
2 state on, at different times, five years maybe,
3 fifteen, maybe thirty years on the three different
4 plots and if this is the same pond with the same
5 sediment with the same loss processes, I would think it
6 would reach steady state at the same time so there's
7 something else changing in this system. Are these,
8 this scenarios are very different as far as different
9 ponds?

10 **DR. RUHMAN:** This is the concentration
11 and the sediment, not the, the sediment of the entire
12 pond.

13 **DR. MADDELENA:** Right, the receiving
14 environment is the pond and the sediment is what you're
15 tracking and it's reaching steady state at very
16 different times so what's different about that sediment
17 that makes that happen?

18 **DR. HETRICK:** Well, first off going back
19 to Dr. Parker's presentation, each one of these
20 scenarios you see a New York grape scenario, a
21 California lettuce scenario and a Florida turf. Those
22 are three different PRZM scenarios so they have
23 different weather profiles that go along with those
24 scenarios and so that's probably one of the driving
25 forces as to why you see differences in the steady



1 state conditions as to what's occurring in the pond.

2 **DR. MADDALENA:** Okay, so, so then, so
3 that leads me to, I guess that makes my next question
4 not very important. It looks to me like the yellow
5 line, there's material going somewhere other than the
6 pond and I was curious if you had a mechanism to figure
7 that out but it may just be that the application is
8 much different. Is there a way to figure out why the
9 mass is there a, let me see. Can you link the mass
10 applied to the mass that ends up in the sediment, in
11 other words, and know what goes elsewhere?

12 **DR. HETRICK:** Yeah, you, you can do a
13 mass balance on using a PRZM exams model. Yeah, you
14 can do that.

15 **DR. RUHMAN:** The amount which is coming
16 into the Florida turf, the run off is very little, so
17 it takes less time, it takes less time to get to this
18 steady state. And what's coming from California
19 lettuce or what's coming from New York grapes, we, it's
20 more run off.

21 **DR. HETRICK:** I just want to add
22 something to this. In looking at these different
23 scenarios, I was glad to see that the turf had the
24 lowest runoff capacity compared to the other scenarios
25 because if it had a higher sediment load compared to



1 our, let's say our California lettuce or our New York
2 grapes or Mississippi cotton, I'd be a little concerned
3 and I would think that it wouldn't make sense, so at
4 least in a categorical kind of a trying to rank these
5 scenarios, it makes a little bit of sense that the turf
6 is the lowest run off scenario.

7 **DR. MADDALENA:** Yeah, it makes sense but
8 it also brings up the question where the material's
9 accumulating. If it's still persistent in the
10 environment, it's accumulating somewhere and you're
11 just not catching it in the pond.

12 **DR. HETRICK:** Well, it could be in the
13 field, too.

14 **DR. HEERINGA:** Dr. Simonich, we have a
15 number of questions, and we'll work our way through
16 them.

17 **DR. SIMONICH:** Staci Simonich, Oregon
18 State University. It seems from your presentation that
19 you're considering partitioning to the atmosphere
20 through the Henry's law constant but I don't see where
21 you're considering the atmospheric half life. For
22 example, it's not listed in the table for the four
23 pesticides.

24 **DR. RUHMAN:** Well, I don't want to say
25 everything, so I left something for my, my colleague.



1 Actually we do, we look at the half life. According to
2 national and international standards if it's more than
3 two day, this was, so we do.

4 **DR. HEERINGA:** Go to Dr. Schlenk and
5 then Dr. Norstrom.

6 **DR. SCHLENK:** Dan Schlenk, ACR. I had a
7 question to sort of follow up on Terry's and Jay's
8 question here on the organic, carbon organic matter
9 component. That's a set value, right, in the PRZM
10 exams model, that is not variable based on the
11 different locations, is that correct?

12 **DR. RUHMAN:** That's correct, yeah, along
13 with the sediment..

14 **DR. SCHLENK:** Is there....I'm just
15 curious is there any mechanism or thought in the future
16 to maybe better characterize that in terms of colloidal
17 size or UM content to in terms of refinement of the
18 model, is that something that's been looked at, or....

19 **DR. HETRICK:** I think if we get into
20 more sophisticated, particularly in the sediment
21 dynamics issues and looking at size fractions of sand
22 silt, clay and different particle sizes, I think we
23 might be able to handle that and I think Dr. Ambrose's
24 talk on WASP will give us some insight into that.

25 **DR. HEERINGA:** Thank you. Dr. Norstrom.



1 **DR. NORSTROM:** Yes, from my experience
2 doing some work around DDT, I know that anaerobic
3 degradation in soils can sometimes be quite important
4 especially if it's flooded. I wondered since you
5 apparently have divided the world up into sediments and
6 aerobic, and soils as aerobic whether you considered
7 adding an anaerobic component?

8 **DR. RUHMAN:** I don't know, I did not put
9 these, you know, the studies which we get is the one
10 which, but we do look at anaerobic system. We have the
11 guideline to do anaerobic soil, an anaerobic soil half
12 life and usually most, most of the cases is less, it's
13 more resistance.

14 In most of the cases which I looked at,
15 there's more resistance there than in aerobic systems
16 but the anaerobic aquatic gives you an idea also about
17 what it would be in an aerobic system soil, soil
18 system.

19 **DR. NORSTROM:** I would think it would be
20 more important in specific site situations where you
21 had flooded soils or very high moisture content.

22 **DR. RUHMAN:** This actually can be used
23 in, we can use the PRZM example, LOEL rises.

24 **DR. HETRICK:** I think when we're doing
25 our simulations, we're looking at conditions that are



1 agronomic conditions where you have crop growth and
2 you're looking at optimal crop growth. I would say
3 under anaerobic conditions that wouldn't be the case.
4 Not to discount the fact that that's not an important
5 thing to consider, but the bottom line is, is that
6 really we're looking at a situation where we're growing
7 crops on it and if redox potential gets too low, crops
8 don't survive.

9 **DR. HEERINGA:** Dr. Thibodeaux.

10 **DR. THIBODEAUX:** Thibodeaux, Louisiana
11 State University. Back to the water solubility
12 question, as I understand it there are really two
13 questions. One is you're finding exceedances in using
14 the exam PRZM model and you also, it's an analytical
15 problem as well in both lab and field?

16 **DR. RUHMAN:** Yep.

17 **DR. THIBODEAUX:** All of those?

18 **DR. HEERINGA:** Dr. Oris and then Dr.
19 Steenhuis?

20 **DR. ORIS:** Jim Oris, Miami University,
21 could you give me an idea of how you define persistent,
22 or is there a cut off or is it based on each individual
23 characteristic or each individual situation, how do you
24 define that?

25 **DR. RUHMAN:** I also am sorry because



1 some other people would say that but I'm going to say
2 it anyway. What we do, we look at lines of evidence
3 and actually we see, look at different lines of
4 evidence of what is happening in the different
5 compartments of the environment and the half life, and
6 we use national/international to give us standards
7 which is like over sixty days and over a few months,
8 but just for our problem formulation to look, see how
9 these compounds need some more concern about than other
10 components where you don't have that, but we do look at
11 it as a line of evidence for our analysis further. Get
12 more, more in depth analysis of the compound

13 **DR. ORIS:** Okay, so that would be
14 defined in the problem formulation for each individual
15 compound?

16 **DR. RUHMAN:** Right, right.

17 **DR. ORIS:** Can I ask one more question?

18 **DR. HETRICK:** May I add to that? One of
19 the concerns that we have is carry over from year to
20 year and that's a consideration and an important
21 consideration in looking at persistence.

22 **DR. ORIS:** So length of growing season
23 would be important?

24 **DR. HETRICK:** Yes.

25 **DR. ORIS:** The other question I had



1 regards to the use of values above solubility. I can
2 understand why you'd want to limit exposure levels to
3 solubility levels but why wouldn't you account for
4 residual pools of material in your estimation of
5 degradation rates, because as the compound degrades, it
6 may in it there's precipitate present or adsorbed
7 material present, wouldn't it desorb or resolubilize?

8 **DR. HETRICK:** You're absolutely
9 correct, and that, if you, that tracks right along with
10 the way we believe our conceptual model is. The
11 problem that we have is that we don't have that written
12 into our EXAMS nor do we have it written in the PRZM
13 into the code to take into account when you get an
14 exceedance of a solubility that you get a precipitate
15 form. Now there is a model that will be presented by,
16 called Agro today that will give you some insight that
17 where they have integrated that precipitation into the
18 model and do exactly as you suggested.

19 **DR. HEERINGA:** Entertain just a few more
20 questions, but Dr. Steenhuis has it.

21 **DR. STEENHUIS:** Tammo Steenhuis, you
22 say that the FD method over predicts? And in order, I
23 mean you choose a degradation rate in order to do this.
24 How did you choose the degradation rate? I mean how
25 are these degradation rates chosen?



1 **DR. RUHMAN:** We, we use the aerobic soil
2 data to generate these because the pesticides may be
3 going into the soil that probably a good thing to do.
4 But...

5 **DR. STEENHUIS:** Why can you not choose
6 the parameter in such a way that it doesn't over
7 predict? You know, you ask later a question about what
8 method is the best. It depends on how you choose the
9 parameters. And it may, I mean...

10 **DR. RUHMAN:** Choosing the method is not
11 only because it's a good method or a bad method, it's
12 also if we have the data to support what we're going to
13 do and most of the times we don't have data for the
14 degradates.

15 **DR. HETRICK:** I don't know if that was a
16 full answer, but I want to try to take a crack at that.
17 Number one, is we recognize that the formation decline
18 kinetics and that approach is the gold standard that we
19 should be striving for but we're realistic in the sense
20 that we don't always have the data to be able to do
21 that and since we don't have the data and we're under
22 time constraints where we can't do an extensive kinetic
23 analysis and sometimes doing a kinetic analysis on four
24 data points doesn't yield much.

25 So the bottom line is that we go through



1 other methods and the other methods, one would be the
2 total residue method and the other method would be the
3 residue summation method, and we're seeking comment as
4 to whether those approximations are reasonable
5 approximations for the formation decline method.

6 **DR. HEERINGA:** Dr. Delorme, and then I'd
7 like to move on.

8 **DR. DELORME:** Just following up on the
9 questions with respect to solubility, you indicated
10 that if you had, you would sometimes like to have data
11 for real water so if you have that versus the distilled
12 water, which one would you use?

13 **DR. RUHMAN:** I would be inclined to use
14 the other one. The real water.

15 **DR. DELORME:** Thank you.

16 **DR. RUHMAN:** But then also you know, the
17 real water is different from one place than...

18 **DR. HEERINGA:** Well, I would like to
19 thank Dr. Ruhman and Dr. Hendrick, Dr. Hetrick for
20 their contributions here. Panel members, I know there
21 are probably residual questions that you want to ask
22 and hopefully we'll have plenty of chance to ask them
23 and certainly before we move on to charge questions.
24 We'll have a general set of questions and I assume that
25 all the members of your staff, Dr. Brady, are going to



1 be here more or less for the duration so okay, at this
2 point in time, I think before we do have lunch, I want
3 to try to stay on at least the sequential schedule if
4 not the chronological schedule or time schedule for
5 this, and Dr. Brady, if you'd like to introduce the
6 next segment.

7 **DR. BRADY:** Thanks very much, Dr.
8 Heeringa. Next series of presentations which will
9 bridge the lunch gap will discuss sediment dynamics so
10 I'd just like to introduce them now and then we can
11 move right into them. Dr. Parker from the
12 Environmental Fate and Effects Division will discuss
13 our current methods in EFED of modeling soil and
14 sediment dynamics.

15 Following the lunch break, Dr. Donald
16 Mackay from the Canadian Environmental Modeling Center
17 at Trent University will provide an overview of the
18 AGRO model. Dr. Frank Gobas from the School of
19 Resource and Environmental Management at Simon Frasier
20 University will discuss environmental fate and food led
21 bio-cumulation models. I'd just like to note that Dr.
22 Mackay and, Drs. Mackay and Gobas are presenting
23 models developed independently from the EPA that were
24 used to evaluate a specific pesticide that was
25 undergoing an EPA risk assessment.



1 We in EPA looked at this modeling work,
2 compared the results to our own modeling efforts and
3 thought it would be worthwhile for Drs. Mackay and
4 Gobas to share their work with this panel. Robert
5 Ambrose from EPA's National Exposure Research Lab in
6 EPA's Office of Research and Development will discuss
7 sediment transport processes and finally to conclude,
8 Dr. Parker will return and present on simulating
9 sediment dynamics for pesticide aquatic eco-exposure
10 assessments, so, we'll start with Dr. Parker.

11 **DR. HEERINGA:** Thank you very much, Dr.
12 Brady. Dr. Parker, welcome back.

13 **DR. PARKER:** Well, thank you again.
14 This is a continuation of the modeling presentation
15 that we started earlier this morning concentrating
16 specifically on the sediment dynamics question. The
17 first question I suppose is why does EFED care about
18 eroding soil and sediment dynamics? I've highlighted
19 in red the portions of what we do that does apply
20 specifically to the sediment dynamics question.

21 The sediment moves from a tree in sight
22 to surface water in three main ways, dissolved in run
23 off water, adsorbed to eroding soil, entrained in that
24 same run off water and drifting in air during spray
25 application and from redeposition of volatilized



1 pesticides. I might say in that latter case that we do
2 simulate spray drift, we have specific methods for and
3 models for simulating spray drift and, but we do not
4 simulate redeposition of volatilized pesticides back
5 into any of the assessment water bodies.

6 Second point very relative to this SAP
7 is that many of the pesticides with PVT characteristics
8 are found largely in the adsorbed phase attached to
9 soil particles in the field or sediment particles in
10 the water body and so simulating soil pesticide
11 requires also accurately simulating eroding soil which
12 carries it from the field into that water body.

13 Each of our two main models simulate an
14 important soil sediment transport process. The
15 pesticide root zone model simulates the transport and
16 fate of pesticide adsorbed to eroding soil from the
17 treated field into the exposure assessment water body,
18 in this case our standard farm simulation pond.

19 Soil eroding from the treated field is
20 estimated by a modification of the universal soil loss
21 equation which is I think the basic work horse of a lot
22 of the edge of field models that simulate run off of
23 pesticide from treated fields and then simulates
24 pesticide degradation and movement within and between
25 the lateral and the benthic model compartments in the



1 EXAMS model.

2 For people that may not be familiar with
3 the universal soil loss equation, there are five or six
4 main parameters that, that are used in that
5 representation of soil erosion to estimate the total
6 amount that the universal soil loss equation as it was
7 originally formulated was based on around 10,000 plot
8 years of field data from a standard plot which was done
9 by the USDA Agricultural Research Service back in the,
10 starting in the '50s and continuing I think on into
11 the, on into the '70s, extensive data base of
12 information on soil erosion. The main parameters used
13 in estimating soil erosion are the erosivity of the
14 rain as it falls on the eroding soil. Erosivity is the
15 function of the energy of the rain and the intensity of
16 the rainfall events in terms of millimeters per hour.

17 Second factor is the erodability of the
18 soil itself which is a function of soil texture and the
19 organic matter content of the soil. The third factor
20 is the protection from the erosive impact provided by,
21 provided to soil by the growing crop, that is a
22 function that increases typically as the growing crop
23 provides more protection from the soil.

24 A cotton sprout provides very little
25 protection from raindrop impact but as that cotton crop



1 grows, you may have a leaf area index of three or four
2 and so by the time you have a full canopy of cotton in
3 the field there's very little raindrop impact on that
4 growing soil and the PRZM model does simulate that
5 growing crop. We have crop protection, the C values
6 for about every two weeks throughout the year
7 representing each of the particular crops.

8 Next factor is the slope and the slope
9 length of the specific site. That is obviously a site
10 specific parameter based on the inclination, the slope
11 of the field and the length of the slope that is
12 exposed to the run off of that. And the last factor is
13 the management practices implemented by the farmer or
14 grower which would include terraces, contour plowing,
15 reduced tillage, leaving proper residues in the field,
16 all of which have specific values for reducing soil
17 erosion.

18 The universal soil loss equation in its
19 original form was predicted an annual average value
20 over a, officially a 22 year, a 22 year simulation.
21 That 22 year average value was not particularly useful
22 in this kind of a model where you're needing to predict
23 soil erosion on a storm by storm basis as you have
24 rainfall events happening throughout the year and so
25 Dr. Jimmy Williams at Texas A&M has modified the



1 universal soil loss equation in several ways that can
2 be used in this kind of a representation.

3 We currently use a modification called
4 MUS. MUS is an acronym that has an acronym in it. MUS
5 is the muscle which is another of the modifications,
6 muscle for small water sheds and you can see that
7 equation there on the screen if you look at the last
8 few, where's my pointer, if you look at these last few
9 factors here, they are four or five of the main USOE
10 factors that are used in the USOE equation, and then
11 these first factors are the ones that make it available
12 on a daily basis for predicting soil erosion.

13 Within the EXAMS model partitioning two
14 benthic sediment is a function of the process that is
15 bringing the pesticide into the water body, pesticide,
16 dissolved pesticide in the run off water is
17 instantaneously partitioned between the water column
18 the suspended sediment, the suspended biota and the
19 benthic sediment based on the partition coefficient,
20 either the Kd or the organic carbon normalized Koc can
21 be used for that.

22 Adsorbed pesticide is a bit different.
23 In the run off water it is initially routed among the
24 four destinations: the water column, the suspended
25 sediment, suspended biota and benthic sediment based on



1 another's exam's parameter called the percent benthic
2 or PR ben. The developers of this model have given a
3 default value of point five and for all pesticides and
4 we haven't seen a reason to change that so that is our
5 default for the percent benthic for partitioning
6 routing of the adsorbed pesticide and then it is after
7 that is repartitioned based on the partition
8 coefficient.

9 Spray drift partitions instantaneously,
10 also the same as the dissolved portion between the
11 water column, suspended sediment, biota, and the
12 benthic sediment again completely based on the
13 partition co-efficient and then once that's happening,
14 all pesticide in the water body and in the benthic
15 sediment zone are continuously repartitioned based on
16 differential degradation within the water compartment
17 and the sediment compartment.

18 So for example, if the pesticide in the
19 sediment department, sediment compartment is degrading
20 much more quickly then you would have a net movement
21 from the water column to the sediment in order to
22 maintain that, the initial Koc value.

23 Looking at enrichment ratios for organic
24 matter and soil, I believe someone touched on earlier.
25 Due to the large surface area of the fines, the silt



1 and clay size fraction of the soil, these size
2 fractions differentially sorb more pesticide than the
3 larger size fractions.

4 Soil erosion also selectively erodes the
5 finer soil particles and the organic matter so you have
6 both of those happening at the same time, selective
7 partition to the finer particles and organic matter and
8 selective erosion of those same particles and so there
9 is an enrichment process going on in between the field
10 and the water body.

11 PRZM does use an organic carbon
12 enrichment process to account for enrichment of the
13 organic matter in the soil but does not have a sediment
14 enrichment process to select for the finer erosion
15 particles in the eroding soil. This is an important
16 slide, this and the next one are two representations of
17 the same scheme. If you look at the PRZM box on the OP
18 standard scenarios on the upper left, you see that
19 pesticide in run off goes directly into the exam's EFED
20 standard pond.

21 The pesticide sorbed to eroding soil,
22 the same goes directly to the standard pond but the
23 eroded soil, which is also predicted by the mass of
24 eroded soil which is also predicted by the PRZM program
25 and the depth of run off water, which I guess becomes a



1 volume by the time you know the area, are not read into
2 the EXAMS pond so you, we do not have an accumulation
3 of sediment from PRZM going into the exam's pond and we
4 do not have eroded soil coming from PRZM going into the
5 exam's pond.

6 This is a verbal representation of the
7 same thing. There are four, well, there are many,
8 many parameters that are estimated by PRZM but these
9 four are estimated and go into the PRZM/ EXAMS transfer
10 file but only the bottom two that the pesticide masses
11 are the ones that actually, actually enter into EXAMS
12 and so many of the questions that we are asking you to
13 take a look at are based on this specific concept that
14 the pesticide mass is moving into the pond but the mass
15 of eroded soil and the volume of run off water are not
16 routed into that pond.

17 The EXAMS, sediment dynamics EXAMS uses
18 a lumped process to represent pesticide mixing between
19 the water column and the benthic zone. Many models
20 specifically represent individual processes.

21 The EXAMS has looked at, from
22 discussions with the developers of EXAMS has looked at
23 those processes and decided that this single lumped
24 process is an adequate representation of that total
25 process and so that is the representation which is in



1 the EXAMS model.

2 That mass transfer coefficient
3 represents sediment settling and resuspension. That
4 represents any wave action within the pond that might
5 cause resuspension or mixing within the bottom
6 sediments, bioturbation caused by either lateral or
7 benthic fauna that may be living in the pond, ranging
8 from bacteria to muskrats and mink I suppose, and then
9 all of these are represented by this mass transfer
10 coefficient with the assistance of the percent benthic
11 or PR ben parameter.

12 This is a general representation of the
13 sediment dynamics processes which I think could be said
14 to represent what happens in a large number of models
15 that deal with sediment dynamics. You can look at
16 these a little more closely at your leisure after the
17 presentation. The area in the oval toward the bottom
18 of this representation looks at the processes that are
19 represented by our lumped mass transfer coefficient
20 rather than representing each of those individually and
21 then does not actually represent....does not actually
22 represent variable.

23 From your white paper, if you look in
24 chapter four which presents most of this information,
25 there are two equations that represent what's actually



1 happening with this mass transfer coefficient. This
2 equation simply states that the change in the poor
3 water concentration as a function of time is, can be
4 expressed as the mass transfer coefficient times the
5 difference in concentration between the benthic poor
6 water concentration which is what's being predicted and
7 the concentration, the aqueous concentration in the
8 water column itself.

9 It should be noted in this case that the
10 aqueous concentrations in this, in this equation are
11 only used as a surrogate Dragon force and do not imply
12 aqueous only transport from the water column to the
13 benthic region. This equation then represents all of
14 the causes of pesticide mixing between the water column
15 and the benthic zones.

16 This is the way that this equation is
17 implemented within the EXAMS program. Again, you can
18 see, you can get more information in your white paper
19 when you're looking at chapter four. The K transfer is
20 the geometry independent water column to benthic mass
21 transfer coefficient, which has a fixed value which you
22 can see there on the right and then that's multiplied
23 by the surface area of the boundary between the water
24 column and the benthic compartment which is the same as
25 our one hector pod so that's ten thousand square meters



1 divided by the total volume of that benthic compartment
2 which again is that ten thousand square meters times
3 the five centimeter depth of sediment, giving us five
4 hundred cubic meters of sediment to which all of the
5 chemical is bound.

6 The percent benthic in EXAMS is the
7 initial routing parameter, as I mentioned before, for
8 incoming sorbed particles. What it actually represents
9 is the routing of the labile portion of the field
10 sorbed pesticide, that which comes off the field
11 already sorbed as it mixes instantaneously into the
12 water column and suspended sediments and the benthic
13 sediment.

14 The EFED default PR ben value, as I
15 pointed out, is zero point five for all pesticides
16 meaning that fifty percent is initially routed,
17 initially meaning day one, routed into the water
18 column, and fifty percent is initially routed into the
19 benthic sediments and suspended sediments and biota and
20 then after that they are repartitioned, continuously
21 repartitioned based on the sediment, based on the
22 repartitioning on the partitioning coefficients.

23 The EXAMS manual describes a method to
24 simulate permanent pesticide burial using a first order
25 rate constant, but the manual also advises that for



1 evaluation and screening purposes, it seems unwise to
2 suppose that buried synthetic chemicals will never
3 reappear.

4 EFED generally agrees with that
5 cautionary advice and currently does not simulate
6 buried pesticide. However, as an example specifically
7 for this presentation to the panel, we did use the
8 first order burial method as described in the EXAMS
9 manual and using our example chemicals three and four
10 to see what impact, see what impact that would meant,
11 that would mean for those, for those chemicals and the
12 next couple of slides you can see the results.

13 The Mississippi cotton cropping scenario
14 is a scenario that produces a lot of sediment, and so
15 we used that as sort of a high exposure case for
16 looking at that. Here we, we compared the non-burial
17 simulation with the burial simulation and looked at the
18 percent reduction as the function of looking at that
19 burial process.

20 The top row there looks at the water
21 column concentration, that difference. The next row
22 looks at the poor water concentration difference and
23 the bottom row looks at the sediment concentration
24 difference looking at this first order rate burial
25 process for pesticide three, also looking at pesticide

1 four and rather than forcing you to look at a lot of
2 numbers and trying to figure out what's what, I
3 actually put them on a single slide here so you can
4 look at what the impact of that burial process does.

5 And as I say, this is not something that
6 we normally do as part of our risk assessment process,
7 but it came up in looking at how we simulate these
8 specific pesticides where you do have a large amount of
9 it that is sorbed to the pesticide, we looked at how
10 that process might be represented within EXAMS if we
11 were to do that and here you can see that the results
12 that are from your, from the two previous, two previous
13 slides summarized so you can see it.

14 I think the reason that the numbers are
15 so much higher, reductions are so much higher in
16 pesticide four is that the Koc of that particular
17 compound is higher than the Koc of pesticide three.

18 So summarizing just this particular
19 presentation, EFED uses the PRZM EXAMS model to
20 estimate pesticide concentrations for ecological
21 exposure assessments. PRZM uses the MUS modification of
22 the universal soil loss equation to estimate soil
23 erosion from the field into the water body.

24 PRZM simulates organic matter enrichment
25 but not fine sediment enrichment in that process.



1 EXAMS uses a lumped mass transfer coefficient process
2 to represent all mixing between the lateral and benthic
3 model compartments and EFED does not currently use the
4 first order process available in EXAMS to simulate
5 pesticide burial.

6 **DR. HEERINGA:** Thank you again, Dr.
7 Parker, and what I'd like to do is entertain questions
8 for about 15 or 20 minutes and then we'll break for
9 lunch. Dr. Thibodeaux.

10 **DR. THIBODEAUX:** Thibodeaux, Louisiana
11 State University. From the water shed to the pond you
12 said that particles, soil being eroded from the water
13 shed were directed away from the pond, is that correct?

14 **DR. PARKER:** No, I may have said that,
15 but I, they're, they're, it's actually the eroding soil
16 is carried by the run off water from the water shed
17 into the pond.

18 **DR. THIBODEAUX:** Could you go back to
19 that slide?

20 **DR. PARKER:** I can. It is number...

21 **DR. HEERINGA:** Is it true that once it
22 hits the pond it disappears though because it does not
23 accumulate?

24 **DR. THIBODEAUX:** Nine, Number 9.

25 **DR. PARKER:** Which, which slide is that?



1 **DR. THIBODEAUX:** Number 9.

2 **DR. PARKER:** Slide Number 9?

3 **DR. THIBODEAUX:** Yeah, I'm looking at
4 both of those dotted arrows, the one that says eroded
5 soil and run off water...

6 **DR. PARKER:** Right, they, they are not
7 used by the EXAMS program. They are in the, they could
8 be, but we don't currently use them. The run off water
9 and the eroding soil which are predicted by the PRZM
10 program are not actually utilized in the EXAMS program.

11 It's only the sediment bound portion of
12 the pesticide and the dissolved portion of the
13 pesticide so it's just the two pesticide masses or
14 three if you include spray drift, that actually enter
15 the EXAMS pond and we don't actually simulate the soil
16 as it flows into the pond or the volume of water as it
17 comes off the water shed so the soil and the water are
18 not simulated by EXAMS but the pesticide dissolved and
19 sorbed to both are simulated by EXAMS.

20 **DR. THIBODEAUX:** So a follow up
21 question. On those two dotted arrows that go to the
22 left, do they contain any of the pesticide?

23 **DR. PARKER:** No.

24 **DR. THIBODEAUX:** Thank you.

25 **DR. PARKER:** All of the pesticide goes



1 to the pond and the sediment and the water are ignored
2 by EXAMS.

3 **DR. HEERINGA:** Yes, Dr. Mehta.

4 **DR. MEHTA:** Yeah, but that means that
5 the burial effect is not simulated...

6 **DR. PARKER:** Correct, correct, we don't
7 simulate burial, but that's one question that we're
8 looking at.

9 **DR. HEERINGA:** Dr. Portier.

10 **DR. PORTIER:** Can you give me some idea
11 of how sensitive the model is to the PR Ben? You chose
12 that 50 percent split. I mean, if you're moving that a
13 little bit does the model really react strongly to
14 that?

15 **DR. PARKER:** The peak concentration on
16 the first day reacts quite vigorously to that as you
17 can imagine, because you're putting, if you're putting
18 90 percent of, if you assume that 90 percent of the
19 pesticide is labile is going instantaneously into the
20 sediment, then that peak concentration in the sediment
21 is much higher, the peak concentration in the water is
22 much lower. But after that initial routing, it's the
23 Koc that then redistributes them based on that
24 particular parameter. So for a sixty day simulation it
25 really doesn't make much difference but if you're



1 concentrating on that peak value it makes a big, it can
2 make a big difference.

3 **DR. HEERINGA:** Dr. Schlenk.

4 **DR. SCHLENK:** Dan Schlenk, UC

5 Riverside. Yeah, just to follow up on a question I
6 asked in the earlier presentation, maybe you're trying
7 to say it here and as far as PRZM simulates organic
8 matter enrichment but not fine sediment enrichment,
9 does that mean again the DOC that's in the pond is not
10 being parameterized in terms of the model or is that
11 even an issue, is that even considered in the model.
12 Or are you just using just a total mass or
13 concentration of DOC in the water at that particular
14 point?

15 **DR PARKER:** The DOC does change with
16 the incoming pesticide...

17 **DR. SCHLENK:** Okay, so like for example,
18 so you're not using the eroded soil component, I see
19 that, but in the water itself is there any size class
20 differentiation of that DOC in the water column at
21 all?

22 **DR. PARKER:** No.

23 **DR. SCHLENK:** In the inner model?

24 **DR. PARKER:** Correct.

25 **DR. SCHLENK:** Is it possible to do that



1 in EXAMS?

2 **DR. PARKER:** EXAMS uses the three size
3 fractions of the soil to based on some Wells and
4 Bracken-Seeks regression equations to estimate both
5 density and water holding capacity and so those are
6 available to us, but the erosion process itself doesn't
7 differentiate between them so we really don't know
8 which size classes are injuring. We know the texture
9 of the soil, the field soil, but beyond that, we don't
10 have that information.

11 **DR. SCHLENK:** One final question, is
12 there any way to estimate colloidal impact in terms of
13 the water column?

14 **DR. PARKER:** No.

15 **DR. HEERINGA:** Dr. Delorme and Dr. Gan.

16 **DR. DELORME:** Just out of curi...Peter
17 DeLorme from Health Canada. Just out of curiosity,
18 where does the assumption of a first order process for
19 burial come from? Is that based in science anywhere or
20 is that just something somebody, one of the developers
21 pulled out of the air? I know you're not using it,
22 but I'm just curious as to where that assumption might
23 have come from.

24 **DR. PARKER:** I'm guessing that Larry
25 Burns when he was very active with the regulatory



1 community and with us and at some point he did some
2 playing with that to see if he could simulate burial.
3 He, as you know, he passed away last November and so I
4 can't ask him that anymore, but I'm guessing that came
5 from Larry Burns. I don't know that there's more
6 science behind it than...

7 **DR. DELORME:** So you don't know if it's
8 based on any empirical data of any sort?

9 **DR. PARKER:** No.

10 **DR. DELORME:** And I have a...what was
11 my second question? I can't remember.

12 **DR. HEERINGA:** You can come back to it.
13 Dr. Gan?

14 **DR. GAN:** Just a question on your
15 enrichment ratio of soil to organic matter, does that
16 vary from soil to soil or do you have a fixed
17 relationship and how important you think that will
18 affect the ultimate fate and transport?

19 **DR. PARKER:** The organic matter is,
20 comes from the data base of soil properties that we use
21 for developing the, developing the scenarios and so it
22 does, that is a function of the original organic matter
23 in the soil and I don't know what the impact of that
24 is, we've never looked at what the impact of that might
25 be. I mean it's something we could do, but we have, up



1 to this point we have not...

2 **DR. GAN:** So does the current PRZM
3 address that process?

4 **DR. PARKER:** Yes, but not the, but not
5 the sediment process.

6 **DR. HEERINGA:** Dr. Hickie and Dr.
7 Doucette?

8 **DR. HICKIE:** Agricultural ponds are
9 often enriched in nutrients from fertilizer use, does
10 EXAMS take that into account in any way in terms of
11 production of algae within the ponds?

12 **DR. PARKER:** No, there is a fixed value
13 for the algae content of the pond. I think if you
14 listen to Bob Ambrose's presentation this afternoon,
15 they actually predict changing algal populations based
16 on water temperature and solar radiation but it's a
17 fixed value in our, in our pond.

18 **DR. HEERINGA:** Dr. Doucette.

19 **DR. DOUCETTE:** Bill Doucette. Have you
20 considered looking at other ways of normalizing
21 absorption other than just organic carbon, especially
22 for certain classes of pesticides or types of
23 pesticides where organic carbons may not be the
24 dominant absorptive site?

25 **DR. PARKER:** If we had the data, we

1 would probably use specific surface as a, at least as
2 an alternative for beaching the soils but that's not a
3 parameter that we get from, as a potential input so the
4 only inputs that the model accepts are the organic
5 carbon normalized version of the Kd itself.

6 **DR. HEERINGA:** Peter, did you think of
7 your second question?.

8 **DR. DELORME:** Yeah, Peter DeLorme. It
9 came back to me. You used the high or a high erosion
10 scenario when you did your burial so given that for one
11 of the pesticides is around 20 percent, do you guys
12 have an idea of where you would bring in burial? Like
13 do you have any idea of criteria because if you look at
14 this if it's a low erosion scenario or a medium, it may
15 not have any effect. I'm just wondering how could you
16 factor that into your sort of risk assessment or your
17 tiered E, or have you given it much thought?

18 **DR. PARKER:** Well, with these high Koc
19 compounds are something. I mean, we've looked at some
20 prior neotroids, but are something that we weren't
21 really dealing with in the beginning so that's
22 something we want to look at. We're actually, in
23 having a number of these compounds that we're starting
24 to look at, we're looking at the parameterization for
25 our early soil parameters to see if they are



1 appropriately conservative to represent this class of
2 compounds.

3 **DR. HEERINGA:** Okay, Dr. Parker, I'd
4 like to thank you again for the presentation and
5 addressing the questions. Panel members will have a
6 chance to revisit questions to all of the presenters
7 before we enter the charge questions. It's time I
8 think we've all earned lunch, and I'm showing just a
9 little bit before 12:25. Let's say we'll reconvene at
10 1:30 instead of 1:15 as shown on the agenda, so 1:30
11 and see everybody this afternoon.

12 **(WHEREUPON,** a recess was taken for lunch.)

13 **DR. HEERINGA:** Okay, let's find our
14 seats, and we'll get underway. Thank you, everyone,
15 and welcome back to the first day of our multi-day
16 meeting of the FIFRA Science Advisory Panel on the
17 topic of Selected Issues Associated with the Risk
18 Assessment Process for Pesticides with Persistent,
19 Bioaccumulative, and Toxic Characteristics.

20 Through the morning session, we heard a
21 series of presentations linked to the white paper that
22 was prepared by the Patent Effects Division, and at
23 this point, before we move on with a...a presentation
24 by Dr. Mackay, I would like to turn it back to Dr.
25 Parker for just a few points of clarification,



1 follow-up on this morning's discussion. Dr. Parker?

2 **DR. PARKER:** Thank you. Over the lunch
3 hour, I received a little bit more information from a
4 couple of my colleagues and answers to a couple of the
5 questions this morning. In terms of the question on
6 the first order...order burial rate using the EXAMS.
7 EXAMS mathematically is a stirred reactor, behaves that
8 way, and so the...the first order process lays down the
9 sediment continuously, and as it enters the pond, it
10 continuously...if it enters the pond continuously, it
11 is automatically deposited continuously.

12 And the way that...the way that
13 half-life value was calculated was to take the entire
14 mass of sediment in each of the rainfall events over
15 the 30-year period and divide that continuously on
16 a...a moment-by-moment basis to...to develop that first
17 order process which then lays down the...lays down the
18 sediment in the pond.

19 On the question of organic matter in the
20 soils and in the pond, the organic matter in the PRZM
21 field is taken from the USDA data base which is the
22 official record of that particular soil as it's used
23 in...in the PRZM scenario, and in the EXAMS the...the
24 DOC is fixed at 5 parts per million for all sites and
25 all simulations. That doesn't...that doesn't vary.



1 It's not...that value is not a function of the organic
2 matter in the soil.

3 And EXAMS has the capability of running
4 flow through it. We just don't...don't choose to...to
5 do that through the eco assessments. We do, as a
6 matter of fact, run flow through...through the index
7 reservoir for drinking water, human health drinking
8 water assessments, because the level of concern in this
9 for a bigger watershed is less. And so, we can still
10 be conservative by running flow through that, but we
11 don't use that for...for ecological risk assessments.

12 And we do have...we are working on
13 developing a variable volume pond that is quite similar
14 to the EXAMS pond except that it has the capability for
15 the water level to raise and lower with evaporation and
16 inflow, and that model will accept sediment on a
17 day-by-day basis as it's...as it's produced from the
18 flow.

19 Did I catch everybody's points? Okay,
20 thank you.

21 **DR. HEERINGA:** Thank you very much.
22 That's very helpful.

23 Before I move on, just one quick
24 administrative note. With...with Myrta Christian's
25 permission, I have a teaching obligation at the



1 University of Maryland early this evening, late
2 afternoon, so I'm going to be stepping out part way
3 through the afternoon session, and Dr. Bucher is going
4 to be taking the chair for the balance of the
5 afternoon. I'll be back tomorrow morning. So, I'm not
6 running out. If you want to know where I'm going,
7 there's that piece of information.

8 Okay, at this point in time, I'd like to
9 recognize Donald Mackay. Is it Mackay? I was told it
10 was Mackay...who is with the Canadian Environmental
11 Modeling Center at Trent University, for an overview of
12 the AGRO model for pesticides. Dr. Mackay?

13 **DR. MACKAY:** Thank you very much. I
14 appreciate the opportunity to share some thoughts with
15 you on the AGRO model. I will be talking about the
16 water quality aspects, and my colleague, Frank Gobas'
17 assignment will be looking at the food web.

18 A few comments. I...I was very much
19 impressed by the white paper that was produced. It's a
20 formidable document, and it certainly covers all the
21 issues, and I compliment the EPA staff for producing
22 it.

23 And I was equally impressed with the
24 qualifications of the analysts. So, I think it's going
25 to be a very useful event.



1 The focus here is on models for
2 pesticides which are more PDT like in properties. I'm
3 going to outline the evolution and the performance of
4 the AGRO model and in doing so compare with EXAMS and
5 then have some concluding thoughts or prejudices on
6 desirable model features for your consideration.

7 Frank and I were given a task to develop
8 a dynamic water quality aquatic food web bio-cumulation
9 model for chemical III, and as you heard this morning,
10 EFED defines a 10 hector field, a 1 hector pond, 2
11 meters deep with input by spray drift and soil erosion.
12 We selected the QWASI, that's quantity of water-air
13 sediment interaction model for the water and the
14 IMA-Gobas model as the food web model, and we modified
15 them for this purpose.

16 Our aim was to produce a realistic
17 model, including all the relevant processes, and
18 especially focusing on more hydrophobic substances.

19 A few words on hydrophobicity, because
20 it's a very important concept here. To a physical
21 chemist, hydrophobicity is fundamentally determined by
22 the activity coefficient of the substance in water
23 which is a measure of the force with which the water
24 matrix is attempting to expel the...the solute
25 molecule. It's not a very happy quantity to use



1 directly. You can use water solubility, and for a
2 liquid solute, water solubility is essentially the
3 reciprocal of the activity coefficient. So, it's
4 hydrophobic substances, some very high activity
5 coefficients and very low water solubilities.

6 The best metric is octanal water
7 partition coefficient which is essentially the ratio of
8 the activity coefficient in water to activity
9 coefficient in octanal, and because activity
10 coefficients in octanal are generally quite constant,
11 range from about 2 to 10, it's a very good indicator of
12 the hydrophobicity, and it's generally accepted as
13 such, and it is used, for example, to calculate the
14 organic carbon water partition coefficient, and TOC is
15 generally about a third of KOW. KOW is also important,
16 because it's usually equated to the lipid water
17 partition coefficient, and it is lipid water partition
18 coefficient that is the major determinant of
19 bio-cumulation.

20 The question then arises, is there a
21 bright line cutoff for hydrophobicity versus
22 non-hydrophobicity? And the short answer is no.

23 About a log KOW of 4, you're beginning
24 to see hydrophobic...hydrophobic character. Above 6,
25 it is strongly hydrophobic, but so 5 is sort of a



1 middle of the road number, and it, by coincidence, at a
2 log KOW of 5, partitioning in a pond between the
3 dissolved phase and the particulate phase is about
4 equal, so that above 5, it is very important to include
5 the chemical sorbed to water. And on page 82 of the
6 white paper, it gives a nice example of this.

7 Hydrophobicity also affects the
8 bioavailable fraction in water by partitioning not only
9 the particles but the dissolved organic carbon,
10 dissolved organic matter. It also controls the rates
11 of respiratory and dietary uptake by fish, and roughly
12 speaking, at a log KOW of 5, there are equal weights of
13 uptake from respiration and dietary uptake. When you
14 go to 6, it's about 90 percent from diet.

15 So, as you go to more hydrophobic
16 substances, bioconcentration, that's uptake from water
17 becomes less important. Frank KOW substances can also
18 have very slow uptake and clearance times, long
19 half-lives. And roughly speaking, at a log KOW of
20 about 5, it takes about a week or so or maybe two weeks
21 for the...the fish to take up the material, half of
22 that is taken up by respiration.

23 So, 5 is sort of a good middle of the
24 road number.

25 Just a little bit of history. I was



1 privileged in the 1970s to work with George Bachman and
2 his colleagues at Athens, and he and his colleagues put
3 together the EXAMS model. My particular responsibility
4 was volatilization in that model. So I was completely
5 familiar with EXAMS at that time, and essentially, I
6 copied it and converted it into a fugacity format, and
7 that became the QUASI model. So QUASI is really now
8 sort of son of EXAMS, but in doing so, I introduced two
9 major changes which I'll mention later.

10 So, the AGRO model is...there is the
11 QUASI model. It leads into a food web model and into
12 other deliberations, and the difference from the
13 existing EFED model which we heard about this morning
14 is that EXAMS replaces it. So, that is the AGRO shell
15 and the models contained in it.

16 So, this is a picture of the QUASI
17 model. There are a number of arrows in this, and each
18 one has a D against it. That represents a process.
19 There's an equation for that process. There are
20 parameters go into it, and I draw your attention to
21 four arrows between the water column and the surface
22 sediment.

23 There is deposition of particles. There
24 is resuspension of particles. There is diffusion from
25 water to sediment or water and diffusion from sediment



1 or water to the water column. And as Ron Parker
2 described this morning, these four processes are all
3 lumped in EXAMS, and I felt uncomfortable about that,
4 and the reason was that when you go to very hydrophobic
5 substances, the sediment deposition and resuspension
6 processes become very much more important than the
7 diffusion processes. In fact, you get to a KOW of 6,
8 you can almost ignore sediment in water diffusion.

9 I also put in burial as a process,
10 because I was mainly interested in having a model which
11 would simulate conditions in the Great Lakes or areas
12 of concern within the Great Lakes. But it has all the
13 usual processes of inflow, exchange with the
14 atmosphere...it also has deposition from the atmosphere
15 which is irrelevant here...outflow, reaction in water,
16 and reaction in sediment.

17 A key modeling principle, I think, is
18 that if a process occurs naturally that affects more
19 than a few percent of the substance's fate, you must
20 include it in the model, but the relative importance of
21 all these processes depends on the chemical's half-life
22 and on its hydrophobicity and on its volatility. So, a
23 fate model should be capable of treating a wide range
24 of chemicals. At least, a user should be aware of any
25 limitations that occur, and this is particularly the



1 case with respect to hydrophobicity.

2 So, that's a list of all the processes
3 which are included in the QUASI model. They are all
4 treated as separate processes with a separate equation.

5 The model also includes partitioning
6 between water and suspended matter and between core
7 water and sediment. It can include the influence of
8 dissolved organic matter, and it can include
9 partitioning to microorganisms in fish and microphytes,
10 as Frank will talk about.

11 It does not treat mixing in the water
12 column. It treats the water column as well mixed,
13 although there are directions which stratify the water
14 column. And bioturbation can be included by increasing
15 the diffusivity between the sediment and the water.

16 So, how do EXAMS and QUASI compare?
17 Well, they both have inflow and outflow of
18 volatilization. They both have degrading reactions.
19 EXAMS does a much better job of treating reaction in
20 that it will help the user obtain, for example,
21 photolysis half-life, QUASI just asks for a half-life,
22 and how you get it is your own business. EXAMS doesn't
23 include sediment burial, QUASI does. And EXAMS, as Ron
24 Parker explained, treats sediment water exchange as a
25 bulk dispersive diffusive process and QUASI, there are



1 four separate processes.

2 Some of the key parameters in the model,
3 Koc, organic carbon partition coefficient. This is
4 usually measured rather than derived from KOW, and the
5 way in which it is measured normally is to measure Kd,
6 that is, the whole solid to water partition
7 coefficient, and then that is divided by the organic
8 carbon content. So, any sorption to mineral matter is
9 actually automatically included, and it's wrongly but
10 actually attributed to organic carbon partitioning.

11 The degradation half-lives are usually
12 measured. You can get field to pond transport from
13 PRZM, which is an excellent model, and it is the
14 deposition resuspension steps that are critical, and
15 these deposition rates can be generic constant values,
16 or they can be values based on local measurements or
17 other sources as I'll discuss.

18 Sediment in water transport, I was going
19 to present some material, and then, to my horror, I
20 discovered that Willie Lick and Louis Thibodeaux were
21 on this panel, and I know you're all putting together
22 your Christmas wish lists of books to buy, so Willie
23 Lick's book on sediment transport should be at the top
24 of the list, followed by Louis Thibodeaux's
25 Environmental Chemodynamics.



1 So, the actors...

2 **DR. THIBODEAUX:** Thanks for the plug.

3 **DR. MACKAY:** The invoice is in the mail.

4 All I'll say is this, and I bow to these guys' greater
5 knowledge of this. The deposition and resuspension
6 rates depend on the size of the pond, the fetch, any
7 flow rates of water, solids characteristic, wind speed,
8 duration, depth, shielding, microphytes, benthic
9 organisms, and so on. There has been an enormous
10 amount of excellent work done on resuspension
11 deposition in lakes like Lake Erie and estuaries, and
12 Willie Lick has been the guru of this for many years.

13 We're dealing with relatively small
14 ponds, and I think applying these lake correlations to
15 ponds is not wise, because they're unlikely to be
16 reliable. Functionally, for small ponds, the
17 measurements are easy. The pond is accessible, and you
18 can make deposition resuspension measurement. So, that
19 is, I think, the ideal source of data for those
20 purposes.

21 And one point is and it came up this
22 morning in Mohammed Ruhman's discussion, if you have a
23 pond, it's essential that the model have some mechanism
24 for loss of chemical, because if there isn't, the
25 chemical will build up and build up indefinitely. For



1 example, if you apply copper ion as a pesticide, which
2 I hope you never do, it will just runoff into the pond
3 and build up until you have a deep blue pond of
4 saturated copper ion. You must have exit processes or
5 the model gets distorted results.

6 So, we went through essentially three
7 volumes...three versions of the AGRO model. The first
8 one, we had an integrative chemical, either steady
9 state, X grams per hour, or a pulse of Y grams or
10 repeated pulses, and we use this to validate that a
11 mass balance was, in fact, achieved, and it worked.

12 We put in constant on what we thought
13 was reasonable but user selectable values of the pond
14 parameters, the transport parameters such as
15 resuspension deposition rates, and you get tabular and
16 graphical output, and Frank used that to calculate
17 organism concentrations.

18 We discovered that the solubility in
19 water may be exceeded, and this is a...a sketch of what
20 you might get. The concentration in water will rise
21 rapidly, usually as a result of spray drift, and then
22 it falls fairly rapidly over a day or two. This is the
23 dissipation process that Mohammed was talking about.
24 And, of course, there is uptake and an increase in
25 concentration in the sediment.



1 And it is very easy to exceed the
2 solubility limit, especially with spray drift, because
3 the solubility of these substances is in the microgram
4 per liter range, and that really worried us. Oh, I'm
5 going to skip that.

6 What is it that causes all the
7 solubility? Well, it's hydrophobicity, a high log KOW,
8 and it's also a high melting point, especially if the
9 molecule has molecular symmetry. I mean,
10 x-chlorobenzene is the classic example. It's something
11 that's going to be a much more frequent issue with
12 hydrophobic and high molecular weight pesticides. It's
13 a problem that I think has to be addressed.

14 The white paper and this morning, they
15 have strategies on how to address this problem. Exam
16 allows the solubility to increase, and that kind of
17 makes the problem go away. From a physical chemistry
18 point of view, that's a little bit naughty, but it
19 works.

20 AGRO goes through the process of
21 allowing for a precipitate reservoir to form which can
22 dissolve once the concentration in water falls below
23 the solubility limit, and that, I think, is more
24 rigorous. The precipitate just sits there in water.
25 It doesn't deposit. It doesn't flow out. It doesn't



1 react. Nothing happens to it.

2 It's not entirely a happy assumption,
3 but it kind of works. So, that's what AGRO does.

4 So, what you get with AGRO is a picture
5 of spikes of concentration corresponding to spray drift
6 from an application followed by input by runoff or
7 erosion from the field, and you have highly variable
8 water concentration and buildup in the sediment which
9 eventually decays, and over a year or two, this is
10 repeated. You can look at it in terms of fugacity as
11 well, and you get essentially the same picture.

12 That concentration pulse propagates into
13 the food web, but it is very highly damped, and the
14 reason for that is the pulse in the water column lasts
15 a couple of days. The uptake time of the fish is
16 measured in weeks. So, the fish never get close to the
17 equilibrium value corresponding to the maximum
18 concentration in the water column.

19 So, the fast sediment water transport
20 reduces the high concentration. It's of short
21 duration, and although the pulse propagates into the
22 food web, the organism functionally is relatively slow
23 to take it up compared to the pulse duration, so it is
24 absolutely essential to apply a dynamic model. The
25 worst thing you can do is take a peak concentration and



1 then multiply it by a steady state bioconcentration or
2 bio-cumulation factor.

3 This, actually, is the old canary in the
4 coal mine philosophy. Steady state models are useful
5 in places like the Great Lakes where you have chronic
6 conditions, but for agricultural/agrochemical
7 processes, you really need a dynamic version of both
8 the water quality model and the food web model, and
9 that's what AGRO seeks to do.

10 You can put in repeated pulses, and over
11 a long period of time, you get results that are close
12 to the steady state value, and as Frank will explain,
13 you can get good agreement with mesocosm registration
14 data. And the short-term water concentration is
15 controlled largely by sediment deposition rather than
16 reaction. So, measuring that dissipation rate gives
17 you that rate, but it's difficult to get a reaction
18 rate out of it, and I'll return to this later.

19 The reason is this. And for those of
20 you who like mathematics, this is my attempt to do it.
21 The differential equation for the water concentration
22 is that, and there's a whole group of five processes
23 which are reducing the water column concentration.
24 There is flow, there is volatilization, there is
25 deposition, there is diffusion, and there is reaction.



1 And the total might be a number like 120 units. It
2 don't matter. Of that, perhaps 100 is deposition.

3 So, to try and extract an accurate value
4 of 5 from that data is basically impossible, and this
5 is just a restatement of the message that Dr. Ruhman
6 gave you this morning.

7 AGRO then move to version 2 in which we
8 had input from PRZM, and then version 3 in which input
9 was again from PRZM, but particles of solids flowing
10 from the field were now included in the deposition
11 process. And this was discussed this morning.

12 So, that arrow in Ron Parker's diagram
13 which went off to the left in...in AGRO, goes right
14 into the pond. And this is important, because you
15 increase the rate of deposition, and that reduces the
16 concentration in the water column, reduces the
17 bioavailability of the chemical, and it reduces the
18 concentration.

19 And burial is now important. Because
20 you're putting more particles into the water, they've
21 got to go somewhere. They go to the sediment, and this
22 results in burial. So, I'm convinced that it's
23 important to include burial.

24 In the white paper, page 91, there's an
25 example, and Ron Parker described it this morning, of a

1 burial half-life of 222 days. That's a long time, it's
2 a slow process, but what that means is every year,
3 virtually all that sediment is buried and replaced.
4 So, over 30 years, in fact, the pond fills up
5 completely, and you no longer have a pond. So,
6 although it's a slow process, it is very important,
7 especially if the degradation rate in the sediment is
8 very slow.

9 So, for accurate simulation of pond
10 dynamics, it is essential to include burial, in my
11 opinion, and I'm going to skip that.

12 So, ideally, I think, the model that
13 should be used should simulate the real world as
14 closely as possible. If you can simulate it, it is
15 capable of validation, and I'd love to see a lot more
16 effort into actually going out and measuring
17 concentrations in real ponds and seeing if these models
18 are producing results that in any way mimic reality, so
19 validation is very important.

20 And if you...I understand completely the
21 desire to apply regulatory conservatism to the results,
22 but I think it should be applied to the results at the
23 very end and not to the model processes. Don't remove
24 a process from the model like burial because you think
25 it's non-conservative. You can do that at the end if



1 you wish.

2 So, PRZM gives flows of chemical and
3 solids and water. I would argue you should include all
4 of these three flows into the water, and putting
5 sediment into the pond results in burial, and it
6 results in faster deposition. Putting water into the
7 pond, especially after severe storm events, increases
8 the volume of the pond, it dilutes the contaminant, and
9 it may result in outflow. And if you want, you can
10 reduce the outflow to a very small number.

11 So, these are just some concluding
12 thoughts for your consideration. I think it's
13 important that the model include...includes all the
14 relevant processes in a realistic manner with realistic
15 parameter values, and it should be validated, if
16 possible.

17 And I would urge you to strive for
18 simplicity consistent with the need for a realistic
19 simulation. A simple model is much more easily
20 interpreted. It's much faster, and you must remember
21 the likely accuracy.

22 If you can get within a factor of 2 or 3
23 of the real numbers, you're doing quite well in this
24 game, in my opinion. So, don't worry if the result is
25 4.1 as distinct from 4.2. You'll never get that



1 accuracy with these models.

2 And you can do sensitivity analysis and
3 a combination of careful interpretation and Monte Carlo
4 methods is I think the way to go. So, we favor a
5 simple two-compartment sediment water model, and that's
6 what we designed, with advice from EFED.

7 And un...in the white paper on page 93,
8 there are other models. These and in EXAMS are
9 excellent models. There's no doubt about it, but
10 they're not designed for this purpose. And I would
11 urge EFED to design their own model for their own
12 purpose. Then, you're free of all the constraints of
13 these other models.

14 And if it's a simple model, it can treat
15 a pond, and it can treat a very gently flowing river.
16 And it can treat the total residue degradation product
17 issue which Dr. Ruhman talked about this morning, but
18 there's no doubt that the...the formation degradation
19 option, the FD version, is the way to go, and with a
20 simple model, it's not all that difficult to include
21 the formation and degradation of degradation products.

22 I'm going to skip the remark on OECD2.
23 There are some difficult but not insurmountable
24 problems with the concept of an overall system
25 half-life, 'cause in a two-compartment system, you

1 basically have at least two half-lives, one that occurs
2 early on and one that occurs later.

3 Weaknesses of AGRO. AGRO does not take
4 into account the pesticide mass that is in the food
5 web. It assumes that the water column is not reduced
6 by the transfer of chemicals into the food web. That
7 could be included, but it's a conservative assumption.

8 We neglect deep or irreversible sorption
9 into organic matter. Often it is found that after a
10 long period of time, chemical sorbed to organic matter
11 is very, very difficult to get out, and it's very
12 non-bioavailable. We ignore the soil type or texture
13 or drain size, mainly because we just didn't have the
14 data to do it, and I think the input of soil solids and
15 the input of water from PRZM will go a large way to
16 alleviate the so-called solubility problem.

17 AGRO is a fugacity model. Some people
18 don't like fugacity models, but you shouldn't be afraid
19 of fugacity. Fugacity and concentration levels are
20 fully inter-convertible. In fact, the EU's model in
21 Europe which is widely used in the REACH program used
22 to be a model called simple bogs, which was initially a
23 fugacity model, and it was converted into a
24 concentration model and Frank's bio-cumulation model
25 can also be written...and we have done it...as a



1 fugacity version.

2 In fact, EPA has a model called
3 TRIM.FaTE which was not in the list which actually uses
4 QUASI treatment of sediment and water exchange with a
5 fugacity approach. So, don't get scared of fugacity.

6 So, I'd like to thank the people who
7 supported our work at the modeling center. You're very
8 welcome to visit our web site for newsletters, and we
9 have all soil models, including models on long-range
10 transport, and thank you for your attention.

11 **DR. HEERINGA:** Thank you, Dr. Mackay.

12 I'd like to give the panel an
13 opportunity...I know we want to hear next from Dr.
14 Gobas, but give the panel an opportunity for any
15 questions of clarification or interchange with Dr.
16 Mackay. Yes, Dr. Biddle man?

17 **DR. BIDDLE MAN:** Don, has AGRO been
18 applied to estuaries, or do you see any special
19 modifications that would be needed to apply it to
20 estuaries?

21 **DR. MACKAY:** It has not been applied to
22 estuaries, and it would require considerable
23 modification. Estuaries are very tricky often because
24 of salinity wedges and things like that, and it's just
25 not suitable for that purpose.



1 **DR. HEERINGA:** Dr. Mehta?

2 **DR. MEHTA:** Yeah, when you talk about
3 including burial would actually reduce the
4 concentration in suspension, you know, if you had a
5 substantially low enough say fine-grain sediment that
6 was very quickly and to the point, you get inert
7 settling, and so, that would mean that you would have
8 to modify your settling velocity function also, because
9 if you didn't do that, then it will, settling in it in
10 that way could actually transport itself out rather
11 than get it buried. So, all I'm saying is that if you
12 include burial it could also involve, more refine some
13 of the other processes.

14 **DR. MACKAY:** Yeah, you're absolutely
15 correct. One of the tricky points is to define that
16 deposition rate, and for very fine-grain sediments, it
17 can be quite slow, but in EFED's use of EXAMS, there is
18 no outflow at all, so that material just can't get out
19 regardless of how fine it is.

20 **DR. HEERINGA:** Dr. Maddalena?

21 **DR. MADDALENA:** So a question, Don,
22 about the...the, about the solubility limit issue that
23 you brought up. I agree we need to, you can't just
24 ignore that. In your conceptual model, do you just
25 create a new compartment essentially at the pure phase,



1 and if so, how do you regulate the...read the solution
2 of that new phase as to solubility? Because it seems
3 like you would just maximize your water solubility over
4 the solid state.

5 **DR. MACKAY:** What happens is if, for
6 example, you're applying pesticide on spray drift,
7 let's say the solubility in water is 1 microgram per
8 liter. Once you mix the pesticide into the water, you
9 get 2 micrograms per liter. What then happens is the
10 model reduces that 2 to 1, and it moves all of that
11 chemical into another compartment that's called
12 precipitated pesticide. And that sits there, and as
13 reaction and other processes dissipate the chemical
14 from the water column and the concentration drops, that
15 precipitate dissolves and feeds the dissolved
16 compartment and keeps it constant until the precipitate
17 goes away completely.

18 So it's a kind of temporary storage
19 reservoir for...that is essentially the model that Dr.
20 Ruhman described this morning.

21 **DR. MADDALENA:** Okay, so I did...maybe I
22 looked down with the chart, but it seems like the water
23 solubility would be flat at that point.

24 **DR. MACKAY:** It would be, yeah.
25 That...that...on that graph, that was the results we



1 got before we...

2 **DR. MADDALENA:** Okay.

3 **DR. MACKAY:** ...put in the solubility.

4 **DR. MADDALENA:** Okay, so you didn't
5 actually, it stayed until the reservoir is gone, and
6 then it goes back to...

7 **DR. MACKAY:** Yeah. So, and now what it
8 would do is it would go up, go along at a steady level,
9 and then come down. I should have put that slide in,
10 thanks.

11 **DR. HEERINGA:** Dr. Simonich?

12 **DR. SIMONICH:** Don, this question might
13 be better asked of Frank, but let me throw it out.
14 Have you...have you modeled amphibians yet in the food
15 web model?

16 **DR. MACKAY:** That would be a question to
17 ask Frank.

18 **DR. HEERINGA:** Hold that one. Dr.
19 Norstrom?

20 **DR. NORSTROM:** Norstrom. Don, with
21 extremely high log KOW substances that precipitate, do
22 you think they will ever redissolve?

23 **DR. MACKAY:** That precipitate because
24 you've exceeded the solubility?

25 **DR. NORSTROM:** Yeah.

1 **DR. MACKAY:** Yes, I think they will,
2 because...because they're very sparingly soluble, the
3 precipitated particles must be very, very small, and
4 very, very small particles tend to have a large air to
5 volume ratio. So, they dissolve fairly fast. I think
6 so.

7 **DR. NORSTROM:** You know, I have a lot of
8 concerns about kinetic phenomena for...for high log KOW
9 compounds, because I think we've ignored that, but I'll
10 bring that up maybe later in the panel discussion. But
11 if it's very small, yes, I suppose it would. If it was
12 large, however, they might lay there forever and never
13 dissolve.

14 **DR. MACKAY:** Yeah, that's right. I
15 don't really know what happens. I suspect a very small
16 precipitate particle of pesticide would probably
17 associate to some extent with the dissolved and
18 particulate organic matter in the water column, and it
19 might well sediment, but I didn't want to include that,
20 because it's a sort of enhanced method of deposition
21 that's a bit suspect.

22 **DR. HEERINGA:** Dr. Abbott and Dr.
23 Thibodeaux and then...

24 **DR. ABBOTT:** I support your comments
25 about the need to validate the model. I wonder if you



1 could suggest a data set that could be adequate for
2 validating, say, the redesigned PRZM that included
3 burial and outflow, or would that data set have to be
4 collected?

5 **DR. MACKAY:** I think, ideally, it has
6 to be collected, but it's not, you know, rocket science
7 to do that. I think there are data out there,
8 and...and at least one or maybe two papers in the white
9 paper that are cited that have data of this type, and
10 because AGRO is flexible...you can usually change the
11 volume, the area and the depth of ponds, and it's...I
12 think it's highly likely that you can find data out
13 there that would...could be used to our data, and, of
14 course, our mesocosm data which are much more tightly
15 controlled which can be bounced against the model.

16 **DR. HEERINGA:** Dr. Thibodeaux?

17 **DR. THIBODEAUX:** Don, it was a nice
18 comparison between AGRO and EXAMS and cleared a lot of
19 things up for me. Back to the solubility idea. It
20 seems to me your way of accounting for it through a
21 precipitate is really a mass routing rather than a
22 process model. Is that correct?

23 **DR. MACKAY:** Yeah, Mm-hmm (indicating
24 affirmatively).

25 **DR. HEERINGA:** Dr. Doucette?



1 **DR. MACKAY:** Well, it...it...it is my
2 attempt to get at a process model, and it's...

3 **SPEAKER:** Good start.

4 **DR. MACKAY:** Thank you, yeah.

5 **DR. HEERINGA:** Dr. Doucette and then Dr.
6 Hickie.

7 **DR. DOUCETTE:** Yeah, I was wondering,
8 you mentioned this model ignores irreversible
9 absorption or combining. Have you played around with
10 the...the scenario within the model if you allowed that
11 process to occur and what...what sort of results there
12 would be? I mean, I realized you're trying to keep it
13 conservative, but conservative is nice but not if it's
14 not realistic all the time.

15 **DR. MACKAY:** I haven't played around
16 with it, and the basic reason is I'm kind of lazy,
17 because it means putting in all kinds of sorption
18 kinetic, desorption kinetic expressions into the model,
19 I was very reluctant to do. So, it's laziness.

20 **DR. DOUCETTE:** Could...could you do a
21 simplification where you basically ignored the kinetics
22 and...and just put a...a certain percentage into a...a
23 compartment as a...as a removal mechanism?

24 **DR. MACKAY:** Yes, you can do that. In
25 fact, it...we've done some work on soils and



1 partitioning from soils to terrestrial invertebrates
2 like worms, and in order to get the model to give the
3 results, we have to put in a fudge factor which is the
4 fraction of the total chemical in the soil which is
5 bioavailable. And it can be something like 20 or 30
6 percent. And so, that addresses the problem that you
7 raised, but I...I feel uncomfortable about it, because
8 I don't know where to get those 20 or 30 percent.

9 **DR. HEERINGA:** We have a few more
10 questions. Dr. Hickie and then Dr. Maddalena and then
11 Dr. Delorme.

12 **DR. HICKIE:** Don, I have several,
13 hopefully, short questions. One is I, earlier I asked
14 about EXAMS and keeping track of carbon budget. Does
15 AGRO do that?

16 **DR. MACKAY:** It doesn't, and if...if I
17 was to continue to develop AGRO, I would want to, you
18 know, keep track of the chemical, keep track of the
19 water, keep track of the mineral and solids and keep
20 track of the organic matter, because the organic matter
21 is a vehicle for moving the chemical around, and it
22 doesn't do that at the moment, and some years from now,
23 I think that is definitely where to go.

24 **DR. HICKIE:** I...I'm particularly
25 thinking of a potential issue of biodilution with algal



1 growth and things of that sort.

2 **DR. MACKAY:** Absolutely.

3 **DR. HICKIE:** And the other one is AGRO
4 has an input of...of the weather records over years and
5 years. Does...does AGRO do that? I'm sorry. EXAMS
6 has that. Does AGRO?

7 **DR. MACKAY:** The weather record goes
8 into PRZM.

9 **DR. HICKIE:** Okay.

10 **DR. MACKAY:** And PRZM, then, gives you
11 the runoff record. So, AGRO doesn't have the...

12 **DR. HICKIE:** I have just one last
13 question. Is...these ponds are very shallow, so
14 sediment incidence is very much wind driven, I would
15 imagine?

16 **DR. MACKAY:** It probably is, and we use
17 the ponds 100 meters across, and it's not a very long
18 fetch, but...

19 **DR. HICKIE:** I...I'm just wondering
20 about variability in winds and storm events and what
21 effect that might have on the burial process.

22 **DR. MACKAY:** Yeah. Well, the whole
23 sediment resuspension and deposition process is highly
24 episodic, and it, you know, Willie Lick has been saying
25 this for many years, and I'm sure the same things



1 happens in...in these small ponds, and I...it should be
2 characterized in some way.

3 **DR. HEERINGA:** Dr. Maddalena and then
4 Dr. Delorme.

5 **DR. MADDALENA:** One more question on the
6 PRZM. You taught AGRO to talk to PRZM, so I'm
7 wondering if the flow, the invecting moving phase that
8 comes from PRZM into AGRO, do you have any control over
9 the fugacity capacity of that moving phase? I asked
10 this question this morning but in...not in fugacity
11 terms though.

12 **DR. MACKAY:** Sorry, Randy. The input to
13 AGRO comes from...through the PRZM, and PRZM has got
14 water and soil into your pond.

15 **DR. MADDALENA:** It does. Do you have
16 control over the fugacity capacity of that water and
17 soil, or is that just a single volt input in the model
18 upstream?

19 **DR. MACKAY:** AGRO doesn't really care.
20 All it wants to know is what mass of solids goes in,
21 what mass of water goes in, and what mass of chemical
22 goes in, and the fugacity capacity of the solids
23 leaving AGRO, it's kind of taken into account by the
24 adsorbed enhancement factor, whatever you actually get
25 when you open in AGRO...in PRZM, but it...it could be.



1 **DR. HEERINGA:** Dr. DeLorme?

2 **DR. DELORME:** Thanks, Don, for
3 enlightening me on fugacity once again. It's been a
4 few years since I talked about it. Anyway, I have a
5 couple of questions.

6 With respect to your statements on
7 dynamic versus steady state models, although I can
8 appreciate using a dynamic model for...for a farm pond,
9 I think one of the issues that we face as regulators,
10 when we look at the PBT substances, they don't stay
11 where they're put, and when they move around, they are
12 persistent. I mean, in the longer term, I think a
13 steady state model in an area like the Great Lakes or
14 in the Arctic may be appropriate for use in some of our
15 regulatory risk assessments.

16 **DR. MACKAY:** Well, I...I...I think that
17 a steady state model is...is quite appropriate for a
18 system like the Great Lakes or the Arctic where you
19 don't have intense spikes of input as you have in the
20 vicinity of an agri pond.

21 **DR. DELORME:** So...but we may need to
22 develop both kinds of...

23 **DR. MACKAY:** Yes, yes.

24 **DR. DELORME:** The other question I had
25 is...and I'm not sure...might...might need to talk



1 to...to Ron about it. I wasn't quite sure how EXAMS
2 and how your model handle temperature. Certainly, in
3 the northern states and in Canada, you have a
4 significant part of the season when the water's frozen.
5 That affects dynamics. You also have a...an effect on
6 metabolism...metabolites, metabolic rate of the
7 organisms that are going to degrade these things. So,
8 I'm not quite sure.

9 You know, the studies we get are lab
10 studies done at 20 degrees, but for a persistent
11 compound, that could result in some changes to the
12 dynamics of that system.

13 **DR. MACKAY:** AGRO does not include any
14 temperature variation, and it certainly doesn't include
15 any ice cover. It just assumes constant temperature
16 conditions, and the properties it uses are the
17 properties that are in...the user puts in and if the
18 user thinks that these properties change with time then
19 they've got to pretend that these changes.

20 Temperature is an important
21 consideration. And here it's like in a secondary
22 effect. And I think for evaluative purposes such as
23 EFED is concerned with, maybe you can ignore it, but
24 there certainly are differences from location to
25 location and season to season.



1 **DR. DELORME:** And the final question I
2 had with respect to your comment about apply regulatory
3 conservatism to the result and not the model processes,
4 as one of the people who...who would be looking at the
5 results, I'm trying to figure out how I would do that.
6 How can I apply conservatism to the results of the
7 modeling rather than in the...in the formulation of the
8 models themselves?

9 **DR. MACKAY:** Well, what I suggest is you
10 run the model with outflow and with burial and get
11 results, look at them, and the results will tell you
12 how important these processes are, and then you can
13 tweak them. You can reduce burial a little bit and see
14 how that affects outflow. In fact, Arthur did that
15 this morning, and that way, you can obtain a...an
16 impression of the sensitivity of the final result to
17 that process, but if you remove burial right at the
18 beginning, you'll never know whether burial was
19 important or not.

20 So, we play games with it, tweak it.

21 **DR. DELORME:** And then that's the answer
22 you want, do the what if analysis.

23 **DR. MACKAY:** Exactly.

24 **DR. DELORME:** And see what the
25 sensitivity relies on, and then you can include that in



1 your risk characterization, and it's up to the risk
2 managers then to take that information and make the
3 decision. Okay.

4 **DR. MACKAY:** Exactly.

5 **DR. HEERINGA:** Let's have one more
6 question from Dr. Thibodeaux, I believe. You pass?
7 Okay, wanted to give you the opportunity for certain.

8 At this point, I'd like to thank you
9 very much, Dr. Mackay. Very interesting presentation.

10 And appending to that is the next
11 presentation by Dr. Frank Gobas who is with the School
12 of Resource and Environmental Management at Simons
13 Frazier University and talking on Application of
14 Environmental Fate and Food Web Bioaccumulation Model
15 for Assessing Ecological Risks of PBT Type Pesticides.

16 Dr. Gobas, welcome.

17 **DR. GOBAS:** Thank you very much, and
18 thanks for inviting me to...to come to this...to this
19 meeting. I...I'm sure I speak for Don as well.
20 We...we greatly appreciate the opportunity to...to talk
21 about something we all share, and that's an interest
22 in...in PBT type substances.

23 And PBT substances are, of course,
24 special. They are different from other chemicals in
25 the sense that they are persistent, of course. They



1 react slowly, perhaps not at all, and they also
2 typically have high KOWs and/or high K_{OH} which gives
3 them high sorption coefficients which ostensibly cause
4 them to sorb strongly to...to particulate matter, and
5 they also have slow elimination rates because of those
6 properties in biota, and as we've already talked about
7 quite a bit, they have, in many cases, high melting
8 points and...and low aqueous solubility.

9 And these characteristics themselves
10 have profound effects in terms of how these chemicals
11 behave and...and how you...how you should model them.
12 And we've talked about the models, and here they are.

13 The...we have an existing model that Ron
14 Parker talked about in...in...in detail which links
15 the...the PRZM model to EXAMS, to a steady state food
16 web model that includes the food web, and the model
17 that Don talked about which was the QUASI model here,
18 and that is part of the newer model which links PRZM to
19 QUASI through a time dependent food web model and
20 to...and to...and the...the food web model. And...and
21 that is the model that...that we...we...we talked
22 about.

23 And, oh, I'm pushing the wrong button.
24 Is there any other button...oh, here we go. Now, the
25 key thing about the slower reaction rates and



1 persistence is that when you start looking at these
2 models is you start to turn off certain rates, right,
3 so Don, this is the...the...the...the sediment reaction
4 rate, persistent...the chemical's persistence. We
5 basically turn that one off. We turn this one off if
6 the chemical is not per...is persistent in the water
7 phase. If you...if the outflow of the chemical is slow
8 or if you turn it off and that becomes no longer an
9 exit route, if the chemical has high...or has a low
10 Henry Law constant, then even that route becomes very
11 small as well.

12 And then, you really end up in the
13 system, and this will probably see in many of these
14 pond systems, where there's really only one net loss
15 rate that...that...that applies to that system, and
16 that's the burial or the net deposition rate. And
17 QUASI has that ability, of course, but EXAMS does not.

18 When we...when you start modeling, and
19 when you compare the two models in terms of how they
20 behave in dealing with inputs of...of...of pesticide,
21 you start looking at two different situations. Is the
22 EXAMS model here really, is it inputs of pesticide into
23 the water column? 50 percent is then moved to the
24 active sediment layer which is the sediment layer that
25 interacts with the water phase, that...that connects



1 with the water phase as well as to the biota living in
2 that system?

3 And here, we've got the buried sediment
4 and there is, of course, no arrow there, whereas in
5 AGRO, you...you...you don't have that extra rate out.
6 And that rate has an important impact, of course, on
7 the...on the concentrations that you would calculate as
8 a result of pesticide input into that pond system.

9 And this is an example. This is the
10 EFED farm pond. Has constant sediment dynamics. What
11 I'm showing you here is...is...is a 30-year simulation.
12 Annual concentration estimates...these are the
13 concentration sediments. And you can see what the
14 difference in including that burial rate does in terms
15 of the calculations. Right?

16 Over a 30-year period, you get
17 substantially different estimates of concentrations
18 in...in that system. Is not correspondingly related to
19 the sediment. The water will really show you the same
20 results. Right? Major differences.

21 Also, when you start to use real PRZM
22 scenarios...and that's here shown for...for the Maine
23 potato scenario...you still get the same kind of
24 results. You see a constant accumulation in the EXAMS
25 model, whereas the AGRO model really provides a lift to



1 that maximum concentration which is totally controlled,
2 really, by that net deposition rate or burial rate.

3 And this is another example. This is
4 the California cotton scenario. And we can see
5 that...that there are some...there are differences, but
6 in all cases, there remain very big differences in
7 concentration estimates between these two models.

8 This is the sensitivity analysis. Here,
9 we look at the impact of the degree of burial on
10 sediment concentrations over time, and basically, what
11 I'm showing you here is the EXAMS output with no
12 burial, AGRO with no burial, and you can see that with
13 increasing burial rates, of course, there's a greater
14 net loss of that substance from the system, and as a
15 result, the concentrations really go down and also,
16 tend to reach a maximum at a certain point in time
17 rather than keep continuing to accumulate over time.

18 Another important aspect of modeling
19 this processes of meta deposition is...is dealing
20 with...oh, sorry. These...this is the sensitivity
21 analysis of the biota. Of course, I've got to talk
22 about biota. That's my job in this life.

23 This is the impact of...this is the
24 analysis for burial rate on the...on the biological
25 data, so these are now concentrations of Perciforous



1 fish. Perciforous fish is a larger 1 kg fish higher up
2 in the food web, and...and you can see how the
3 concentrations in these fish really vary as a function
4 of time and as a function of the burial rate, and,
5 again, you can basically see that a higher degree of
6 burial will give you lower concentration estimates.
7 Right?

8 And the fish really respond to the water
9 concentrations and the sediment concentrations, and
10 whatever happens to those concentrations will have an
11 immediate impact on the levels in them, in the food
12 web.

13 And important aspect of...of dealing
14 with these...modeling these net deposition rates is
15 actually dealing with this active sediment layer. The
16 active sediment layer is used by modelers to describe
17 the amounts of sediment that interact with the water
18 phase.

19 In many cases, that's hard to define,
20 and it's really hard to state, you know, what depth
21 should one choose in these models, what, you know, to
22 what depth do chemicals still interact with the water
23 phase and interact with the biological systems that
24 live in that system as well.

25 So, that's a key...key issue in terms of



1 how you...how you find and how you set an active
2 sediment layer. So, what I'm giving you here is
3 basically a sensitivity analysis on...on...on selecting
4 these values.

5 Typically, what...what happens is that
6 for fresh water systems, these rates or these
7 thicknesses are a little bit smaller than the order, in
8 the area of 5 to 10 cm. In marine systems, because of
9 tidal actions, the active sediment layers are typically
10 much larger in...in these fate models.

11 The impact of selection of these numbers
12 is shown in here where I basically have shown you the
13 concentrations in the sediment. This is pesticide 3
14 again, effects farm pond, these are the deposition
15 parameters, 30-year simulation, and now I'm using
16 different thicknesses of that active sediment layer.

17 And basically, what the active
18 sediment...the thickness of the active sediment layer
19 does, it determines the response time of the chemical
20 concentration in sediment. The thicker the layer, the
21 slower the response time.

22 And what it doesn't really do is it
23 doesn't really change that maximum level, that steady
24 state level, that if you were to take the simulation
25 longer, that you would have achieved. That's fairly



1 independent of the selection of that thickness.

2 This is the impact of this...the...the
3 active sediment layer on the biological systems, these
4 are concentrations in fish, and here we can see, again,
5 that the thickness of the sediment layer has...has some
6 effect on the concentration of the biota, but it is
7 relatively small. That...that's good news, that in
8 terms of selecting that parameter, the selection is not
9 that sensitive or the...the concentration estimates
10 that you derive is not that sensitive on the thickness
11 of that layer except for the time response which is
12 quite sensitive to that sediment thickness.

13 And these are, of course, all model
14 simulations, and model simulations need to be compared
15 with real data to see if we're on the right wavelength,
16 and that's what I've tried to do here. And so here,
17 now, we're...we're trying to see the behavior that's
18 predicted in these models is actually realistic.

19 And we...we don't...I'll show you some
20 examples later, but the example that I've shown here
21 is...is...is...is an example for...is an example for a
22 really big pond which is Lake Ontario, and where we
23 basically have seen over the past an input of PCBs over
24 the years in that, then followed by sharp declines in
25 the PCB inputs over the years.



1 And what you tend to see in this...this
2 little box here are really the concentrations in the
3 sediments, and we can see how they have responded over
4 time. They have gone up, and as soon as the loadings
5 actually went down, soil concentrations went down. And
6 the concentrations in these sediments were also...or
7 these decline rates were also mimicked to a certain
8 degree in the biological systems as well. So,
9 concentrations in a number of fish species like rainbow
10 snell, lake trout, and also perch species fell as a
11 response to those declining sediment concentrations.

12 And I think that the...the point here is
13 that when loadings go down in systems that I think are
14 comparable...we're looking here at PCBs. They are
15 persistent chemicals. Loss rates of...for Lake Ontario
16 for outflow are low, and we...we basically have
17 somewhat comparable situations that shows that when
18 these loadings stop, the concentrations will drop.

19 I think that's important, because if you
20 would...and the other point I was going to try to make
21 here is after these concentrations drop, you tend to
22 see a rate of concentrations decline, and they tend to
23 follow the rate that you would expect from the net
24 deposition rate of that system which, in this case here
25 for...for Lake Ontario, is about 5.5 years. And in the



1 end, what you're seeing is that when these loadings
2 actually stop, the concentrations will start declining
3 at rates that are comparable to the burial rate.

4 It's probably one of the best
5 indications that we have that burial rates can control
6 the central dynamics in, in this case, a big system
7 like...like a lake.

8 And this is, of course, what you would
9 expect from...from EXAMS if you did not have that
10 burial rate and you did not have the loss rate through
11 transformation and you have no loss rate through
12 volatilization. And the only result that you're going
13 to get is...is for something like...like that, and I
14 think in the Lake Ontario example, the point is that we
15 don't really see that.

16 The other aspect that I would like to
17 spend a little bit of time about is...is about slow
18 excretion rate of PBT substances. The slow elimination
19 rate of chemicals have a very important effect in terms
20 of modeling and controlling the behavior of chemicals
21 in biological organisms.

22 Slow elimination rate basically means
23 the chemicals reach steady state very, very slowing.
24 So, in many cases, they don't reach steady state. And
25 I think that's important to keep in mind when we're

1 running these models, because the...the model that's
2 often used to...to apply to the biological system is a
3 steady state food web model. And for many of these PBT
4 substances, you don't reach steady state.

5 For that reason, we...we have replaced
6 that with a TINY TIMS model. And I think that can have
7 a major impact on...in...in terms of what kind of
8 concentrations you're going to see in...in the
9 biological systems.

10 This is an example. This is pesticide
11 number 3. Has a log KOW of 5. If you tried to put
12 that in...in Perciforous fish, it's about a 1 kg lipid
13 content of 6 percent, it takes about 189 days to get to
14 95 percent steady state, a half-life time of 44 days.
15 Right?

16 And you can see that the elimination
17 rate, of course, mimics that. The same kinetics apply
18 to the elimination phase, in this case the elimination
19 phase is largely controlled by gill elimination which
20 is represented by this K2 value which is the largest
21 elimination rate and...and the largest elimination rate
22 constant of all the losses, which is gill elimination,
23 fecal excretion, and roe. You can see for this
24 particular chemical, elimination through the gills is
25 controlling the time dynamics, but the time dynamics



1 are slow, very slow.

2 When we go to a chemical with a log KOW
3 of 8.1, pesticide 4, that uptake curve is even slower.
4 Right? It takes more than 1000 days to...to get to
5 steady state. Right? And the elimination kinetics
6 which is actually quite interesting is actually no
7 con...no longer controlled by...by this gill
8 elimination which is K2. It's not controlled by fecal
9 excretion either. It's really controlled by...by KG
10 which is the growth rate of the animal. So, the
11 elimination is really controlled by growth.

12 Now, that...that has important
13 implications when you start exposing organisms to
14 pulses of chemicals in water and...and sediments, and
15 this is an example, pesticide 3. This is an actual
16 scenario, Maine potato scenario. And the output is
17 from PRZM, and what I'm showing you here are
18 concentrations in water over time, and this is at 168
19 days. These are four applications, and you can see how
20 the water concentration responds through those four
21 applications of pesticide 3.

22 Now, if you would run the steady state
23 model to calculate the concentrations in the fish, this
24 is what you would get for...for Perciform fish.
25 That's the 1 kg fish. You can see, of course, you



1 know, the, the, the pulses in the water concentration
2 are mimicked by similar pulses and in the
3 concentrations in the fish.

4 However, the fish, of course, cannot
5 respond to those concentrations that fast, and this is
6 more the type of response that you would expect to see,
7 and that's the time response given by...by...by a time
8 dependent model. And you can see the differences
9 are...are significant.

10 This is an example of now a 30-year
11 simulation. Pesticide 3 again. PRZM linked to AGRO
12 model. These are the concentrations in the water that
13 you would expect to see over that 30-year simulation,
14 and if you run the steady state model, you see the same
15 pulses again, and you get this. If you run the time
16 dependent model simulations, you get that. Right? And
17 this is for a small fish.

18 If you do this for a bigger fish, these
19 are the steady state concentrations. These are the
20 concentrations of the time dependent model. And I put
21 them on the same scale here so you can easily compare
22 them.

23 You can see, of course, that there are
24 major differences. And these differences can really
25 make an enormous difference when you do the risk



1 assessment. If this is your cutoff value that you're
2 comparing these concentrations to, you can obviously
3 see you're far below it, and if you run the steady
4 state model, you get to see instances like...like this
5 where you would, of course, exceed those threshold
6 concentrations.

7 This effect that Don already talked
8 about of this...this temporal effect in the food web
9 where, basically, concentrations are dammed or cannot
10 achieve their steady state values increases when you go
11 up the food web. Basically, when you go from smaller
12 to bigger organisms, this effect becomes greater.
13 Also, when you increase the...the lipid content, this
14 effect becomes bigger.

15 And also, when you go to higher KOW
16 pesticide, this effect only becomes bigger. So, the
17 effects that I've shown you so far for pesticide 3, has
18 a log KOW of 5. This differences are much, much
19 greater when you go to a chemical with a log KOW of 4.

20 And so far, again, I've talked about
21 models. It's important to...to make sure that when we
22 start using these models, that these models are
23 reliable, and I think the best way to do that is
24 actually by comparing the models to actual data. In
25 this case, what I'm really concerned about is the



1 temporal dynamics to how do these temporal dynamics
2 that we're using in the...in the AGRO model and in the
3 tem...in the food web model, how do they stack up, are
4 they reliable so that you can make reliable
5 calculations with...with your model.

6 I'll show you two levels of comparisons
7 here. The one is for a...a comparison with laboratory
8 studies, typical BCF stuff, the BCF test that you may
9 be familiar with where you expose fish to chemical
10 concentration in the water and in the water only, and
11 you follow the concentrations in time in the water and
12 in the organism, and you can use that then to calculate
13 the rate constants, and those rate constants of uptake
14 and elimination are telling you about the temporal
15 response of the model.

16 So, what I'm going to do here is give
17 you some examples of how these models fare. This is
18 pesticide 3, bluegill sunfish, two exposure scenarios
19 at different concentrations. These are the rate
20 constants that we should look at. The uptake rate
21 constant for pesticide 3, it's 380, 330, and this test
22 more a calculation of about 366.

23 Elimination rate constant here, 0.04.
24 0.04, 0.056, and the steady state fairly comparable.
25 Bioconcentration factor is fairly comparable and the



1 steady state fairly comparable. So, it's a good
2 example where...where we see a reasonable performance
3 of the model calculations and in terms of providing us
4 with estimates of rate constants.

5 This is pesticide 4. Pesticide 4 is
6 interesting. Here, what we've basically done is we
7 have performed the model, and by mimicking, really, the
8 bioconcentration test, basically, we see the model
9 coming up with a rate constant of 385. BCF study is
10 600.

11 Now, the total elimination rate constant
12 is interesting, 'cause it's totally controlled by
13 growth in the BCF test. So this is really a growth rate
14 constant, controlled totally by the conditions of the
15 test, and we've taken that number and compared that to
16 the reported value, 0.023, and the BCFs are roughly the
17 same. T95s are quite comparable.

18 I think when you look at the report,
19 you'll see major differences between how...how the BCF
20 results differ from...from the results of this model.
21 It's largely because of this effect, growth, and we
22 see...let me show you how important it can be.

23 There's a little lesson there. And
24 these are really the growth data in the bluegill
25 sunfish experiment. These animals were growing quite



1 rapidly, from about 13g at the beginning of the test to
2 about 130g...well, it would have been 130g in about 180
3 days. This fish would have been about 1.3 kg at the
4 end of a year.

5 Typically, a fish cannot grow that fast,
6 and these are the growth rates that are typically used
7 in the model which are much smaller, more reflective of
8 growth in the...in the field. And as a result, you
9 get...you get enormous differences between the BCF
10 results...and this is the model outcome for the BCF
11 results...and field conditions. Right?

12 Here, you see this large amount of
13 growth that totally controls the elimination rates.
14 And growth also controls the elimination rate in the
15 model, but that growth rate is much smaller.

16 And another lesson in here is really
17 that when you start doing...running these BCF tests for
18 chemicals with low KOWs of that magnitude, 8.1 in this
19 case, you really start to measure the properties of the
20 fish rather than the properties of the chemical, and
21 you have to really watch out for that when you start
22 using those results and using them to predict
23 situations in the field.

24 This is the...the final part of the
25 simulations. Here, what I'm going to show you is how



1 these time dynamics of this food web, in this case, the
2 food web bio-cumulation model, how it compares to the
3 real data. What I'm doing here is basically taking
4 the...the water concentrations and sediment
5 concentrations in microcosm studies and using them as
6 input to the food web bioaccumulation model to
7 look...to estimate the time dynamics of that model, and
8 then we're going to calculate the concentrations in
9 various biota and then compare them to the observed
10 values to see for any agreement.

11 These are the...the results. This is
12 for macrophytes. This is what we predict, blue line.
13 This is what is observed. And you may see a difference
14 of where...we're actually really proud of this result.
15 These are...or this is...this is not a logarithmic
16 axis. These concentration differences are actually
17 really small.

18 So when...and there...there's no fudging
19 in this model. There's no calibration. So, we
20 basically see a reasonable agreement of time dynamics
21 between model and data.

22 These are crustaceans. I'll flip
23 through them quite quickly so you get a bit of a feel
24 for it. This is sea brown mussels. This is snails,
25 and these are fish. And, in general, what you tend to



1 see for this particular pesticide is a fairly good
2 agreement in terms of time response, and I think
3 that's...that's encouraging.

4 And I also tried to re...we...we also
5 tried to fit here the...the combined model, so now
6 we're looking at evaluating the time dynamics of the
7 combined AGRO and food web model. Right? By taking
8 the pesticide application, putting in the AGRO model,
9 letting the AGRO model calculate the concentrations in
10 fish and water. The biota picks it up, and then we
11 calculate the concentrations in...in the food web to
12 see how these models behave.

13 And pesticide 3, and the two models
14 we're running here combined. There are two pesticide
15 applications at 370 intervals, and we're comparing
16 concentrations. And this is for water, and we can see
17 how...how that behaves. And this is it for
18 macrophytes. And we get a similar behavior, basically
19 telling you that the...the AGRO model does a good job
20 in predicting the time dynamics of concentrations in
21 these microcosm studies.

22 So, we have a few con...conclusions.
23 First, I think that we all agree that the very high
24 persistence of these chemicals and the high sediment
25 absorption coefficients of PBT substances create a



1 strong linkage between the fate of the pesticide and
2 the sediment. Right? And the sensitivity analysis
3 that we...that I've shown you confirms that linkage,
4 and it shows you that concentrations of these PBT type
5 substances in water, sediment, and biota can be
6 expected to be directly related to the magnitude of
7 sediment deposition which is a key part of what
8 controls the fate of the sediment.

9 Sensitivity analysis also shows that the
10 thickness of the sediment layer affects the temporal
11 response of the chemical concentrations but not so much
12 the long time steady state response of the
13 concentration.

14 The monitoring data, the little bit that
15 we have, but I think there are some other examples that
16 we can draw from, show that sediment dynamics play a
17 key role in controlling temporal response of
18 concentrations of PCBs in lakes and other persistent
19 chemicals as well.

20 There are some good examples. Lake
21 Ontario is a good one. Another one is in San Francisco
22 Bay where you really can really see the effect of net
23 sed...of net sediment deposition on the fate of the
24 substance.

25 Including net deposition, therefore,



1 seems to be a logical next step to make the...the
2 models, the environmental fate models, more realistic.
3 I think this is especially important for PBT type
4 substances, because they don't have an extra loss
5 through reaction and transformation.

6 And EXAMS...or it can, as we've learned,
7 include that process, but at the moment, I think in
8 most applications, the sediment dynamics and especially
9 net deposition is not included, and I think that can
10 have major impact on the levels that you're going to
11 calculate.

12 On the biological side, PBTs have slow
13 excretion rates, require a long time to reach steady
14 state. As a result, they don't really reach steady
15 state quite often, especially in situations where the
16 chemical is applied on an episodic basis, the
17 pesticides.

18 The application of steady state
19 bio-cumulation models to PBT type substances under
20 conditions of time variable exposure concentrations
21 may, therefore, produce unrealistic concentrations
22 in...in...in...in wildlife.

23 Also...and this is something that I
24 tried to put in and maybe I'll regret it, but I think
25 we should exercise very great caution when using BCFs

1 for PBT type substances in exposure assessment. I
2 think that in many cases, we can make major errors
3 using these BCF data in the risk assessment.

4 I've shown you the effect of growth. I
5 haven't shown you the effect of dietary exposure which
6 is a key...key exposure route for PBT type substances.
7 It can further only increase the difference between the
8 BCFs that you see in the test and the real values that
9 are observed in the field, and we're really talking
10 orders of magnitude here. So, we can make big mistakes
11 there.

12 So, be very cautious or don't do it at
13 all perhaps. Be careful in the use of these BCFs.

14 Finally, the model results for AGRO, I
15 think, are encouraging. Temporal dynamics of the
16 pesticides in...or pesticide 3, at least, and we also
17 looked at two other pesticides. I don't have the data
18 for you, but they...the model did fairly well in
19 describing the temporal dynamics.

20 It's a flexible model as well, so
21 it...it can be parameterized to represent varying
22 degrees of net deposition, so if you want to
23 parameterize it for a no net deposition environment,
24 you can.

25 I don't think...AGRO, I think, will



1 improve exposure assessment of PBT and non-PBT
2 substances. I think there is still some work that
3 needs to be done in the parameterization of these net
4 deposition rates. I think there is some uncertainty
5 still there, what are the appropriate values to use.

6 And, finally, a...a...a...something we
7 learned or we learned when we went through this
8 exercise is that when you start doing the modeling,
9 it's often interesting to do it in...in...in a two-step
10 way where you verify and apply, and that's perhaps
11 something I learned out of this exercise. Typically,
12 what we're doing with our models is we parameterize
13 them for the pesticide management scenarios, and we run
14 the exposure analysis.

15 And this is maybe a...a very useful way
16 as well. When you take that model and parameterize it
17 for the field conditions that you've got data for and
18 you test your model first with the data, you calibrate
19 it, then produce a new model, a calibrated model which
20 is again parameterized for your management scenario to
21 do the exposure analysis.

22 This will allow you to deal with...with
23 many processes that the model is poorly equipped for
24 dealing with for certain chemicals, perhaps, that it is
25 not truly designed for, or if you're dealing with



1 metabolism and it's poorly characterized, there is a
2 possibility to calibrate these models and then use the
3 calibrated model for the actual management scenario.

4 I'll leave it there. Thank you for your
5 interest.

6 **DR. HEERINGA:** Thank you very much, Dr.
7 Gobas. I'm sure there are some questions, and we'll
8 begin with Dr. Simonich.

9 **DR. SIMONICH:** Thank you, Frank. I have
10 three questions. The first is, are amphibians included
11 in your model?

12 **DR. GOBAS:** No. That's easy.

13 **DR. SIMONICH:** Should they be?

14 **DR. GOBAS:** Yes. This is a good one.
15 No, I...I think you're absolutely right. It...it...I
16 think we still see a lot of risk analysis are done for
17 fish, and we're very good at...at...at...at making
18 estimates for fish, but we often stop at fish, not
19 necessarily, but in some cases, we do, and we should
20 realize that there is much more out there than fish.

21 And especially for PBT substances, this
22 is important, because for a...for the few examples that
23 we have, we typically see examples of wildlife effects
24 in...in higher trophic levels, not necessarily in fish,
25 but in marine mammals, in birds, and amphibians,



1 perhaps, as well. So, we should definitely broaden our
2 horizons and include more organisms and...in...in our
3 risk assessment methods.

4 **DR. SIMONICH:** Second question. On a
5 slide on model sensitivity, it shows that EXAMS and
6 AGRO with 0 percent burial deviate from each other
7 after about 25 or 30 years.

8 **DR. GOBAS:** A little bit, yeah.

9 **DR. SIMONICH:** What would cause that?

10 **DR. GOBAS:** Well, these are really minor
11 differences in...in...in how these models run. I don't
12 know the exact answer to your question right now. We
13 would have to look that up in...in more detail.

14 But these models are...are fairly
15 similar in the way they behave, but there are some
16 minor differences, for example, in the way sorption is
17 calculated, the transfer of mass, for example, from the
18 water phase into the benthic phase. That's set at a
19 value of 0.5. In AGRO, it's calculated, and when we do
20 the calculations, you know, the equivalent value is
21 about 0.89, and that may be one of the factors that can
22 cause these differences.

23 And...but the differences are minor
24 enough that you can say that the models for the AGRO
25 with no burial will produce...at least in that scenario



1 that I showed...similar results as...as EXAMS.

2 **DR. SIMONICH:** And my last question,
3 is...do you consider the soil...the half-life of the
4 chemical in soil and how that chemical may be
5 resuspended or released into the environment each year
6 with piling? Because I think currently, we see some of
7 the past PBT pesticides that are now banned, we still
8 see them deposited in ecosystems each year, and, I
9 think, in part, due to the persistence in the soil and
10 the annual piling of soils in volatilization.

11 **DR. GOBAS:** My understanding is that
12 PRZM takes that to...into account to a certain degree.
13 So, there's runoff from the field into the pond in
14 included, and in that calculation, weather conditions
15 and changes in weather conditions...and...and Ron
16 Parker really explained it well...are taken into
17 account. So, that's really in the PRZM part.

18 Is that..did I answer your question?

19 **DR. SIMONICH:** Yes.

20 **DR. BUCHER:** Dr. Meador?

21 **DR. MEADOR:** I wasn't clear if
22 bioturbation's part of your model.

23 **DR. GOBAS:** Well, bioturbation is really
24 part of the resuspension process.

25 **DR. MEADOR:** So you, in a sense this is



1 obviously more important than others and it will
2 probably keep burial from going deeper, and the
3 variants are really good about ...

4 **DR. GOBAS:** Yes.

5 **DR. MEADOR:** ...keeping the soil mix. So
6 not only effluent water but actually it gives you a
7 human variant.

8 **DR. GOBAS:** Absolutely.

9 **DR. MEADOR:** So, how do you...what's the
10 parameter? How do you actually quantify that?

11 **DR. GOBAS:** That's a good point. That's
12 why I had in my conclusions, you know, that still more
13 attention is needed in characterizing what the
14 appropriate resuspension rates are in ponds of this
15 kind.

16 **DR. MEADOR:** Okay. It's really a
17 physical process.

18 **DR. GOBAS:** Yes.

19 **DR. MEADOR:** Okay.

20 **DR. BUCHER:** Dr. Thibodeaux?

21 **DR. THIBODEAUX:** This question is
22 directed both at Don and Dr. Gobas. Going back a few
23 years, I have seen models go from what I call a
24 thermodynamic base, and now we seem to be having
25 problems, one of them exemplified by the fact that the



1 solubility is limited. And also, I noticed on your
2 models, there is a definite time shift kinetic-wise
3 between sources and what ends up in the fish.

4 And you made the point blank statement
5 that bioconcentration factors are getting us nowhere.
6 Do you think the time is right for future emphasis on
7 transport processes in these models?

8 And, for example, you keep bringing up
9 the idea of particle deposition which...in your
10 transport. It's not an equilibrium process. It's not
11 a reaction process. As we move ahead...and, of course,
12 we hear dynamics from every presenter's lips. We also
13 see time series of concentrations.

14 So, the only question is, do you see
15 maybe we should put...haven't we...haven't we arrived
16 on partitioning? Do we need to do more on
17 partitioning, or are we at the point of diminishing
18 returns? Shouldn't the kinetics come forth, because
19 it's plain to me at this time that's the things that
20 need to be tended to.

21 And, by the way, bioturbation is not a
22 deposition process.

23 **DR. GOBAS:** No, no, the resuspension
24 process...

25 **DR. THIBODEAUX:** No, it's not that

1 either. Anyway, question to both you and Don on that
2 point.

3 **DR. MACKAY:** My answer is yes.

4 **DR. THIBODEAUX:** The question is
5 partitioning. You know, we've done partitioning.
6 Everybody does partitioning. Very few people do
7 transport kinetics. Is that maybe a blind spot that
8 now needs to be fixed?

9 **DR. MACKAY:** Yeah, I think you're
10 absolutely right. There is an enormous literature on
11 basic solubility and thermodynamics and
12 bioconcentration and so on, but over relatively short
13 time periods and episodic inputs, it just doesn't
14 apply, and kinetics is a mass transport in the sediment
15 water process and into the fish and from the fish, it's
16 very much kinetically controlled, and it's basically a
17 mass transfer phenomenon and it has to be quantified.

18 **DR. GOBAS:** One instance, it does not
19 achieve these equilibria in time, so it's the time
20 course to these partition coefficients that is really
21 controlling the...the concentration.

22 **DR. THIBODEAUX:** Kinetically controlled?

23 **DR. GOBAS:** Kinetically controlled.

24 **DR. THIBODEAUX:** And mobility
25 controlled?



1 **DR. GOBAS:** Well, yes, yeah, and
2 especially for these PBT substances, because they
3 behave so slowly because of their properties. The
4 release rates from organisms in particle is very, very
5 slow which basically means that you do not get to see
6 these equilibria ever being achieved. The environment
7 changes too quickly.

8 **DR. THIBODEAUX:** I'm not saying that
9 these parameters shouldn't be in the model, at least
10 not at that valid concept except it's outdated now.
11 Not outdated in the sense we don't need it, but the
12 emphasis of research should move away from partitioning
13 onto how fast, because my first law of chemodynamics is
14 the only way you're going to get partitioning in any
15 phase is to diffuse it from its source into that phase
16 so that fusion and transport has to come before
17 partitioning. Do you agree with that?

18 **DR. GOBAS:** Yeah, I would agree with it.

19 **DR. THIBODEAUX:** Thank you.

20 **DR. BUCHER:** Dr. DeLorme first, and then
21 Dr. Norstrom.

22 **DR. DELORME:** Just a couple of
23 questions, possibly clarifications. I think it...it's
24 good to see this...this work and sort of have my eyes
25 opened a little bit on what's going on out there with



1 temporal courses and...and what not, but as an
2 ecologist, I always wonder where do you bring in the
3 ecological reality.

4 I think of something like a forage fish
5 which may have a life span of two to three years
6 maximum. You've got a...in some systems, you're going
7 to have a lot of your chemical tied up in the biota,
8 and that's going to cycle back and forth into the
9 sediments and through the microbial populations, et
10 cetera, et cetera.

11 I mean, the reality is the stuff just
12 doesn't disappear if it's persistent. I mean, it's
13 being slowly degraded. So, I mean, is there room for
14 moving some of these things into the model at some
15 future date?

16 **DR. BUCHER:** Before you answer that,
17 could everyone speak into the microphones so that
18 everyone in the room could hear, please?

19 **DR. GOBAS:** I don't exactly understand
20 the question.

21 **DR. DELORME:** Well, okay, if you take a
22 look at your...one of your slides, you looked at
23 the...the bioconcen...or food web bio-cumulation model,
24 and you've got, you know, it looks like for forage
25 fish. Okay? Reality is, I mean, you're...you're



1 stating a steady state isn't reached for hundreds of
2 days in some cases.

3 **DR. GOBAS:** Right.

4 **DR. DELORME:** It might exceed the life
5 span of some of these organisms.

6 **DR. GOBAS:** That's right. Yeah, that's
7 correct.

8 **DR. DELORME:** And so, I mean...I mean,
9 it's another consideration. You know, the biological
10 component or compartment where the chemicals end up, I
11 think, is an important component in the model to
12 consider the dynamics of exchange not only to the
13 sediment and the water but also between the biota and
14 the sediment, et cetera, et cetera.

15 **DR. GOBAS:** Yeah, I fully agree.
16 That...that's why we developed the time dependent food
17 web model, yeah.

18 **DR. DELORME:** The other...the other
19 point I have has to do with the amphibians. I think if
20 we're going to look at amphibians, we have to look a
21 redefining what our receiving water body is, because I
22 don't think a 2 meter, 1 hector pond is, you know,
23 appropriate. You have to bring in some ecological
24 relevance there. Just as an aside.

25 **DR. BUCHER:** Dr. Norstrom?



1 **DR. NORSTROM:** Thanks so much for
2 bringing this whole business of...of equilibrium
3 partitioning and dynamics in. I've felt for a long
4 time that it's extremely important to these processes.
5 We're living in an era where everything that was
6 happening with chemicals was fast compared with
7 everything else, so we could get away with it, but in
8 this particular case, we can't. So, for some of these
9 chemicals, I think we have to be dealing with dynamic
10 systems..

11 One of the things...

12 **DR. BUCHER:** Speak into the microphone,
13 please.

14 **DR. NORSTROM:** All right. Well, as
15 close as I can get to it without sort of swallowing it.

16 I presume that the reason for this
17 rather short depuration half-life in the white paper
18 on page 139 for chemical 4 is due to growth dilution.
19 I had a question on that. I wondered how something
20 with a KOW that high could be depurated into the
21 half-life of 30 days, but that's the bluegill sunfish.

22 **DR. GOBAS:** Yes. It's growth dilution.

23 **DR. NORSTROM:** The...the other comment
24 I'd like to make is that I don't know...I used to be a
25 physical chemist in the dim distant past. Actually, it



1 wasn't a Ph.D. then, but if I remember correctly,
2 equilibrium constants like log KOW are actually ratios
3 of rate constants, strictly speaking. They're not just
4 ratios of concentrations at equilibrium.

5 And so, a partitioning constants in that
6 sense can theoretically be dynamic, and we could have
7 situations where two chemicals with the same log KOW
8 would actually have very different rates of transfer
9 between the two media. If the solubilities were
10 different in the two, you could have different rates of
11 transfer. Is that correct? I...I'm...sort of in my
12 simplistic view of things, that's the way I would look
13 at it.

14 **DR. GOBAS:** I...I think you can look at
15 it both ways. At equilibrium, the weight of the flux
16 in and the flux out become equal, and this was a cause
17 and effect. I tend to look at it from a thermodynamic
18 point of view. The equilibrium corresponds to equal
19 chemical potential or equal fugacity in the two phases,
20 but at the same time, the fluxes are equal.

21 So, it's just, I think, a different way
22 of saying the same thing.

23 **DR. BUCHER:** Dr. Hickie?

24 **DR. HICKIE:** A couple of questions. One
25 is does your dynamic food web model still use



1 equilibrium partitioning into plankton?

2 **DR. GOBAS:** The...no, it's not.

3 **DR. HICKIE:** Okay. Second question,
4 then, is in this model, you have one grouping of 1kg
5 fish.

6 **DR. GOBAS:** Mm-hmm (indicating
7 affirmatively).

8 **DR. HICKIE:** And you're running it for
9 30 years. Is it the same 1kg fish, or are you...are
10 you reintroducing a new fish that has acquired some
11 burden of contaminant before it joins the 1kg fish
12 study?

13 **DR. GOBAS:** That's a...that's a good
14 point. In this simulation, the answer is no. So, this
15 was the same fish. You can do it and create new
16 generations of fish.

17 **DR. HICKIE:** You're actually getting
18 population turnover and...

19 **DR. GOBAS:** Yes. That was not done in
20 this example, but you can, and we have done that.

21 **DR. HICKIE:** Okay. Third thing just
22 comes back to sediments. You gave your example of the
23 decline of PCBs in Lake Ontario suggesting back when
24 you wrote that paper that the half-life was 5.5 years,
25 and, really, since about 1985, that has stalled, it is



1 virtually no change, so I'd just like to hear your
2 comment on how sediment burial has come into play in
3 explaining that.

4 **DR. GOBAS:** Well, the...I think the
5 answer is that the...the loadings have not kept going
6 down. So at a certain point, the loadings have put a
7 lid on that going down of the concentration, and so,
8 the example I've shown you is not ideal, but, of
9 course, many...in most...most cases, the environment is
10 not ideal to demonstrate some of these more theoretical
11 points.

12 And all the data
13 that...that...that...that were included in that study
14 indicate that if the loadings would have continued to
15 drop, that's the rate of decline in concentration that
16 would have been expected. Initial decline was actually
17 seen, but it didn't last long enough because of the
18 loadings. The loadings didn't go down anymore.

19 **DR. NORSTROM:** In that then can you
20 separate out the change in loadings from the rate of
21 burial?

22 **DR. GOBAS:** Yes, yes, you can. In the
23 model, you can, but the point of the example was to
24 demonstrate that when...that when loadings stop,
25 concentrations don't just stay the same forever. It's



1 not a continuous accumulation. The system actually has
2 ways of...of...of eliminating chemicals even when they
3 are persistent ones, and the key one that was
4 identified in that study and also in the study that Don
5 did earlier on...on...on the same topic was that
6 sediment burial is the key loss route for PCBs in that
7 system.

8 **DR. NORSTROM:** Thank you.

9 **DR. BUCHER:** Dr. Maddalena?

10 **DR. MADDALENA:** Frank, thank you
11 for...really, a lot of kudos for saying here's the
12 model and in this last slide, here's how you use it.
13 I...I appreciate that.

14 I wondered if you could elaborate just a
15 little bit on what you mean by calibration.
16 Specifically, I'm interested in is there a formal
17 process that you like to use for your food web model,
18 and if so, were the results that we saw that looked so
19 nice, were they calibrated previously, or were they raw
20 inputs and here's your output?

21 **DR. GOBAS:** No, what I've shown you is
22 not calibrated. So, these are just...just the raw
23 calculations, but in terms of getting to bio-cumulation
24 issues, there's...the issue of metabolism is a really
25 important one. Organisms in...in...in many cases, have



1 the ability to metabolize chemicals. These rates can
2 vary tremendously between the organisms or at various
3 times of the year and under various conditions.

4 It's...it's not possible at this point,
5 although we're making some progress lately, especially
6 Joan Arnett who worked on this issue or wrote a thesis
7 on this, but we're still not there in terms of
8 calculating metabolic transformation rates of...of
9 chemical in...in biota.

10 And that may be an issue for pesticides
11 that are metabolized, since we do not have that
12 capability to estimate what these metabolic rates are.
13 The calibration step provides you with a way to take
14 metabolism into account.

15 **DR. BUCHER:** Are there any other
16 questions at this point?

17 (No response.)

18 **DR. BUCHER:** Okay, thank you very much
19 for those presentations.

20 I think we'll move on now to the last
21 presentation before the break. It's Dr. Robert
22 Ambrose, Ecosystems Research Division, National
23 Exposure Research Laboratory at ORD of EPA, on Sediment
24 Transport Processes in Pesticide Models.

25 **DR. AMBROSE:** First, I want to say it's

1 good to follow these previous two talents, I've
2 followed the careers of Dr. Mackay and Gobas to some
3 degree and hold them in high regard, and I particularly
4 do want to say up front a couple of things. One, how
5 you set up and use the model, I think, is more
6 important than which model you choose or which
7 processes happen to be explicitly represented in the
8 models, because we often implicitly set up and use a
9 model in...in the right way. If we have good process,
10 we can still get a good result from a model that is
11 less explicitly process based.

12 I, too, have a couple of other models
13 for consideration, but I did want to say that latter
14 point.

15 And another prefatory comment from the
16 start is, no, Dr. Thibodeaux, these models do not have
17 bioturbation, either, but they are representatives of
18 that process in the same deficient way. We should be
19 better on that in the future.

20 I should also...I'm sorry. I have to go
21 back. I won't go back, but just to say that Dr. Earl
22 Hater is the co-author of mine. He's the real expert
23 in sediment transport processes.

24 I'm going to be talking to some degree
25 about sediment transport processes and their



1 applications in models, and yet, most of these
2 processes are flowing through some stream systems, and
3 the focus here is really on ponds, so I'm going to talk
4 about ponds as well. I'll go through the process part
5 of it maybe too fast in order to get through on time.

6 This is the conceptual diagram, and the
7 main point I want to make here is that the chemical
8 concentration is what we're after in this fate model.
9 It's informed by, its course by the sediment processes,
10 so I'm going to focus on the sediment processes, but
11 you have to keep in mind that they're not an end in
12 themselves here, at least, but a means to get better
13 chemical concentration.

14 Soils dynamics, I do believe, is
15 important, and that's been well covered in previous
16 talks, so this lists different ways in which I believe
17 soils dynamics are important, and we end up in the
18 bottom and buried below the bioturbation depth. I want
19 to say it potentially sequesters chemical from biota.
20 I think it's an important loss process, but still a
21 comment, I think, that originally came from Larry
22 Burns, it might be unwise to assume that buried
23 chemicals stay buried forever, and that's a regulatory
24 type of decision. In any case I, myself, do like to
25 include burial and other processes explicitly.



1 Now, given that they are important,
2 there are some technical issue that we have to address
3 when we're applying sediment transport models. To some
4 degree, there are similar technical issues with any
5 kind of modeling.

6 Spatial heterogeneity has to be
7 recognized, and these real environments which we
8 represent as a simple two-layer pond, are really a
9 combination, or a simple stream. They're never really
10 simple when you get down to the details. When you
11 focus in, they're infinitely complex.

12 There's always spatial heterogeneity
13 that we do not take into account in the models. Can't
14 get away from it.

15 There's temporal variability as well,
16 and at some point, the process-based model that you
17 have will not represent branding in motion, for
18 instance. There's no need to, of course, but at some
19 point, the models break down temporally as well as
20 spatially.

21 We also have to recognize in the
22 sediment realm, there's a virtual continuum in the
23 sediment out there. It's not just one type or two or
24 three. The models will inevitably have two or three or
25 maybe ten, but they don't have everything, and it goes



1 all the way from gravel down to dissolved organic
2 matter or colloids, et cetera.

3 Finally, we have to recognize the
4 availability of input data. We're always limited by
5 that. No matter how good a job you do calibrating the
6 model, getting test data sets, when you apply it
7 somewhere else, you won't have all the force in
8 functions. Even something like rainfall, you might have
9 good daily rainfall that might be 20 miles away, and
10 it's not going to be the same rainfall as your site.

11 So, you have to recognize these, so
12 given these issues which will always be there, and
13 given that we want to do a better job representing
14 reality, what, Dr. Einstein, should we do? What is the
15 goal of building the models?

16 And I...this has been sort of a...a
17 guiding philosophy. I think a lot of people do share
18 it, make things as simple as possible, but not any
19 simpler. Which of course, begs the question of what is
20 simple as possible.

21 So, how complex should the model be that
22 we're trying to build up? I have several points to
23 make here, and I'll try to make them reasonably fast.
24 We can discuss it later.

25 First of all, it's obvious that some

1 environmental systems are more complex than others. An
2 estuary is a lot more complex than a farm pond. Small
3 streams can be quite complex, so it's not just the size
4 of the water body that makes it complex.

5 Some pollutants are much more complex
6 than others. Salinity or a monoamine dye tracer is not
7 the same thing as, say, mercury.

8 Finally, management questions. Some
9 management questions that are asked are relatively
10 simple to answer and can be answered with conservative
11 assumptions, the screening kind of models. What is a
12 safe screening model, say. But other management
13 questions are very difficult. Some management
14 questions evolve. Well, how long is it going to take
15 to clear out that estuary? What is a safe level to
16 clean up this site to, given the possible flooding that
17 might happen.

18 Keep in mind that when you design the
19 model, you might be asked one question and design a
20 perfectly good model for that question, but there's
21 always mission creep. Managers will then say well,
22 okay, that's good, what if...and so, it might be good
23 to have a model a little bit more complex and capable
24 than the question right at hand and anticipate the next
25 one, like what was asked earlier about, in a sense,



1 buffer strips, what happens if runoff from the field
2 goes over another portion of land, what happens there.
3 So, you do have to recognize that.

4 Now, if your model is too simple, there
5 are some consequences, and I think we all recognize
6 them. If you miss key processes...and let's just take
7 burial as a...as a potentially key process for some
8 chemicals...you might not be...you might not
9 extrapolate correctly to the future. You might...your
10 model might be wrong.

11 You might not actually be able to
12 address even relevant management questions. If you
13 have a steady state model, you cannot use that directly
14 to answer questions about how long will it take to
15 clean up.

16 It might be a perfectly good model, but
17 it might not be defensible in an adversarial review,
18 and we've all seen adversarial reviews where models are
19 attacked unfairly. Sometimes, it's fair, sometimes
20 unfair, but just sometimes it's better just to go ahead
21 and say okay, I don't think it's important, but we'll
22 put it in anyway.

23 Now, there are some consequences to
24 overly complex models, however. It can add unnecessary
25 data collection, computational burdens, and you'll see



1 a little bit of that later in my talk.

2 Some people say it adds to uncertainty.
3 I don't necessarily buy that. I'm not sure,
4 philosophically, how more knowledge can lead to less
5 knowledge, but some people that have studied this that
6 are smarter than me in statistics assert that.

7 But I think the other thing is it shifts
8 the focus away from the problem at hand into something
9 that might be endless analysis. Coming from the Office
10 of Research and Development, endless analysis sounds
11 fine to me, but the regulatory agency, you need to keep
12 your eyes on what is the question at hand. So, I have
13 seen cases where too complex a model gets you
14 sidetracked.

15 Okay, let's launch into some of the
16 transport processes. This is a cartoon slide, and we
17 have...it has...does not have a picture on here of
18 internal biotic production of organic matter. I will
19 say right at the start that one of the models I'll be
20 talking about, the ERB model, was...does do internal
21 biotic production and keeps track of the organic matter
22 as a separate state variable.

23 And we generally divide the world into
24 cohesive and non-cohesive solids. We have the settling
25 and deposition processes for both erosion, scour or



1 entrainment, bed load, and down in the sediment bed,
2 we'll have consolidation and burial.

3 So, I'm going to go through some process
4 equations that will cover some of the...most of these
5 processes, and first of all, just to recognize in a
6 flowing system, we have velocity profiles and the sheer
7 stress profile, and the sheer stress at the bottom
8 tends to be a property of that system that drives
9 the...the exchange of the solids and the chemicals
10 associated with the solids between the bed and the
11 water column. So, the tail's a B.

12 So, calculating the different kinds of
13 stress, the sheer stress that you can calculate the
14 grain-related bottom sheer stress or skin friction
15 factor is, I am told, from my esteemed co-author, is
16 the proper one, and this is the formula given, the key
17 here is that bottom sheer stress is a function of
18 velocity squared, and it's an inverse function of the
19 log of the...of the depth. That's another
20 parameterization in there.

21 Now, settling. Non-cohesive settling is
22 a function of the particle diameter and the density of
23 the particle along with viscosity of the water. There
24 are different expressions. Stokes is...is something
25 that's been around for a long time. Notice that it's



1 a...a function of the particle diameter squared and the
2 density of the particle minus the density of the water.

3 A more complex expression than Ryn...and
4 I'm not sure if I'm pronouncing his name right, so
5 somebody could correct me right here...Ryan...Ryn,
6 okay, thank you. I wasn't sure about that. I had
7 three different pronunciations.

8 The...this breaks down the settling
9 velocity into three regimes. The top regime is the
10 same thing as the Stokes comes out, and once you do the
11 math here, it's the same thing as the Stokes velocity.

12 And the bottom regime...and the Stokes
13 is again a function of diameter squared and...and rows
14 of this. The bottom is a function of diameter to
15 the...the square of the...the square root of the
16 diameter and the...and the density, and there's a
17 transition zone.

18 So, you can see you can get it more
19 complex and probably more realistic.

20 Now, that's settling. What's
21 deposition? If you have spill water, they should be
22 the same, but there's a probability of a particle
23 sticking, and if you...if the water moves, that
24 probability goes down, and if the water moves fast
25 enough, the particle won't stay on the bottom.

1 So, there's a parameterization of this
2 alpha term, probability of deposition, which is
3 more...goes from 1 to 0 as shear stress goes from 0 to
4 a critical value. That critical value can vary quite a
5 bit.

6 By the way, when you have a pond
7 that...that has no outlet, it doesn't matter what the
8 resuspension velocity is. The burial rate is equal to
9 the mass coming in. Resuspension just makes the water
10 column concentration of solids higher, but burial rate
11 still stays the same at equilibrium.

12 Going into non-cohesive entrainment,
13 there's velocity, $WT \text{ bar}$. There's entrainment which is
14 mass flux based, and these are based on particle
15 diameter and density along with the bottom shear stress
16 and the critical shear stress.

17 There are different formulas, many
18 different ones out there. Van Ryn's expression here
19 is, I believe, used in the model that Oldhager is
20 working with, and you can see that it's a function of
21 the particle diameter and the shear stress over the
22 critical shear stress or critical shear stress
23 minus...the shear stress minus the critical over the
24 critical to the 1.5 power. Again, times a shields
25 number. So, this will vary with particle size.



1 There are more complex formulations.
2 There's one from C.N. Parker. I don't follow that
3 literature well. I just know that they do collect
4 data. They do spend their lives on this. It
5 represents the processes but still needs to be
6 parameterized, and I'm going to get back to that at the
7 end.

8 But for cohesive sediment resuspension,
9 this is a Lick formulation here. Functionally, looks
10 same as the Van Ryn. It's a multiplier times...times
11 shear stress minus the critical value to a power. It's
12 just the multiplier and the power will be different,
13 and you'll notice that this is not by particle size,
14 but it's for the cohesive hit.

15 There's a wide range of values that
16 represent the different cohesiveness of the different
17 types of soils or sediments, and they have to be
18 determined experimentally and/or with model
19 calibration. I understand that there are experimental
20 apparatus, the set plumes that can be used to get these
21 model parameters and constrain the model or constrain
22 this part of the model, this equation, better.

23 There's bed load transport, and I'm
24 not...well, some models have it. The good models, good
25 sediment transport models so.



1 And, finally, I want to mention burial.
2 Generally, our models will do this by mass balance, so
3 the excess mass goes into a settling velocity or
4 settling mass flux.

5 Given those sediment transport
6 processes...and those aren't all, but that's...I'm
7 trying to...trying to stay somewhat within my
8 time...there are other things that are not covered
9 usually in our models, because of their complexity.
10 Stream bank erosion is one, though people are working
11 on it.

12 Watershed erosion and delivery by
13 particle size has been mentioned before. Generally,
14 the watershed models give us total erosion and would
15 parameterize that total erosion with particle size
16 fractions from the parent soil, perhaps modified by
17 some enrichment ratio. Nevertheless, they don't treat
18 this erosion and delivery explicitly by particle size.

19 Flocculation in fine-grain sediments,
20 there are ways to do that implicitly. I understand
21 that explicit formulations are somewhat lacking.

22 Bed load armory, I understand they're
23 implemented in...I'm not sure if it's just like Van
24 Ryn's or, Willie, whether I can pronounce your...SEDS?
25 SEDSLESAY...just go ahead and...okay...which has



1 several particle sizes which are needed to do the
2 armory.

3 And, finally, no model will handle
4 fine-scale heterogeneity and temporal dynamics if you
5 get fine enough.

6 Now, I want to move toward the models
7 and example output. EXAMS is on the simple end. The
8 EFDC model was a SEDS CLJ process based algorithms on
9 the other end of the spectrum, and then WASP, the one I
10 know personally the best and work with end up with...at
11 the intermediate algorithms.

12 Now, EXAMS scientific modules, it does
13 do flow continuity, although in the farm pond example
14 here, it...it, you know, that was bypassed as just
15 water dumped into the pond, but it..it will do flow
16 continuity and do variable flow as well. Constant
17 geometry, however, so it won't do small streams very
18 well, but I think it will do ponds just fine.

19 Solids balance is not simulated
20 explicitly. You input the total suspended solids in
21 the water column and the benthic solids, and that's
22 used descriptively. It does do organic chemical fate
23 in a detailed way.

24 You've seen this before, this picture
25 before, and there are a couple notes I wanted to make

1 on it. I've been taking notes during the earlier
2 talks.

3 The lumped mass transfer coefficient
4 which takes into account the poor water diffusion
5 settling and resuspension...don't worry about
6 that...it's not just poor water diffusion of dissolved
7 chemical. Larry did this in such a way that it
8 actually turns over the solids as well and takes into
9 account the water column solids, the benthic solids,
10 and their partition coefficient in the water and the
11 sediment.

12 So, if you have a high partitioning
13 chemical, it's not going to overlook the mixing process
14 for it. You know, this poor water diffusion won't do
15 much for high partitioning chemicals, EXAMS will. So,
16 it does cover sort of a solid turnover implicitly.

17 What it doesn't do here is this is a
18 symmetrical process. The solids going down is equal to
19 the solids going up which is okay. That, I think,
20 handles bioturbation turnover reasonably well, but what
21 it doesn't handle is you can have excess solids that
22 leads to burial. This is just turning it over, and if
23 you add a decay term on the bottom, that will kind of
24 vary it, but you didn't have the excess solids feeding
25 it, so it's not quite the right thing. So, it doesn't



1 have an asymmetrical exchange there of the solids.

2 But you can put a constant first order
3 rate in, and it will do something. Again, the way you
4 use the model, how you parameterize it, is more
5 important than the model. You can probably
6 parameterize this to handle solids if you take a more
7 complex model and sort of match these models up. Okay,
8 enough of that.

9 Environmental fluids dynamic code, EFDC
10 is on the high end of complexity for hydrodynamics.
11 It's typically applied to estuaries, three dimensional.
12 It's got various versions out there. It's got a little
13 bit of a version control problem.

14 Our hydrodynamics link was lost, and we
15 use that down in Region IV a lot for the estuaries.
16 It's a very personal, very complex, and capable model.
17 Does the salinity, temperature, hydrodynamics, and Earl
18 Hater's been working with it to add the solids
19 balances.

20 So, it's got directly coupled sediment
21 and contaminant transport, wetting and drying of flood
22 plains and mud flats, tidal marshes, near-field mixing
23 in it, hydraulic control structures, et cetera.

24 A model like this desperate needs good
25 software to help you run it. It's very difficult to



1 run. It takes a lot.

2 The work on grid generating...grid
3 generation code, there's one almost available. It's
4 almost impossible to do it right by hand.

5 A sediment transport process is in it,
6 are virtually the ones that I covered earlier. It does
7 not, as far as I know, include internal production.

8 It's applied here to a Superfund site,
9 Pucitonic River. There are two different modeling
10 regimes, the upper and the lower. It's gotten in as a
11 Superfund site with PCBs. A couple notes here I want
12 to make sure I cover. Earl Hater is doing the bottom
13 portion of it, about 30 to 35 km at a stretch. 4800
14 computational cells that includes the flood plain,
15 water sediment in flood plain, 5-year simulation. I
16 show one year from it. Takes three days to run on the
17 computer.

18 So, we're talking about very high end.
19 You're not going to keep running this over and over
20 with different scenarios. You know, you turn it on and
21 take a long weekend or something.

22 It's embedded in, like a lot of models,
23 in...in...it's like the other models, HSPF feeds the
24 sediment to EFDC here, and there is a, I think, QEA. I
25 can't even read it. It says...there's a bio-cumulation



1 model as well.

2 HSPF modeling domain, you can see the
3 sub-watershed, and this would be typical of setup for
4 SWAT and HSPF, but I won't go into how you set those
5 up.

6 And, finally, some example output.

7 There are five years of example output with PCB data
8 below this Superfund site. These are log scaled, so
9 you can see the extreme variability in the stream
10 system covering flood plains as well as the seventh.

11 So, that's a very high end of what you
12 might do in a flowing system.

13 I want to spend the rest of the time on
14 the intermediate end. WASP seven is a very general set
15 of water quality modules. It will do internal stream
16 transport using kinematic wave routing, so it will have
17 variable flow velocity, depth, width. It also will
18 have outflow arrears equations, so if you have ponded
19 reaches, it can do outflow over sills and weirs.

20 Or it can be linked with external hydro
21 models so you can apply it at estuaries such as the
22 FDC. It does solid balance silt, sand, and particulate
23 organic matter in the water column and sediments, and
24 it's got some different water quality modules that are
25 independent but now, as of this year in a project I've



1 done, linked together if you want them to be, or you
2 can run them independently.

3 The Heat Mounts module is taken from
4 C40W2, and so, James Martin put that together in MOS.
5 It takes solar radiation, MET data, wind speed, et
6 cetera. Predicts water temperature along with
7 pathogens and other things.

8 The water quality module, we have an
9 advanced mutual module that's similar to many other
10 advanced mutual modules around nutrient cycling, three
11 species of phytoplankton, benthic algae, the organic
12 matter fraction, dissolved oxygen and carbon.

13 This can be run independently, or you
14 can run the...or it can take the output temperature, et
15 cetera, from the heat model. Likewise, it produces an
16 intermediate file that includes temperature and then
17 the biotic substances, the production rates, et cetera,
18 that feed forward to the mercury and organic chemical
19 models.

20 So, you can run organic chemical models
21 as a simple model, a simple pine models with input, or
22 you can run them linked with very detailed variable
23 biotic.

24 Okay, the same geometry with a kinematic
25 wave routing is based on hydraulic coefficient, so you



1 can, depending on what coefficients you set, you can
2 have U-shaped stream reaches or V-shaped stream
3 reaches.

4 The sediment transport processes, you
5 know, the same general ones but they're not as detailed
6 process based at this point. In the past, ROSS would
7 allow the user to specify deposition and resuspension
8 velocities. We now have internally in a test version
9 in our own internal projects, both based on stream
10 velocity to power, and we're not even going to publish
11 that, because we're going to go ahead and put in the
12 standard shift stress formulations. The results you
13 see here are based on velocity to power...velocity
14 minus critical velocity to a power.

15 The solids kinetics in ROSS, we have
16 biotic solids and inorganic fines linked together in
17 sands, and you can input the production rates, have
18 them vary in time, and with temperature and dissolution
19 rates.

20 Okay, gonna show a few pond simulations.
21 First one is chemical only. It's EXAMS like, it's not
22 exactly the same as EXAMS, because the sediment-water
23 exchange is a little bit different. The sediment
24 chemical version is the standard ROSS type of
25 simulation. We're going to do this with steady loads



1 and then unsteady loads.

2 So, basically, I'm trying to isolate the
3 effect of burial on the pond on this.

4 It's a standard pond that I set up
5 hopefully close to the EFED pond, 2 meter, 1 hector,
6 and for the steady case here, just steady silt
7 and...and PON and sand input as well as water input.
8 You have to make an evaporation rate to match the input
9 in order so there wouldn't be outflow, because ROSS
10 will predict a variable water column and outflow.

11 Internal production, I just did a, at
12 least at first for this a constant. Our production
13 rate constant and dissolution rate in the upper
14 sediment layer. We have two sediment layers defined
15 here, 2 cm and 3 cm so the total is a...is a 5 cm
16 layer. Deposition and resuspension in this...at this
17 point are constant, but they vary in the next
18 simulation. And then, the three chemicals I just
19 picked.

20 I tried to get a span of partition
21 coefficients from low to high and biodegradation rates
22 in the upper sediment from low to high, because the
23 active burial will be different for the high
24 partitioning chemicals. It will be more important for
25 those than it will be for the lower partitioning,



1 higher decay chemicals. And the note, those chemicals
2 are not the same as the OPP chemical 1,2, 3. These are
3 just chosen here for purposes of this talk.

4 And there are some results. Water
5 column...since I have steady input, no outflow, the
6 concentration of chemical in this 20-year sim...solid
7 in the 20-year simulation is constant. The sediment
8 bed on the bottom left...and once we have constant
9 density, it does a mass balance, and if there's more
10 mass than...more mass coming in, the upper sediment
11 layer will rise or fall, and then, at a sediment time
12 step, we'll bury chemical out.

13 So, you can...you can see that...that
14 the comp...the composition, sand, silt, organic matter
15 in the sediment bed will change over time if you have
16 done it in simulation, and burial velocity on the
17 right-hand side is...is calculated here, 0.4 cm/year.
18 In the steady input, that will match the solids coming
19 in, solids plus the internal production rate.

20 Now, on the left is a chemical only
21 simulation. On the right is the sediment chemical
22 simulation. There's not a...you know, with something
23 this small, mainly the thing that I want to call your
24 attention to, chemical 1 is the...the low partitioning
25 chemical. The difference between the left and the



1 right which is due to burial is about 6 percent for
2 chemical 1, and 26 percent for chemical 2.

3 Chemical 3, the higher partitioning
4 chemical, it's greater than 33 percent. Likely to be
5 50 to 100 percent, but 20 years is not a long enough
6 simulation to get any kind of steady state when there
7 is no burial. When there is burial on the right-hand
8 side, you see that it got to steady state.

9 I think these kind of match the
10 simulations, in a sense, you saw earlier with the other
11 models, and it would be good to check these models
12 against each other. Usually, you learn something.

13 Finally, an unsteady simulation, I took
14 run-off and erosion from the Suratt model which is
15 applied to Middle Swamp in North Carolina, and I just
16 adjusted that and put it into this farm pond
17 simulation. 6-year meteorological record, and on that
18 simulation with ROSS, I also had simulated variable
19 production, and I put that into this as well, so it's
20 internally biotic production.

21 The chemical concentrations were just
22 set to 1 g/L in the runoff water, and as you can see,
23 like you've seen in many earlier simulations, you get
24 spikes for the runoff events. Here, you'll see on the
25 bottom right spikes in the burial rate now as well.



1 And on the bottom left, you can see the composition of
2 the upper sediment layer varying slightly, buffered.

3 And this is the chemical concentration.
4 Water column on the upper right. So, again, you can
5 see variability there.

6 How important is that variability? I
7 think it's probably good to simulate it and then take
8 the average rather than do a steady state simulation.
9 And, in fact, OPP does that in simulation. They just
10 don't do it with the solids, but they do it with the
11 chemicals. Perhaps we'll find a way to do it with the
12 solids.

13 I've got some Middle Swamp applications
14 for stream system that shows the 12 digit HUC, and it's
15 got 12 reaches in it. This is output, typical kind of
16 output you'll get at the mouth. This is the lake
17 modeling system with temperature, biotic production,
18 and solids. Temperature on the bottom right. You can
19 see the seasonal variations.

20 The...the depth and width and velocity
21 are varying dramatically. And the bottom right shows
22 some burial rates coming from this excess. I think
23 it's not calibrated properly yet, so it's not a final
24 result, but we have a lot of excess solids coming in
25 this agricultural area. I don't really believe those



1 production rates, but those are the burial rates, so
2 this is the type of output you'll get in a stream
3 system as opposed to a pond system.

4 And rushing on to the conclusions,
5 'cause we either have a late break or miss the break,
6 one of the two.

7 Process based equations are available to
8 represent sediment transport in diverse water bodies,
9 and I think that they capture the trends that you want
10 to capture. And I think simulations, particularly in
11 streams, can be improved by incorporating those, and
12 we're going to be...we are doing that in ROSS now.

13 But they also rely on site-specific
14 parameterization. We have to pay attention to how
15 we're going to do that if we use them.

16 The simulations will always be limited
17 by...by the data that we have to drive them, and I do
18 think that case study tests are going to be important
19 between the models and with real data to properly
20 parameterize and properly use whichever suite of models
21 is chosen here.

22 So, I think that's the main...most of
23 the points I wanted to make, and it's faster than I
24 usually talk, so I'm going to take a breath here and
25 turn it back to the moderator.



1 **DR. BUCHER:** Thank you very much, Dr.
2 Ambrose.

3 I think what we'd like to do is give
4 everybody a chance to take...catch their breath, and
5 we'll take about a 15-minute break now and come back
6 and address questions to you, if you wouldn't mind
7 coming back at that time. And we'll see where we are
8 in the afternoon then and adjust accordingly.

9 So, come back at about, oh, five after.
10 **(WHEREUPON , a brief recess was taken.)**

11 **DR. BUCHER:** Okay, I think we can begin.
12 Take your seats, please.

13 **DR. AMBROSE:** Before the questions, I
14 did want to mention that in ROSS, we do...in the heat
15 model, we do ice cover, and that does affect, it feeds
16 forward and it does affect gradation and volatization.
17 There was a question earlier about that in another
18 model.

19 **DR. BUCHER:** Okay. I've been asked
20 again to remind folks to get close to the microphones
21 and speak loudly.

22 We can now take questions on the last
23 presentation. Yes, Dr. Mehta?

24 **DR. MEHTA:** You know, the last two
25 presentations, both of those emphasized resuspension



1 and deposition. You know, many lakes in Florida, they
2 are like 2 meters deep, and the waves are one second or
3 less because of the short phase, and so the waves don't
4 reach 2 meters depth...okay...typically, unless you
5 have a storm, and then you have the sub-micron size
6 particles. What happens is that you get this, you get
7 two layers, basically. You get a lower layer of
8 sub-micron particles with high density, and then you
9 got an upper layer which is basically a water.

10 Basically, what happens is that due to
11 wave action and the boundary layer that it creates,
12 even though you have no exchange within the bed and the
13 water column, you do have mixing of the two waters, the
14 lower particle-concentrated water and the upper one.
15 And so, it...it's like a classical mixing process
16 between two fluids.

17 And so, in...in...in...in fact, in many
18 of those lakes, that's the primary process and not
19 classical erosion and deposition except when you have
20 strong winds and hurricanes and so on. So, it looks
21 like that mechanism could be simulated as well to
22 determine how the nutrients or contaminants exchange
23 between the top of the water column and the bottom of
24 the water column.

25 The other comment I had was regarding



1 the effect of temperature. You know, the effect of
2 temperature on erosion is substantial, and, in fact,
3 what happens is that when you bring the temperature
4 down, the erosion rate decreases quite a bit. A lot of
5 these models actually are not applicable to the
6 situation that you describe, because without the
7 temperature effect, you will be grossly over-predicting
8 the rates of erosion and also the second thing is
9 because of viscosity of the fluid exchanges, especially
10 the viscosity's high use of these sub-micron particles.

11 So, there are a lot of these processes
12 that...you know, you made a statement that process
13 based equations are really, like to say that they are
14 available, but they do not capture a lot of the
15 phenomena that you see both due to effect of
16 temperature and due to sub-micron particles and the
17 effects of waves.

18 **DR. AMBROSE:** I was looking real quick,
19 the effect of temperature on viscosity is certainly in
20 some of these equations, but there might be other
21 temperature effects that are not captured.

22 As to the...the other point you made, I
23 think that goes into a general point about how you set
24 up a model is more important. You know, certainly WASP
25 and I'm sure EXAMS, and I'm sure that the...these other



1 models could be set up with a bottom boundary layer but
2 settling down to, at some exchange between the two
3 fluid layers.

4 If...if...if that can be characterized
5 well enough, I'm sure the models are robust enough to
6 capture that in some way, and it may be that we ought
7 to set up a pond with two water column layers. That
8 might be a recommendation.

9 **DR. BUCHER:** Are there other questions?
10 (No response.)

11 **DR. BUCHER:** Thank you very much, then,
12 Dr. Ambrose.

13 Next we'll move on and hear from Dr.
14 Parker again concerning Conclusions On Simulating
15 Sediment Dynamics for Pesticide Aquatic Ecological
16 Exposure Assessments.

17 **DR. PARKER:** Well, thank you again, and
18 hello again. I'm going to provide a few very brief
19 summary comments, and...and then add a few
20 considerations which I hope may just assist in...in
21 your deliberations and questions over the next few
22 days.

23 Dr. Ambrose has showed us that in
24 modeling sediment dynamics, we can be about as complex
25 as we wish and still not approach the ultimate



1 complexity of nature which is...is far, far beyond what
2 we will ever be able to...to model. Dr. Einstein
3 in...in Bob Ambrose's slides reminds us to make things
4 as simple as possible but not any simpler, and we, in
5 EFED, ask ourselves what does that admonition mean for
6 us, and...and I'm sure you'll be asking yourselves that
7 question.

8 In the EFED modeling presentations,
9 we've seen a summary of...of current EFED methods
10 and...of aquatic exposure modeling and at least a brief
11 rationale for...for their use and why they're useful
12 for us. And Dr. Mackay and Dr. Gobas' presentations,
13 we have seen how other scientists have looked at these
14 same issues and...and come up with some similarities
15 and...and some differences.

16 I thought it was very interesting in
17 looking at the quotes, Dr. Ambrose's quote from Dr.
18 Einstein, that young Hans Einstein would take up, based
19 on that quote, would take up such a...a complex issue
20 to...on which to base his career, and I'm sure there
21 are other people in this room who have marveled on the
22 complexity of the issues that they work with every day.

23 EFED faces a unique set of
24 considerations that are, I think, different from all of
25 the other EPA programs. I guess we all think we're



1 unique, but we really are unique. EFED performs
2 exposure assessments for national risk assessments and,
3 occasionally, for more limited areas.

4 And each of our simulated sites
5 represents exposure not only for that single modeled
6 location but also for hundreds or thousands of
7 additional sites. So, we're looking for our...our
8 representations are...are much wider than just looking
9 at a specific...looking at a specific site.

10 Our current risk assessment methods
11 require a single concentration duration value for each
12 exposure assessment endpoint, as we were pointing out
13 this morning, for each crop on the pesticide label.
14 Many times, we have 400 crops on a pesticide label, so
15 that becomes a...a major consideration, and each of
16 those crops has a unique growing area that is a
17 function not only of soil and climate but also of
18 the...of the market for the product or processing
19 facilities which may or may not be...may or may not be
20 available.

21 EFED's single farm pond is static by
22 design in order to provide an appropriate conservative
23 surrogate for other surface water, and in looking at
24 that other surface water, certainly much of that
25 is...is flowing surface water in which case the



1 sediment dynamics are entirely different, and burial
2 may happen on a temporary basis but very rarely on a
3 permanent basis. It may be buried by one medium-sized
4 storm that comes by, and it may...it may be buried for
5 a while, but the next time a bigger storm comes by,
6 it's...it's very much unburied and moving on
7 downstream.

8 And even though looking at burying DDT,
9 for example, for...for a period of time, it doesn't
10 necessarily stay buried, and we don't want farmers that
11 have to dredge their farm ponds in case that it does
12 fill up in 30 years. If they're dredging their farm
13 ponds, we don't want them to have a...a hazardous
14 material that they're having to...that they're having
15 to deal with.

16 EFED has explored using a flowing stream
17 for higher tier exposure assessment as a response to
18 a...a previous SAP. That SAP recommended that we
19 evaluate some of the basin scale models, and we've made
20 some effort and some progress toward...toward
21 doing...toward doing that. Certainly, for higher
22 tiers, that is...is an option for us.

23 We do use that single EXAMS parameter,
24 the mass transfer coefficient, to represent mixing
25 caused by a variety of...of...of causes that would

1 certainly stir up the bottom portion of...of even a
2 static...a static pond that causes mixing, and there
3 again, looking at how appropriate is this single value
4 for is it...is it complex enough to represent what we
5 need to represent in terms of mixing between the water
6 column and the...and the benthic layer.

7 And, again, looking at the...the
8 admonition for...for EXAMS that synthetic chemicals may
9 not...the assumption that they may remain buried may
10 not always be the appropriate.

11 In light of the new hydrophobic
12 pesticides that we've been looking at more recently,
13 EFED is debating the appropriate level of
14 conserva...conservatism and the factors which impact
15 soil erosion. We...we realize that in a couple of
16 these farm ponds, they were actually filling up in...in
17 30 years which was certainly not our intention. Our
18 intention in...in modeling 30 years of...of rainfall is
19 to look at the temporal variability from year-to-year
20 based on wet years and dry years and not having a...not
21 having a pond fill up, so that we have had a number of
22 internal discussions in looking at whether those are
23 actually appropriately parameterized.

24 So, that's basically the end of my
25 summary. If anyone has clarifications or additional

1 questions on modeling, I'd certainly be happy to try to
2 answer them.

3 **DR. BUCHER:** Questions for Dr. Parker?
4 Yes, Dr. Maddalena?

5 **DR. MADDALENA:** Yes, the last comment
6 you made was in reference to wet years, dry years. If
7 you focus on the PRZM which is the source model for the
8 pond model, what happens in PRZM on wet year, dry
9 years? Do your applications accumulate on a dry year,
10 for example, or is there...I don't know what the
11 chemistry is in PRZM, if there's actually...if that has
12 a fate model contained within it as well.

13 **DR. PARKER:** Yes, yes, PRZM has,
14 basically, the same inputs as...as EXAMS, so the
15 pesticide stays in the field until it...until it
16 degrades or...or sorbs or...or a few small rainstorms
17 without runoff will slowly move that...that pesticide
18 down into the ground water. So, between movement,
19 beaching into the ground water or the vadose zone
20 and...and runoff, there is less and less chemical in
21 the field for runoff each time a new storm comes by.

22 So, typically, in looking at the...the
23 output values from PRZM, the two or three major runoff
24 events will happen within a week or so of...especially
25 for a chemical that has somewhat...somewhat of a short



1 half-life. The three major events of...for runoff and
2 high concentrations will happen within a week or so
3 after the...after the pesticide has been...has been
4 applied.

5 So, you do, yes, you do definitely have
6 degradation and binding in the field the same as you do
7 in the...in the water body.

8 **DR. BUCHER:** Dr. Simonich?

9 **DR. SIMONICH:** I guess a more specific
10 question about PRZM. Does it include a piling term, a
11 term where...a scenario in which you can have a
12 persistent pesticide that maybe could be depleted in
13 the top layers of the...the soil and, in annual piling,
14 be moved back up to the...the air/soil interface?

15 **DR. PARKER:** Yes, in short. It's more a
16 case, typically, of moving it downward in that the...by
17 the time you plow a second year, there's very little
18 left from applications of the...of the previous year.

19 But you'll...you do sometimes pull a
20 disk after you apply on the same swath across the
21 field, and so, that is mixing it to a deeper and deeper
22 level.

23 PRZM model allows us to put it in as a
24 band on the surface, as a T band partially on the
25 surface and partially incorporated, incorporated to

1 most any depth that...that we wish, depending on
2 the...the recommendations on the pesticide label,
3 decreasing concentration with depth, increasing
4 concentration with depth so we can really put the
5 chemical wherever the label wants us to put the
6 chemical, wherever the label wants the farmer to put
7 the chemical to make it most effective for the crop
8 that...and seed treatments. We've modeled seed
9 treatments in which the seeds are pre-treated with the
10 chemical, and the seeds go in at a specific depth. And
11 so, we put the chemical at that depth as well.

12 The extraction teams in pulling the
13 chemical out of the surface soil and before it runs off
14 is...is decreasing with depth down to 4 cm, I believe,
15 so if most of your chemical is in the surface, you get
16 a lot more chemical in runoff than if most of it
17 is...is...is deeper.

18 So, those are all factors as well that
19 impact the amount of chemical in...in the runoff
20 water.

21 **DR. SIMONICH:** And I'm just wondering if
22 in the scenario of a more persistent and more
23 hydrophobic pesticide, if you could have a scenario
24 where piling might increase concentrations towards the
25 surface at the air/soil interface compared to a less



1 persistent, more water soluble chemical. I'm not sure
2 of the answer to that, but I'm thinking probably it
3 could be an important role in that. It may be
4 different for different types of chemicals.

5 **DR. PARKER:** I haven't really thought
6 about that as an issue, but I know in some of the
7 pyrethroids that 99 percent of all of the chemical will
8 come off in the sorbed phase with eroded soil. So,
9 maybe 1 percent actually comes out dissolved in
10 those...in the...in the water and then stays dissolved
11 immediately anyway in the...in the EXAMS pond, and 99
12 percent will come off with the...with the eroding soil,
13 and that tends to be the case with a couple of these
14 examp...example chemicals.

15 **DR. BUCHER:** Are there any other
16 questions?
17 (No response.)

18 **DR. BUCHER:** Thank you very much. Oh,
19 yes, Dr. Maddalena.

20 **DR. MADDALENA:** One more...

21 **DR. BUCHER:** One more question. Sorry.

22 **DR. MADDALENA:** ...question. Sorry. To
23 follow back and forth with Dr. Simonich over there, the
24 accumula...we have to think differently now with these
25 particular class of chemicals. I think the answer you



1 gave is perfectly logical for the very classic
2 chemicals that do degrade rather fast, but even your
3 test case had some that will last in soil for thousands
4 of days in which case if you don't have rain and you
5 don't have even those particles removed, you could
6 conceivably have some accumulation right at the
7 surface...

8 **DR. PARKER:** That's true.

9 **DR. MADDALENA:** ... where over the
10 course of 20 years, you could plow that in, in which
11 case you probably would bring it back up.

12 But thinking of just the surface now and
13 just that bound phase, is there an off site dust
14 movement loss pathway from the PRZM model? Because
15 I've seen California on a windy day, and I'm wondering
16 if that is captured somehow for the very persistent
17 pollutants.

18 **DR. PARKER:** You know, I've heard
19 of...of that happening in nature in which dust
20 particles will carry an amount of pesticide sometimes a
21 great distance, but PRZM doesn't...PRZM doesn't
22 simulate...doesn't simulate that. I would think that
23 could happen and probably does, but we don't simulate
24 it.

25 **DR. MADDALENA:** Okay, thank you.



1 **DR. BUCHER:** The final speaker today,
2 Dr. Sappington of the Environmental Fate and Effects
3 Division, Office of Pesticide Programs, Assessing
4 Pesticide Bio-cumulation in Aquatic Food Webs.

5 **MR. SAPPINGTON:** Thank you. I looked at
6 the agenda, and I'm the last talk for today, and I'm
7 the last talk before lunch tomorrow. Teaches me I need
8 to look at the agenda when it's being made a little
9 more closely.

10 Okay, what I'm going to go over, keeping
11 in mind the time, is a little bit of background on
12 bio-cumulation, some terminology, as well as the types
13 of data we typically receive. I'm going to walk
14 through some of the key challenges that we face and
15 review some of the available methods. And in doing
16 this, I'm not talking about specific models per se like
17 Dr. Ambrose went through with the sediment dynamics and
18 water quality modeling, but more of the types of
19 approaches, laboratory measured, field measured values,
20 as well as foodweb models.

21 And then I'm going to provide a summary
22 of...of where we've applied these types of methods for
23 two example pesticides.

24 A couple terms should be familiar, but
25 just to make sure we're starting off in, in the same



1 nomenclature, bioconcentration represents uptake of a
2 chemical through water only, in the case of aquatic
3 organisms through routes of respiration or dermal, and
4 it's typically characterized as the bioconcentration
5 factor or BCF.

6 Bioaccumulation, on the other hand,
7 includes bioconcentration, but it also addresses other
8 routes of exposure should they be available in that
9 situation, and that's characterized as the
10 bioaccumulation factor. And those are just ratios, or
11 you can derive them in different ways.

12 Usually, you're interested in the ratio
13 that corresponds to a steady state accumulation where
14 uptake and elimination are...are canceling each other
15 out and the concentration has leveled off over time.

16 And for what we've heard several times
17 today, for the types of chemicals that we're talking
18 about, non-aqueous exposure routes can be important,
19 and in that case, some of the metrics that we look to
20 are trophic transfer factors or biomagnification
21 factors which are ratios of chemical concentrations in
22 one trophic level to the next. And for these
23 compounds, it's usually best to do them on, compounds
24 that partition preferentially into the lipid phase, to
25 do this on a lipid normalized basis.

1 This is the conceptual model I explained
2 earlier, and the bioconcentration processes come into
3 play here. Bio-cumulation includes, again, the trophic
4 transfer. And the types of receptors we're interested
5 in, even though it's aquatic bioaccumulation, we're
6 concerned about not only the aquatic organisms but what
7 organisms that depend on them for their food. So,
8 piscivorous wildlife, for example.

9 Types of data we commonly see are fish
10 bioconcentration studies as well as the octanal water
11 partition coefficients, and less commonly, we might
12 have bioconcentration measured in lower organisms such
13 as the oyster, we might have food chain transfer
14 studies, as well as field mesocosm studies.

15 But these...these studies are only
16 conditionally required, depending on the lower tier
17 assessments. They're not required. And even the BCF
18 study for fish is required only when the KOW, log KOW
19 exceeds 3.

20 I want to take a...this one slide and
21 walk through bioaccumulation assessment, just provide a
22 thumbnail in another Agency program, the Office of
23 Water. I used to work in the Water office and was
24 involved in developing this methodology with other
25 people at the Office of Research and Development, and I

1 guess it shows you that you can leave an office, but
2 the issue tends to follow you around wherever you go.

3 And what...what the problem was in...in
4 the Water office was how to derive water quality
5 criteria that incorporated bioaccumulation and that
6 incorporated these other routes of exposure. This was
7 in the context of estimating concentrations in biota
8 that would be consumed by humans.

9 That particular method recognizes the
10 different types of data that are available, ACS and
11 field bioaccumulation factors as well as a factor
12 that's indexed to the sediment concentrations, the
13 biota sediment accumulation factor. It also employed a
14 food web model, an earlier version that was developed
15 by Dr. Gobas.

16 Bioavailability is handled by examining
17 the freely dissolved concentrations, and I'm talking
18 here about the mutual organic compounds, as well as
19 lipid normalization. And so, there's a three-phase
20 system in which you had freely dissolved chemical,
21 chemical sorbed to DOC, and chemical sorbed to POC.

22 And this underwent peer review, and as
23 part of that, we looked at some data sets...and this
24 topic has come up today...to try to evaluate the
25 performance of these different methods as well as the



1 bioavailability corrections that we were making, and
2 despite a lot of data being out there, what we found is
3 that the type of data sets we needed were ones in which
4 you had samples that were co-located in space as well
5 as time and all the ancillary measurements as well,
6 particularly for things like DOC and...and lipid
7 fraction.

8 And so, the data sets that...that came
9 out of the screen were largely those from the Great
10 Lakes Green Bay Mass Balance Study, the Hudson River
11 PCB data base, Lake Ontario which included PCBs as well
12 as chlorinated pesticides, and a location in Louisiana,
13 and the results from this evaluation were published by
14 Dr. Burkhardt who's in the back of the room in ES&T in
15 2003.

16 We also had peer reviewed these sets of
17 approaches for application in the Great Lakes as well
18 as for national application, so some of which you see
19 in the white paper are, or actually, a lot of which
20 reflects the thinking that had evolved in other Agency
21 programs.

22 Current challenges, obviously,
23 addressing accumulation via the diet, addressing
24 concerns regarding persistence and potential
25 accumulation over long time periods, and Dr. Gobas



1 mentioned the importance of metabolism, and that
2 is...that is extremely important when applying either a
3 dynamic or a steady state through a bioaccumulation
4 model. And it's not so much the math as it is getting
5 the correct data for in vivo metabolism rates.

6 And I know our Office of Research and
7 Development and other...other groups are working very
8 hard at trying to evaluate ways in which we can infer
9 in vivo metabolism, either from in vitro data or
10 from...even from field data.

11 Understanding environmental degradates
12 and how they may impact bioaccumulation of internal
13 residue, and addressing bioavailability for how they
14 handle further chemicals.

15 Now, I'm going to provide just a cursory
16 overview of the strengths and limitations of different
17 methods, and this was partially addressed in an earlier
18 question about using measured or estimated data, do we
19 have kind of a...a strict preference in that case,
20 and...and the answer was no. It really varies
21 depending on the quality of information from, from each
22 of the studies and the nature of the problem.

23 But in general, for the laboratory
24 bioconcentration studies, they do not...well, they're
25 good at, obviously, measuring uptake from the water,



1 but they exclude other routes. The characterization of
2 exposure is one of their strengths, because, typically,
3 that's measured fairly rigorously over time, and they
4 also address the notion of...of biotransformation but
5 only in the accumulating organism, not in the
6 food...not what may occur in the food chain.

7 And so, the extent to which different
8 organisms have different biotransformation rates will
9 not be addressed here.

10 Environmental realism and multi-season
11 exposure are a limitation of these tests for...for
12 fairly obvious reasons, and I would just loosely
13 classify them as a...sort of a moderate level of
14 effort. They do take a couple of months to run,
15 depending on the length of the depuration phase
16 In comparing that to the food web models, the advantage
17 here is you can address uptake through other exposure
18 routes.

19 Characterization of exposure is sort of
20 equivocal, because it really depends on the confidence
21 you have in the inputs to the model, and many times,
22 these are estimated concentrations. They don't have to
23 be; they can be measured, but in the context of...of a
24 new chemical, we're often left with...with using
25 predicted concentrations.



1 Metabolism, I mentioned earlier about
2 the issue of having proper data, and environmental
3 realism is an issue, because all models are
4 simplifications of reality, and we're having to make
5 assumptions regarding food web structure and...and
6 assumptions regarding environmental parameters such as
7 temperature and...and so forth.

8 One nice advantage is that to the extent
9 that we're concerned about multi-season exposure and
10 accumulation, we can run these models for long periods
11 of time and get an assessment of that, and they are
12 convenient in terms of level of effort.

13 Now, the field mesocosm studies,
14 experiments conducted in the field on...on small
15 outdoor aquatic systems, again, have a number of
16 advantages similar to the food web model with respect
17 to uptake pathways, and the ability to characterize
18 exposure really depends on the study.

19 Sometimes, it's done well; other times,
20 it's...it's not done well. But they do incorporate any
21 metabolism that might occur within the organisms or the
22 food chain that's used in that particular study, and I
23 think they do address environmental realism
24 relatively...relatively well, although again, it
25 depends on the study design.



1 Difficulty here is they're often
2 conducted for just a few months, and so, the issue of
3 multi-season exposure isn't addressed, and, frankly,
4 the...the amount of effort that goes into these studies
5 can be quite high.

6 And lastly, field monitoring data which
7 was...is available but, obviously, only for those
8 chemicals that...that are either out...out in the
9 environment or if there's an experimental permit to
10 conduct such studies for new chemicals have...can
11 address multiple exposure routes as well as multiple
12 seasons and have, obviously, a high degree of
13 environmental realism.

14 Oftentimes, however, the biggest
15 limitation with these studies, with monitoring studies,
16 is getting an adequate characterization of exposure in
17 the relevant environmental compartments, both spatially
18 as well as temporally.

19 So, I'm going to walk through some of
20 the assessment questions with respect to
21 bioaccumulation or aquatic bioaccumulation that would
22 come up during the problem formulation phase.

23 And, basically, we...we have to evaluate
24 where the chemical is going to be found in the
25 environmental compartment, issues related to



1 persistence that we talked about this morning,
2 the...how likely an exposure, dietary exposure, may be
3 important, how degradates may affect both
4 bioaccumulation as well as toxicity, and what
5 about...what are our primary ecological receptors of
6 concern. This defines, really, the scope of...of the
7 bioaccumulation assessment, including the food web
8 structure and...and so forth.

9 Metabolism we talked about, and how long
10 does it take for the compound to reach steady state in,
11 in organisms, and I'll go into this in a little more
12 detail in subsequent slides. The other thing from a
13 toxicity perspective is asking the question, well, what
14 duration of exposure is...is toxicologically relevant
15 to the assessment endpoint that...that I'm using? Is
16 it a short term or is it long term exposure that's
17 really driving the...the chronic risk?

18 In most cases for these compounds, we're
19 worried about chronic effects.

20 The next question is having an
21 understanding of how bioavailability might affect
22 pesticide bioaccumulation. As Dr. Mackay indicated,
23 although there are no real bright lines here, once you
24 get above a log KOW of 5, you start really
25 impact...bioavailability and absorption to dissolved



1 and particular organic carbon becomes increasingly
2 important.

3 And that's...that's important in
4 interpreting the results of different studies, because
5 the bioavailability conditions may be very different.

6 And then, understanding how the
7 different approaches predict bioaccumulation and can we
8 explain differences where they do occur. Is there a
9 rational explanation for them?

10 So I'm going to walk through now the two
11 example pesticides, and this is the profile that sort
12 of relates to some of the early...previous questions I
13 just outlined. This is pesticide 3, and the KOW range,
14 depending on the isomer, the dominant isomer is 5.1,
15 KOC of...of roughly 30,000, so we expected a partition
16 to sediment, and aquatic photolysis, as measured, is
17 relatively short, but in the system's deeper and more
18 turbid systems, it's not considered to be a...a
19 dominant loss process.

20 Exposure routes, based on models such as
21 the ones Dr. Gobas has developed, we expect dietary
22 exposure not to be a dominant contributor but also not
23 to be completely negligible. So, it is a factor at
24 this KOW but just not necessarily a dominant one, and
25 that's, again, assuming no metabolism.



1 Environmental degradates were not a
2 major issue with this...this assessment, and the
3 ecological receptors I'm going to present were
4 piscivorous birds and mammals...I'm just going to
5 present the results for...for birds, because they were
6 the more sensitive of the two taxa.

7 Regarding metabolism, while we didn't
8 have in vivo metabolic rates, we, in our
9 bioconcentration study and I believe the mesocosm
10 study, degradates were measured in biota, and they were
11 relatively minor, so that gives us some confidence that
12 perhaps the biotransformation is...is not going to be a
13 driver.

14 In steady state based on the BCF study,
15 the depuration rate constant was 90 percent steady
16 state, was achieved in approximately 50 days. So,
17 there will be a time lag between, even if it's just a
18 single organism, a time lag between the exposure
19 concentration in water and the accumulation in the
20 organism.

21 Critical exposure period, it was 80, and
22 reproduction related endpoints, we assumed that to be
23 roughly 30 to 60 days, to correspond with durations of
24 accumulation in the parent and deposition in the eggs
25 from that study. And BCF values on a wet weight basis



1 are shown here, and we also had information from our
2 mesocosm study.

3 So, what were the objectives here?
4 First was to evaluate potential exposure to piscivorous
5 birds, incorporating trophic transfer and any pesticide
6 carryover. The second objective was to compare
7 bioaccumulation models that were run in a steady state
8 as well as the dynamic mode.

9 And the third objective was to evaluate
10 the sensitivity in model predictions to assumptions
11 regarding sediment dynamics, and some of this...well,
12 and in doing this, we...we used the AGRO model, and we
13 used an earlier version, the version 2, which had
14 constant parameters for the deposition, resuspension,
15 and the burial rates.

16 General approach, the first one was to
17 use PRZM/EXAMS to give us our predicted exposure
18 concentrations and the model published by Arno and
19 Gobas for the food web in the steady state mode. We
20 also ran this model in a dynamic mode, and Dr. Lawrence
21 Burkhardt was one who...who developed a code for the
22 model in order to run it in the dynamic mode.

23 And we also ran, as I mentioned earlier,
24 simulations with AGRO which, of course, is in the
25 dynamic mode and includes sediment dynamics.



1 This is a schematic of basically what I
2 went through, but it shows approaches 1 and 2 where not
3 only was the objective to estimate concentrations in
4 biota but also to see how the...the different types of
5 models compare in terms of the predictions, and in this
6 case, it's the dynamic and the steady state mode.

7 And so, what we did was on the steady
8 state application, we used as input to the steady state
9 model, 60-day average concentrations. The maximum
10 60-day average concentration with a return frequency of
11 1 in 10 years, and that's the same process that Dr.
12 Parker explained earlier this morning. That was for
13 water and sediment concentrations.

14 And, again, that reflects the time to
15 reach steady state, roughly, as well as the critical
16 exposure period, we think, is appropriate based on the
17 toxicological endpoint. And then we simply put those
18 values in...into the model and produced an estimate of
19 bioaccumulation into...I mean, in the food web.

20 For the dynamic approach, we...we
21 imported the daily values, not...not a single value,
22 for water, sediments, temperature, and in this case,
23 temperature did vary. We used a month-to-month
24 variability function here, and you'll see the impact of
25 that shortly. And, again, in the same...same model but



1 just running the dynamic mode.

2 Okay, there's a question about
3 appropriateness of steady state model predictions, and
4 I just wanted to illustrate that here and in terms of
5 how they might be used, even in highly dynamic
6 situations. To illustrate this, we...we did a run of,
7 with PRZM/EXAMS with short water and sediment
8 half-lives, and this was done to maximize the
9 variability in concentrations in the a...a biotic
10 compartment, that is, in the water and sediments.

11 This is a plot just from one...one year
12 from that simulation. This is with pesticide 3. The
13 black lines, the spiky black lines here represent the
14 dissolved water concentration, and the top line
15 represents predicted concentration in piscivorous fish,
16 and so, you see the time lag that...that we would
17 expect based on the measured time to reach steady
18 state.

19 Now, if, as Dr. Gobas pointed out, if we
20 were to take a daily value, a daily maximum value, from
21 the exposure time series and import that into the
22 steady state model, we would have very high
23 predictions, and...but what is...what is happening here
24 is that the organism is essentially integrating
25 exposure from the water column as well as the food,



1 but, again, for this chemical, water column is...is a
2 dominant uptake pathway over time.

3 And so, what we did was to take an
4 average, a 60-day average concentration, of the water
5 and sediment concentration. The other lines here
6 represent other components of the food web as well as
7 the sediment.

8 Another interesting point here, just to
9 illustrate, is that the other components of the food
10 web display faster accumulation kinetics. So, that's
11 also important to keep in mind, depending on the
12 organism that's driving the risk assessment.

13 So, what we did in order to try to
14 compare apples and apples is we took a 30-year time
15 series PRZM/EXAMS run...runs, and we took the maximum
16 value that correspond to a given average. Okay? So, a
17 1-day average, a 60-day average, 188...180-day average,
18 and...and an annual average. We took those maximum
19 values across the entire time series for water and
20 sediments and imported those into the steady state food
21 web model.

22 Then what we did with the dynamic model
23 is to actually not distill the data down into a single
24 value but import all the daily values but choose the
25 same averaging period, in this case, for the tissue



1 concentrations. So, we would compare the 1-day average
2 tissue concentration predicted by the steady state
3 model with the 1-day...I mean, predicted by the dynamic
4 model with the imported 1-day average of water and
5 sediments to the steady state model. And we did that
6 for each of the averaging periods.

7 And the plot on the lower right here
8 shows a comparison of those results. This is for North
9 Carolina cotton scenario. The top line represents the
10 predictions from the steady state accumulation model,
11 and these are at different application rates, so they
12 don't really pertain to the...the assessment in the
13 white paper, but the point here is that yes,
14 absolutely, if you were to put a 1-day value into the
15 steady state model as input, you're going to predict a
16 very high concentration relative to the dashed line,
17 the purple dashed line here is the results from the
18 1-day max from the dynamic model.

19 However, when you start to increase your
20 averaging period, you start to see a convergence
21 between the steady state and dynamic modeling results.
22 And we think that reflects, basically, the degree of
23 temporal dampening in the system but also the degree of
24 variability in the system. So, you can get similar
25 results even in highly dynamic situations.



1 Now, the third approach was to run the
2 AGRO model which has been explained earlier and to
3 compare that to the PRZM/EXAMS modeling results. As we
4 had a number of input parameters, I'm just summarizing
5 the major ones here, and KOW, we used the higher value
6 for the dominant isomer. Application rates. In terms
7 of half-lives, we have 268 days in the water and...and
8 stable in the sediments based on the fate information.

9 Lipid fraction are shown here, and these
10 are all kept the same between the two models. These
11 values represent median values for the different
12 trophic levels, and as one...one aspect, we can pick
13 deterministic values, but lipid fraction varies quite
14 widely across species as well as within the same
15 species in the function of reproductive status and so
16 forth, and this was a very sort of middle road value.

17 We zeroed out the flow, essentially, in
18 the AGRO model to be consistent with EXAMS, and then
19 the two models looked at addressed solubility like
20 we've already discussed earlier, EXAMS just having the
21 concentrations capped at solubility and in AGRO having
22 them capped but then having the excess in the reserved
23 pool which is dissolved back when concentrations in the
24 water dip below solubility.

25 Two factors we...that were different,



1 major factors that were different. One was the organic
2 carbon content and total suspended solids. The value
3 used in AGRO was...was about 50 percent higher
4 than...than that used in the PRZM model.

5 These values, when you look at USGS data
6 for concentrations of particulate organic carbon, if
7 you were to convert this to POC based on the assumed
8 TSS at 30 mg/l, these values correspond to the upper
9 90th to 95th percentile in lakes and reservoirs across
10 the country, and...but keep in mind that...that those
11 lakes and reservoirs are likely to be much less turbid
12 than our typical farm pond.

13 So, where we are in sort of the
14 distribution of values of farm ponds is still somewhat
15 unclear, but that's where these values shake out in
16 terms of their represent...representativeness.

17 And the sensitivity analysis indicated
18 that this was a sensitive parameter, basically a 50
19 percent increase here resulted. When we did the
20 sensitivity analysis with AGRO, resulted in a 50
21 percent drop in concentrations in tissue as a result of
22 the impact on bioavailability and water column
23 concentrations.

24 None with regards to sediment dynamics.
25 None were explicitly assimilated with...simulated with



1 EXAMS, and the constant values here were used in AGRO.

2 Here are the results in terms of the
3 60-day, maximum 60-day average, EECs, for in the water
4 column as well as in sediment, and, again, you see with
5 the asterisks here we had high-end scenarios.

6 I should have mentioned that each of
7 these scenarios represents the low and high end for
8 that particular crop group. We actually modeled quite
9 a number of scenarios. I just distilled it down
10 to...to these, but we were rubbing up against the
11 solubility limit.

12 Results here predicted for
13 concentrations in tissue, again, with the steady state
14 approach, are shown in this plot for the six different
15 scenarios, and the different bars represent different
16 components of the food web, the higher red bar being
17 the piscivorous fish, and these are on a...a wet weight
18 basis.

19 And the band here shows the relationship
20 of these predicted steady state concentrations to our
21 toxicological value in diet for birds, the NOAC and the
22 LOAC. So, we have exceedances here of our NOAC in all
23 six cases but also our LOAC in five out of six.

24 Now, I'm going to go into the dynamic
25 modeling approaches. The left-hand panel at the top



1 shows the dissolved water concentrations predicted
2 using PRZM/EXAMS, and I'm just showing the cotton
3 scenario here. The blue lines represent California
4 cotton, and the red represents Mississippi cotton which
5 we discussed earlier, is a...a high-end scenario in
6 terms of sediment loads to...to the system.

7 And what's obvious in the water column
8 concentration with Mississippi cotton is that the
9 pesticide loads are great enough that the solubility
10 limit is reached in about 6000 days, and we forced,
11 basically, truncated the values at that limit. And for
12 the Mississippi cotton scenario, we do not reach that
13 limit, although there is gradual increase over time,
14 and this is partially reflected in the sediment profile
15 where we see the increases over time.

16 With the AGRO model, again, the same
17 scenario with the parameters that I mentioned earlier.
18 You see a much different profile from the water column
19 concentrations. We do not have a gradual increase over
20 time, and we see a much more variable concentrations.

21 We were bumping up against the
22 solubility limit on certain peak periods, but we
23 weren't staying at those limits like we were with the
24 PRZM/EXAMS model. And the sediment concentrations, it
25 took about ten years to finally level out at...at a



1 steady state concentration in both of these scenarios.

2 Okay, how does that translate to
3 predictions in piscivorous fish? This is the same
4 power scheme used for the abiotic concentrations.
5 Again, this is PRZM/EXAMS with the dynamic versions of
6 Arno & Gobas being run. What we see is a gradual
7 buildup over time to about 6000 days and then this
8 oscillation at a...basically an oscillating steady
9 state.

10 What we think is occurring here and
11 what's interesting is...is a previous...you remember
12 from the previous plot, we essentially had a flat line
13 with regards to the...the water concentration. We had
14 variable temperature. Seasonal variation in
15 temperature, and that affects the uptake rate constants
16 as well as the growth rate, and we think that that's
17 what this is representing here, is the variation
18 in...and due to temperature changes.

19 And the sediment concentrations follow
20 a...a similar pattern...I mean, at forage fish. The
21 avian LOAC is...is shown here as well.

22 Again, we have the different predictions
23 using the AGRO model. I've put for reference avian
24 LOAC here, and we only have one spike of piscivorous
25 fish that reaches up to that level. So, again, a very



1 different picture. We do not see this long-term
2 accumulation. We think that's due to the sediment
3 burial being included in that model.

4 This is the statistics for the same plot
5 for the dynamic results showing in terms of the EECs
6 are the 1 in 10 year return frequency. And, again, a
7 large difference between the EECs in tissue predicted
8 with the EX...PRZM/EXAMS as input to the same model
9 versus the AGRO.

10 This table just summarizes the results,
11 and I...I threw in sort of what might be an empirical
12 approach as well where we would use a BCF times the
13 average water column concentrations, and we see
14 relatively good agreement between the steady state and
15 dynamic approach, although I will say that this is not
16 a rigorous test, because if you think back to the
17 profile of tissue concentrations, basically, these EECs
18 are returning something close to year 27, because we
19 have a...this...this buildup over time. And so, both
20 models...the EEC is approaching that sort of steady
21 state value at the end of the assessment.

22 Okay, so general conclusions, the first
23 of which, it does appear that pesticide 3 appears well
24 behaved in terms of the assumptions of no metabolism,
25 and that's based on the biotransformation information



1 that we have from the BCF study as well as if you take
2 and look at normalized bioconcentration factor from
3 that study and compare it to the KOW, they're in the
4 same ball park, although, admittedly, there's a wide
5 range in lipids there. But you're...you're in the same
6 ball park, and even if you used the...the low and high
7 end, we're within a factor of 2. So, we think that
8 that supports the notion that metabolism is not a
9 driver.

10 And the rate constants are relatively
11 similar between the ones predicted using the model and
12 that derived from...from the Booneville study.

13 Again, the steady state and dynamic
14 modeling results produced similar tissue-based EECs,
15 but what's critical here is the choice of the averaging
16 period. It is, as Dr. Gobas has showed, clearly not
17 appropriate to just take a daily value and put it into
18 a steady state model.

19 And depending on the critical exposure
20 period, there may be situations where you simply can't
21 use the steady state model, because if the dynamics are
22 such that you're worried about very short-term
23 concentrations in fish tissue and you have a...a highly
24 temporally dampened system, a steady state model will
25 not give you that short-term variation or something



1 that you could use to estimate that. But in this case,
2 the results were similar.

3 And in that regard, I'm going to show a
4 plot that was included in the technical support
5 document to support the bioaccumulation methods within
6 Office of Water and also published by Dr. Burkhardt in
7 2003 in ET&T, and this is a plot that illustrates the
8 effect of hydrophobicity on predicted accumulation
9 kinetics in...in fish.

10 The top line shows predicted
11 concentrations or simulated concentrations in the water
12 column for a reach in the Mississippi River, so highly
13 variable situation. The panel B shows the scaled
14 concentration that's predicted in piscivorous fish for
15 different KOWs, assuming that this water profile
16 applies to different KOWs, and sediments were included
17 in this as well.

18 And what you see here, the lower KOW
19 values go from 2, and the highest goes up to 9, and
20 what you see is at the lower KOW values, concentrations
21 basically mirror those in...in the water column,
22 concentrations in fish, but as you move up the KOW
23 scale, the predicted concentrations start to dampen
24 temporally to while...to...to where they basically are
25 very poorly responsive to changes in...in exposure



1 concentration. And this is over a year time period
2 change here.

3 And this information was used in this
4 publication to actually inform how you would go out and
5 do a bioaccumulation study in the field, and the
6 questions there are much like the questions in the
7 context of the steady state model, and that is well,
8 how often do I need to sample? How...how...what is the
9 interval between sampling periods that most...is most
10 appropriate? Do I need to keep the samples co-located
11 in time, or do I need to, basically, sample fish tissue
12 at one point but sample water column over a, say, a 30-
13 or 60-day period leading up to the sampling of fish
14 tissue?

15 And based on this and other information,
16 recommendations were made on, basically, how to design
17 field studies for estimating bioaccumulation factors.

18 Moving on with the conclusions,
19 obviously, it's very clear that the bioaccumulation
20 predictions are extremely sensitive to assumptions
21 regarding...to the inclusion of sediment dynamics as
22 well as the...I didn't show the results, but if you put
23 different values for burial and deposition, they are
24 sensitive to those values.

25 They're also sensitive to what we assume



1 regarding KOW, and...and here, we're assuming that it's
2 a...a known quantity with no variation, and that's
3 obviously not the case. Lipid fraction is highly
4 variable. Organic carbon fraction is variable.

5 There is an example in the white paper
6 where these parameters were...were varied according to
7 assumptions regarding their distribution and used in a
8 probabilistic fashion. So, that's certainly an option
9 to consider to the extent that the risk assessment is
10 sensitive to these parameters.

11 Key uncertainties include application
12 and parameterization of the sediment dynamic routines,
13 what values are appropriate for farm ponds.
14 Bioavailability above solubility, what do we really
15 assume here, and is the laboratory-measured solubility,
16 how accurate is that for field situations, or how
17 representative is that, I should say. And variability
18 in key input parameters.

19 I'm going to move on to pesticide 4.
20 This is the profile. Dr. Gobas introduced this as
21 well. High/low KOW. High organic carbon partition
22 coefficient. Degradation in term...is...is not a major
23 concern. We suspected that there was something going
24 on possibly related to metabolism, although it appears
25 that it could be related more to the growth dilution.



1 We had large differences between the measured
2 bioconcentration factor in Booneville and what we would
3 estimate using the model. And that's also reflected in
4 the steady state value.

5 We also had concerns at this high log
6 KOW about bioavailability in terms of uptake through
7 the gut, and a trophic transfer study was conducted as
8 part of this with rainbow trout being fed oligochaetes
9 and you see that biomagnification factor there on a
10 lipid basis.

11 We also had information with respect to
12 accumulation through the sediment route of exposure
13 with oligochaetes in two different studies, and we also
14 had a...a mesocosm study that simulated realistic
15 concentrations for spray drift. And this study was
16 done with the formulated product, and it's suggested
17 that maybe the bioavailability of the compound was
18 greater in...in the formulation versus the active
19 ingredient.

20 So, general approach here, again, was to
21 say okay, we have different methods, so let's...let's
22 give them a...a shot and see what they predict but keep
23 in mind some of the limitations of the methods. So,
24 empirical data, we have the BCF, the biomagnification
25 factor, and the biosediment accumulation factor.



1 We have the Arno & Gobas model. We ran
2 that with no adjustments to the rate constants. And we
3 also ran it...and I'm calling this the hybrid approach
4 where we used information from the empirical studies to
5 inform the rate constants in the model, including the
6 trophic transfer values.

7 We...because the different empirical
8 studies capture different exposure routes, we used...we
9 apply them differently for each exposure route and then
10 sum them up. So, accumulation in water, we selected an
11 EEC in the water column of 0.15 parts per
12 billion...that was converted to parts per billion...and
13 that is the solubility limit measured in the laboratory
14 for this compound, and that also corresponds to
15 the...the highest...we reached this limit based on the
16 highest exposure scenario for...for the crops that we
17 studied, and we applied the steady state
18 bioaccumulation factor derived here and came up with a
19 predicted steady state concentration.

20 We also applied the biomagnification
21 factor to estimated concentrations in food, and the
22 range here represents values in food predicted from a
23 range of sediment, predicted sediment concentrations.
24 We came up with those values as representing uptake
25 from food, and we summed them to come up with a range



1 of total accumulation, again, just a...a rough steady
2 state estimate.

3 We also ran the model in default mode
4 with no change in the uptake and elimination rates and
5 other parameters. We used the same screening inputs
6 for water and pore water, so these are...are very high
7 values, and we obviously came up with very high values
8 predicted in tissue.

9 The next...the third approach was to use
10 some of the information that we gleaned from the
11 measured studies, uptake and elimination rates from
12 water and food for fish. We used the same screening
13 level inputs, and we looked at predicted outputs in
14 forage and piscivorous fish, and they ranged from 32 to
15 5.8 respectively in this case, because the piscivorous
16 fish, the food uptake parameter, the BMF,
17 biomagnification factor, was low, and so, they are
18 consuming forage fish but not getting the trophic
19 transfer that you would expect.

20 And when we...actually, the bottom plot
21 used is the trophic transfer factor, and the top plot
22 uses the elimination rate and the uptake rate from the
23 BCF study.

24 And this just compares those results in
25 reference to the chronic dietary effect levels for



1 birds and for mammals, and we have ranges of two orders
2 of magnitude. So, we weren't comfortable, in this
3 case, with the default assumptions, although this issue
4 of growth dilution will have to be evaluated, and it's
5 certainly possible that the empirical approach,
6 if...the juvenile bluegill which were actively
7 growing...and I believe that's part of the...the
8 study...study recommendations, and so, with a compound
9 that's so hydrophobic and has such...is predicted to
10 have such slow elimination, growth dilution becomes
11 extremely important.

12 So, this is...this is important to
13 consider in designing these studies and requesting
14 studies from the...from the registrants.

15 Conclusions, pesticide 4,
16 we...we...doesn't appear to adhere to all our
17 assumptions, at least with respect to the oral uptake
18 with...with...what's being predicted by a food web
19 bioaccumulation model. We did attempt to use the
20 empirical data for directly estimating bioaccumulation,
21 adjusting for kinetic parameters, but there's some
22 uncertainties here.

23 There's another aspect to these studies
24 that is relevant, and that's the use of co-solvents.
25 And, again, these are used, in part, to achieve



1 concentrations in stock solutions that are appropriate
2 in a diluter series, and they introduce uncertainties
3 in terms...in terms of the bioavailability of these
4 compounds in these studies.

5 And it's also important to consider the
6 assumptions in the models that are being used as well
7 as in the empirical data, careful evaluation of those
8 information for applying them in pesticide risk
9 assessments.

10 And for this compound, we had a wide
11 range in variability in KOW, and I just...we just
12 picked the middle value, but obviously, we go two
13 orders magnitude of KOW, we're going to get a...a wide
14 difference, and it just points out that we need to keep
15 these factors in mind when...when...and not be overly
16 precise in our estimates.

17 And that's it. Thank you very much.

18 **DR. BUCHER:** Okay, thank you very much.
19 Are there questions? Yes, Dr. Mehta?

20 **DR. MEHTA:** Okay. You know, you showed
21 that the Kine dependent model is...works much better
22 than the previous model which is not surprising, I
23 mean, the dynamic effects are very much part of nature,
24 but do you anticipate additional changes, additional
25 improvements in the model that the Arno & Gobas model



1 that you...you think might help you, 'cause now you're
2 talking...if you had used that model, that model, if it
3 becomes a standard, it would be used for several more
4 years. So, would you be interested in seeing more
5 things in that model?

6 **MR. SAPPINGTON:** It's a good question.
7 I think what comes to mind more right now...I mean,
8 that model is a considerable refinement of the earlier
9 model, in '93, and it addresses kinetically based
10 accumulation in...in lower parts of the food web. It
11 has a major advantage there.

12 I think I would pay attention, in
13 particular, to our assumptions regarding the input
14 parameters. We saw the effect of what we think are
15 temperature differences and...and we often will just,
16 you know, assume a constant temperature for our
17 PRZM/EXAMS scenarios, and I think that keeping in mind
18 the representativeness of our input parameters for the
19 different regions that we're modeling, I think I would
20 certainly evaluate that very carefully.

21 In terms of modeling itself, I mean,
22 I...I think we have to pay attention to different types
23 of food webs. This is a very simplistic food web, and
24 keep in mind that...that different food webs may return
25 different results, particularly benthic versus



1 pelagic-driven food webs, especially since these
2 compounds are going to be found on a mass basis
3 preferentially, in the sediments.

4 But in terms of the under...underlying
5 architecture, I don't have, you know, major
6 recommendations other than to try to get a better
7 handle on this, this metabolic transformation.

8 We did talk about earlier the idea of
9 incorporating different year classes and addressing
10 different life stages, if you will, of organisms, and
11 that certainly could be added in here, although I
12 hesitate. I mean, all of these sort of additions and
13 layers of complexity, I think, should first start with
14 a question of do we really need to do this, and so,
15 what's particularly useful is that we have something
16 that will point us in the direction and lead us down a
17 logical path for conducting any of these types of
18 refinements.

19 And so, if we got into, for example,
20 modeling different life stages which have different
21 lipid contents and different growth rates and so forth,
22 I'd first want to know if the results were even
23 sensitive, you know, likely to be sensitive to that.
24 So, I'd want to apply it in a very careful tiered
25 fashion, because we're doing a lot of these assessments



1 in a...in a given year, and, you know, oftentimes,
2 we'll have a pretty short time frame in which to work
3 with.

4 **DR. BUCHER:** Dr. Norstrom?

5 **DR. NORSTROM:** Can you tell me
6 whether...I couldn't quite get it, and I've forgotten
7 from my previous reading of the Arno & Gobas
8 paper...whether temperature depends if respiration
9 rates is included? I know temperature depends on what
10 oxygen content is.

11 **MR. SAPPINGTON:** I believe the uptake
12 rate constant is temperature dependent, the K1 value.

13 **DR. NORSTROM:** I know it's back there,
14 so the answer is yes, I gather?

15 **MR. SAPPINGTON:** Yes.

16 **DR. NORSTROM:** Okay.

17 **DR. BUCHER:** Yes, Dr. Hickie?

18 **DR. HICKIE:** You have a very elegant
19 dynamic, I would say, lower food web model, and if you
20 go beyond fish and we...we're using a very simple
21 approach to deal with birds and mammals that are eating
22 fish or aquatic invertebrates. And I'm just wondering,
23 when do we need to have dynamic models for some of
24 those animals?

25 I know it's a tremendous amount of work,



1 but it...but I can see in some of your scenarios where
2 fish concentrations are just bouncing around LOACs or
3 NOACs. There comes a point where we need to do that.

4 **MR. SAPPINGTON:** Yes, and that gets back
5 to that critical exposure period, and if it's
6 relatively short, 30 to 60 days, and you're modeling
7 with the IAC with the terrestrial organisms just
8 bouncing around, then that will lead to questions about
9 temporal differences in the diet of...of...of the
10 terrestrial organisms, how that might affect your
11 actual exposure rather just...I mean, essentially, by
12 drawing that line, you're assuming that...that their
13 entire diet is...is...is comprised of, in this case,
14 pisciv...piscivorous fish.

15 We do have quite a bit of information
16 about the dietary preferences, and...and so, this is
17 a...a simplification of that. We can start to
18 fractionate the diet, estimate trophic position, but in
19 terms of doing that on a...a temporal scale, looking at
20 how that might change over time, I can certainly see
21 where it...where it would...could be important but,
22 also, could be fairly challenging as well, I think.

23 **DR. HICKIE:** It...it's just classically
24 a lot of PDT chemicals where you look for effects is on
25 those higher animals, because biomagnification factors



1 are often considerably higher.

2 **DR. BUCHER:** Anybody else?

3 **DR. NORSTROM:** Just a supplementary to
4 that, I think in point of fact, it's more likely that
5 piscivorous fish are going to be eating the forage fish
6 than they are piscivorous fish in most cases, from my
7 experience, anyway, in dealing with Great Lakes
8 ecosystems.

9 **MR. SAPPINGTON:** Or the piscivorous
10 birds eating the...

11 **DR. NORSTROM:** They're eating air life
12 as well, the same as lake fowl. They're not eating
13 lake fowls. In point of fact, it's...it's quite
14 conservative.

15 **DR. BUCHER:** Yes, that was Dr. Norstrom.
16 Last chance? Yes, Dr. DeLorme?

17 **DR. DELORME:** More out of curiosity than
18 anything else for compound, for pesticide 3, why didn't
19 you consider fish as an endpoint of concern, given that
20 they're bioaccumulative?

21 **MR. SAPPINGTON:** The studies we had for
22 fish indicated that pesticide 3 was not toxic up to the
23 solubility limit in...in the fish, and so, we did not
24 do the bioaccumulation modeling on the lower trophic
25 levels. We could have, but we had no real toxicity



1 endpoint that corresponded...you know, they were not
2 toxic at the limit of solubility.

3 **DR. DELORME:** So, you didn't have any
4 like full life cycle?

5 **MR. SAPPINGTON:** We...we had one full
6 life cycle test that was modified to look at pulse
7 exposures, but, again, the endpoints were above the
8 measured solubility in the system, and a co-solvent was
9 used, so you ended up with a tox endpoint above
10 solubility.

11 **DR. BUCHER:** Yes, Dr. Thibodeaux?

12 **DR. THIBODEAUX:** Thibodeaux, Louisiana
13 State University. Why fish? Are they easier to corral
14 and catch and measure concentration? On farmland, why
15 not deer, bobwhite? Or earthworms? Why fish?

16 It's a...remember, it's a chemical
17 engineer asking these questions.

18 **MR. SAPPINGTON:** In terms of the
19 bioaccumulation you mean?

20 **DR. THIBODEAUX:** Yeah. Fish is a food
21 source where these others aren't?

22 **MR. SAPPINGTON:** Well, the entire
23 aquatic food web would be, you can predict the
24 concentrations in that entire food web. I didn't
25 present the results, but we had information on



1 concen...bioconcentration by earthworms, in these
2 studies, and Kris Garber will be talking about the
3 whole aspect of terrestrial bioaccumulation tomorrow,
4 and that's just an area that's not as well developed as
5 the aquatic system. The...the methods, largely, came
6 out of the...the aquatic tox arena, and we know it's
7 important, and, frankly, part of the reason why we're
8 having this SAP is to start asking questions about
9 bioaccumulation not only in aquatic but in terrestrial
10 food webs as well.

11 **DR. BUCHER:** Yes, Dr. Meador?

12 **DR. MEADOR:** Keith, are you actually
13 measuring basic metabolism, or are you just talking
14 about total elimination rates?

15 **MR. SAPPINGTON:** In terms of the
16 metabolism estimate, that's based on measurements of
17 the concentration of the metabolites in tissue. So,
18 it's not a rate as much as it is looking at the total
19 residue and...and radioactive residue and then actually
20 measuring the components of that, and I would...

21 **DR. MEADOR:** And they have different
22 rates over time if you measured over time and you
23 looked at the formation of metabolites.

24 **MR. SAPPINGTON:** Right.

25 **DR. MEADOR:** Which could be useful for



1 some assessments.

2 **MR. SAPPINGTON:** Yeah, I agree. I mean,
3 we have the...the advantage here of...of having the
4 opportunity to be proactive in the design of some of
5 these studies, particularly if they're follow-up. If
6 we have major uncertainties related to metabolism, we
7 can go back and request some additional studies.

8 And that's, in fact, what happened here
9 in pesticide 4. Some of that was...reflects...I
10 presented it sort of as one point in time, but part of
11 that information reflected going back and...and getting
12 additional information to address uncertainties.

13 **DR. MEADOR:** Yeah, for the long term,
14 you'd like to know what the toxicity is of these
15 metabolites.

16 **MR. SAPPINGTON:** Right.

17 **DR. MEADOR:** And you had said that
18 today.

19 **MR. SAPPINGTON:** Right, absolutely.

20 **DR. BUCHER:** Okay, looks like we've
21 reached the end of the first day of the meeting of the
22 EPA FIFRA for Selected Issues associated with the Risk
23 Assessment Process for Pesticides with Persistent,
24 Bioaccumulative and Toxic Characteristics.

25 Tomorrow, we will convene at 8:30, and



1 we will continue with presentations from the Agency.
2 There will be time after that for public comment, and
3 then we will go into the section of the meeting where
4 the discussants answer the charge questions.

5 Is there anything that you'd like to say
6 before we break up?

7 **MS. CHRISTIAN:** Just a reminder. I
8 mentioned this morning there is a big meeting tomorrow
9 morning at 8...at 8:30 with DOD. They expect the line
10 for breakfast to be longer than normal, so please plan
11 accordingly.

12 And I look forward to seeing everyone
13 tomorrow, and thank you to everyone.

14 **DR. BUCHER:** And I'd like to ask the
15 committee to convene just for a few minutes in the room
16 where we had the meeting this morning.

17 Yes, Dr. Lick?

18 **DR. LICK:** Is it okay to leave things
19 here?

20 **DR. BUCHER:** You can leave papers here,
21 yes.

22 **DR. LICK:** What about changes in the...

23 **DR. BUCHER:** We're going to cover that
24 just briefly in...in this meeting right now in the
25 other room here.



1 (WHEREUPON, the meeting was recessed at 5:30 p.m.)
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1 CAPTION
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4 The foregoing matter was taken on the date, and at the
5 time and place set out on the Title page hereof.

6 It was requested that the matter be taken by the
7 reporter and that the same be reduced to typewritten
8 form.

9 Further, as relates to depositions, it was agreed by
10 and between counsel and the parties that the reading
11 and signing of the transcript, be and the same is
12 hereby waived.
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2 COMMONWEALTH OF VIRGINIA

3 AT LARGE:

4 I do hereby certify that the witness in the foregoing
5 transcript was taken on the date, and at the time and
6 place set out on the Title page hereof by me after
7 first being duly sworn to testify the truth, the whole
8 truth, and nothing but the truth; and that the said
9 matter was recorded stenographically and mechanically
10 by me and then reduced to typewritten form under my
11 direction, and constitutes a true record of the
12 transcript as taken, all to the best of my skill and
13 ability.

14 I further certify that the inspection, reading and
15 signing of said deposition were waived by counsel for
16 the respective parties and by the witness.

17 I certify that I am not a relative or employee of
18 either counsel, and that I am in no way interested
19 financially, directly or indirectly, in this action.

20

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25 SUBMITTED ON OCTOBER 28, 2008



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