

**U.S. Environmental Protection Agency  
Science Advisory Board**

Final Minutes of Public Meeting February 22, 2006

**Committee:** EPI Suite Review Panel. (Roster attached)

**Date and Time:** February 22, 2006 from 1 - 3 Eastern Time (See attached Federal Register notice, Volume 71, Number 21, Page 5317-5318, February 1, 2006)

**Location:** By telephone only, run from room 3610E, 1025 F Street Northwest, Washington D.C.

**Purpose:** The purpose of this teleconference is to prepare the Panel for the review through briefings and a discussion and clarification of the charge. (These materials are posted at the SAB's website, [www.epa.gov/sab](http://www.epa.gov/sab) and will be found in the FACA file for this meeting)

**Materials Available:** The following materials were distributed before the meeting:

1. agenda
2. preliminary charge
3. roster and biosketches
4. website description of EPI Suite  
(<http://www.epa.gov/opptintr/exposure/docs/episuite.htm>)
5. website to access EPI Suite  
(<http://www.epa.gov/opptintr/exposure/docs/EPISuitedl.htm>)
6. presentation overheads for Patel & Boethling (available on SAB website and in FACA File)

**Attendees:** Because this was a conference call, there are no sign-in sheets.

All panelists were present for most or all of the call. The attached roster and biosketches provide more information on the panelists. Briefly, they are:

The chair, **Dr. Michael J. McFarland**, Utah State University and members:

**Dr. Deborah H. Bennett**, University of California

**Dr. Robert L. Chinery**, Environmental Protection Bureau of the  
New York State Department of Law

**Dr. Christina E. Cowan-Ellsberry**, The Procter & Gamble Company

**Dr. Miriam L. Diamond**, University of Toronto

**Dr. William J. Doucette**, Utah State University

**Dr. David A. Dzombak**, Carnegie-Mellon University

**Dr. Anton J. Hopfinger**, University of New Mexico

**Dr. Michael W. Murray**, National Wildlife Federation

**Dr. Thomas F. Parkerton**, ExxonMobil Biomedical Sciences  
**Dr. Kevin H. Reinert**, AMEC Earth and Environmental  
**Dr. Daniel T. Salvito**, Research Institute for Fragrance Materials  
**Dr. Hans Sanderson**, Soap and Detergent Association  
**Dr. Louis J. Thibodeaux**, Louisiana State University

(Drs. Dzombak and Salvito were not able to stay until the end of the call.)

Associate Director for Science, Anthony Maciorowski and DFO Kathleen White from the SAB Staff Office were present for part or all of the call.

The following individuals from EPA's Office of Pollution Prevention and Toxics (OPPT) in the Office of Prevention, Pesticides, and Toxic Substances (OPPTS) were present: Neal Patel, Cathy Fehrenbacher, Bob Boethling, David Linch, Lawrence Libelo. No other EPA staff were on the call.

The following members of the public were present:

John Carbone, Ph.D., Senior Scientist, Toxicology Environmental Sciences, Toxicology Department, Rohm and Haas Company. [JCarbone@RohmHaas.com](mailto:JCarbone@RohmHaas.com)

Gerry Wood, [GerryConsulting@cs.com](mailto:GerryConsulting@cs.com)

Layla Batarseh, Supervisor, The Environmental Review Group, OFAS/CFSAN/FDA, [layla.batarseh@fda.hhs.gov](mailto:layla.batarseh@fda.hhs.gov)

David J. Kent, Keller and Heckman LLP, [Kent@khlaw.com](mailto:Kent@khlaw.com)

Diana Graham, Ph.D., Keller and Heckman LLP [graham@khlaw.com](mailto:graham@khlaw.com)

Noel C. Scrivner, PhD, P.E., DuPont Fellow, DuPont Engineering, Research & Technology, [noel.c.scrivner@usa.dupont.com](mailto:noel.c.scrivner@usa.dupont.com)

Jayashree Srinivasan, Accelrys, [jsrinivasan@accelrys.com](mailto:jsrinivasan@accelrys.com)

The total number of people who participated in the call was approximately 35.

## **Summary**

The meeting went largely according to the agenda (attached)

At the end of the meeting, Dr. McFarland summarized major points for the Agency.

The following is a chronological summary of the meeting.

## **1. Welcome, Roll Call, and Opening Remarks**

The DFO took roll, introduced herself, and opened the meeting by saying that EPI Suite Review Panel was begins its review of the EPI Suite Model on today's call.

The DFO explained that the EPI Suite Review Panel is a panel of the Science Advisory Board, which is a chartered committee under the Federal Advisory Committee Act (FACA). The chartered board will consider the Panel's report before it is transmitted to the Administrator. Such reviews almost always require editorial improvements before the report can be finalized and transmitted. It is possible, but rare, for the Board to return a report to a Panel for further work.

This Panel was formed according to the process detailed in the draft booklet "Overview of the Panel Formation Process at the EPA Science Advisory Board" available on the SAB website. A widecast Federal Register notice was published on January 31, 2005 allowing individuals and institutions to nominate candidates for consideration for service on the Panel, a short list of candidates was posted for comment on September 21, 2005, and the final panel formed after the SAB Staff completed its review of information regarding conflicts of interest, appearance of lack of impartiality, and appropriate balance and breadth of expertise, knowledge and experience needed to address the charge.

All members of this panel have provided information, including confidential financial statements protected under the Privacy Act and information about points of view on the matter to be discussed. The SAB's Ethics and FACA Policy Officer, who is also an Alternate Deputy Ethics Official, has reviewed all these materials. This official, together with the SAB Staff Office Director, who is the Deputy Ethics Official for the SAB, in consultation with the SAB Ethics and FACA Policy Officer, who is the Alternate Deputy Ethics Official for the SAB, have determined that there are no outstanding ethics issues concerning any of the panelists. No waivers, were needed or considered for any of the panelists. In addition, the panelists have completed a one hour on-line ethics course specifically designed for the SAB.

All discussions and deliberations of the panel, its interactions as a body or as individual panelists with the public, including the Agency, as they relate to this review, are to be conducted in my presence. As the Designated Federal Officer I am required to ensure that the requirements of FACA are met. In essence, I act as a chaperone for the process.

We have received one written public comment which has been posted at our website. The slides for the Agency's presentation have been posted there and emailed to those individuals who contacted us to say they would be present on this call. There have been no requests from the public for oral comment on the agenda for today's call.

She then turned the meeting over to the SAB's Associated Director for Science, Tony Maciorowski, for a brief welcome and then to the Chair, Dr. Michael McFarland.

## 2. Briefings by OPPT

At 1:20 Neil Patel introduced the Panel to the structure of the Office. The attached handout from OPPT, entitled, *Overview of EPI Suite™: Software for Chemical Property and Fate Estimation*, (pages 1- 4) capture his major points. OPPT is responsible for assuring that industrial chemicals for sale and use in the U.S. do not pose unacceptable risks to human health or the environment. This is accomplished through pollution prevention, safer chemicals, risk reduction, risk management and public understanding. OPPT is responsible for: Pre-manufacture review of new industrial chemicals; Testing, assessment, and risk reduction of existing industrial chemicals; Management of “national chemicals” (e.g. PCBs); International chemical issues; Pollution prevention advocacy; Partnership programs, e.g. HPVC Challenge, Green Suppliers Network, DfE, and Green Chemistry. His remarks concerning the partnership programs were more descriptive than the handout; partnerships include the High Production Volume Challenge, Green Suppliers Network, Design for the Environment, and Green Chemistry. In all of these, physical-chemical properties are important. They use data where available. Where not available OPPT needs to estimate the properties. There were no questions for Patel.

At 1:20 Bob Boethling began a briefing on EPI Suite using slides (5 - 36). He described EPI Suite, which estimates physical/chemical properties and environmental fate and transport and runs estimation programs sequentially with chemical structure as only input. Again, his presentation followed the attached slides very closely and he was careful to state which slide he was speaking from at any particular time.

Boethling addressed components of EPI Suite using Slides 8-1. Dzombak asked for a little more information on Biowin (Slide 11). Boethling said the full literature is available through the EPI Suite program. Biowin 1 and 2 were the oldest, originally called the biodegradability probability program. The summary of the mostly qualitative weight of evidence evaluations is captured in the environmental fate data base. The next two are Biowin 3 and 4 which is the result of a survey of biodegradation experts asked for their advice on the biodegradability of 200 compounds. Biowin 5 and 6 are the most recent. They model the famous Midi date of 800 - 1000 chemicals.

Biowin 1 and 2 provide a binary classification to predict speed of biodegradation. Biowin 2 and 4 provide a semi-quantitative estimate of biodegradation in days, weeks, months or longer. Biowin 5 and 6 give a fast but based on the Midi 301C data

Slide 13 shows the opening screen as it appears to users and Slide 14 provides an extensive list of caveats. The next slides addressed method details, accuracy and validation. At slide 18, Miriam Diamond, who had looked at the statistics in the help file, asked if there was a policy direction as to what was acceptable. Boethling responded that he knew of none and observed it was a good SAB type issue. Fehrenbacher also thought there was no standard policy on what would be an acceptable level of accuracy. She thinks it is a case by case determination.

Slide 23 describes the users of OPPT models, not just EPI Suite. Many different kinds of people and organizations use the models (industry, research consultants, federal employees, state and local governments, EPA offices other than OPPT, and others).

Slide 24 provides information about the use of EPI Suite in OPPT programs. Dzombak, who gathered EPI Suite is not especially useful for metals or their compounds, asked about the kind of data required for the PMN programs, especially data that EPA might prefer to use instead of these tools. Boethling responded that the submitter is only required to submit what data is in its possession, but there is no up-front requirement for testing. OPPT would like to receive measured data for everything EPI Suite estimates and more. Only 5% of the submissions include any basic physical-chemical data. That's why EPI Suite is used in PMN assessments and other programs where they do not have measured values.

Bob Chinery asked if there were actionable regulatory criteria for physical-chemical values. Boethling thought there were criteria for the persistent, bioaccumulative, and toxic substances. He's concerned about Chinery's use of the word "actionable" as he doubts any action under TSCA has ever been taken on a KOW alone. EPI Suite is also used to provide inputs to ECOSAR. ECOSAR (Ecological Structure Activity Relationships) is a personal computer software program that estimates the toxicity of chemicals used in industry and discharged into water. The program predicts the toxicity of industrial chemicals to aquatic organisms such as fish, invertebrates, and algae by using Structure Activity Relationships (SARs). The program estimates a chemical's acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity. EPI Suite (and other programs) can be used to estimate the octanol/water partitioning coefficient ( $K_{ow}$ ) when measured values are not available. The coefficient is an input to ECOSAR. ECOSAR is not included in this review; another office is responsible for ECOSAR.

Diamond asked whether ions as well as protonated compounds were addressed by EPI Suite; Boethling agreed that was the case and discussed the difficulties (and expenses) of programs that would estimate the relevant values, including the freely available SPARC. SPARC is a general purpose calculator for situations where suitable measured values are not available. Examples include newly-developed chemicals, those that have had little environmentally related data collection, or where chemical parameters are not available at an environmentally relevant temperature or pH. SPARC Performs Automated Reasoning in Chemistry (SPARC) was jointly developed by US EPA and the University of Georgia.

When Parkerton asked if OPPT uses SPARC as a check against EPIWIN, Boethling responded, "occasionally". Parkerton then asked whether there was a process by which OPPT regularly and systematically reviews new data on model predictions. Boethling said it is done as funding permits, which it doesn't very much. Salvito spoke about altering the SMILES notation to change the prediction. A member of the public, Scrivener, said they have some correction factors for ionizable compounds if you know the pH of the environment in which they will find themselves. Boethling isn't familiar with it, but it sounds like the kind of technology that should get more attention.

Using slide 26, Boethling spoke to the High Production Volume Chemicals, a data intensive program.

Slide 27 illustrates the combination of user-friendly software with a policy that allows some estimates. Sometimes applicants submit estimated values instead of measured values even where the measured values exist. The combination could make EPI Suite harder to use. Right now OPPT is adding information, as illustrated on slides 28 - 29. They would welcome suggestions.

The remaining slides provide information on recent and ongoing changes in EPI Suite. Slides 30 - 35 describes the last major changes in the version of November 04 which, in its technical aspects, is the same as what the Panel is reviewing. Slide 36 describes additional changes that are planned. Deborah Bennett asked about how to get more information on how to get more information on these changes. Boethling gave an example. It is an ongoing work assignment. The SAB has not been asked to review these plans. Fehrenbacher said this is outside the scope of the review. panelist noted that the last charge question addresses improvements to EPI Suite.

Cowan- Ellsberry asked about how estimates in one module affected others. In response to a question on multiple values in the literature, Boethling noted that the physical property data base displays selected values, not all values. Slide 29, under data quality considerations, provides a description of how these decisions are made. Boethling thinks this is an area where EPA is making improvements and can do more.

Parkerton asked about experimental values, observing that sometimes a short description of the reference, not a full citation is provided. HELP talks about the experimental data base, but that isn't so useful. Even recognizing that not all the data are included, how do you get the full reference for the selected value used? Boethling responded that some modules list the full references for all the data. PhysProp, however, is not so smooth. You have to go to the Syracuse Data Base linked files to get the full reference.

### **3. Charge to the Panel and Discussion**

At 2:15 McFarland thanked Patel and Boethling and began discussion of the charge. OPPT had officially transmitted the charge after the preliminary assignments had been made. The chair and DFO asked the Agency to point out any substantive changes to the charge as they are discussed. Addressing the preliminary charge question-by-question, he asked the Panel what additional information was needed to provide a basis for responding. Panel members also sought guidance on the depth of the response desired.

The difficulties were question specific. Some are easily addressed now. The more difficult ones are about validation and appropriate use. While the Panelists can do something now, they cannot complete their responses until they have more information. Therefore, they hope to have more material from EPA, especially on uses, before the weekend. Fehrenbacher said OPPT can provide references to the panel before the weekend, but thinks uses will best be addressed by presentation.

## 5. Public Comment

There were no public comments.

## 6. Discussion of Next Steps

The DFO would interact with Agency staff to obtain the supplemental information for distribution to the Panel. The DFO and chair would prepare a revised timeline for distribution to the Panel. Panelists would begin their writing assignments and send them to the DFO

There were no further comments or questions and the meeting adjourned at 3:15

Respectfully Submitted:

/S/

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Ms. Kathleen E. White  
Designated Federal Official

Certified as True:

/S/

\_\_\_\_\_  
Dr. Michael J. McFarland, Chair  
Katrina Soil and Sediment Plan Workgroup

The following are available at the SAB website and in the FACA file for this meeting:

1. Federal Register Notice
2. Agenda for the meeting
3. Workgroup roster
4. Biosketches
5. Preliminary Charge
6. *Overview of EPI Suite™: Software for Chemical Property and Fate Estimation\**
7. Email approving the minutes

\* Due to differences in format, this document could not be incorporated into the minutes, but a copy was posted at the SAB website and one will be found in the FACA file as well.

[Federal Register: February 1, 2006 (Volume 71, Number 21)]  
[Notices]  
[Page 5317-5318]  
From the Federal Register Online via GPO Access [wais.access.gpo.gov]  
[DOCID:fr01fe06-73]

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ENVIRONMENTAL PROTECTION AGENCY  
[FRL-8027-2]

Science Advisory Board Staff Office; Notification of Three Public  
Teleconferences and a Meeting of the Science Advisory Board EPI Suite  
Review Panel

AGENCY: Environmental Protection Agency (EPA).  
ACTION: Notice.

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SUMMARY: The EPA Science Advisory Board (SAB) Staff Office announces  
three public teleconferences and a face-to-face meeting of the SAB EPI  
Suite Review Panel to review software developed by the Office of  
Pollution Prevention and Toxics known as the Estimation Programs  
Interface (EPI) Suite. An agenda and documents for this teleconference  
will be posted on the SAB Web site at: <http://www.epa.gov/sab> prior to  
the call.

DATES: Public teleconferences of the SAB EPI Suite Review Panel will be  
held on Wednesday, February 22, 2006, Wednesday, March 1, 2006, and  
Wednesday, April 5, 2006, from 1 p.m. to 3 p.m. eastern standard time.  
The face-to-face public meeting will be held March 7-9, 2006, from 9  
a.m to 5:30 p.m. eastern standard time.

ADDRESSES: The public teleconferences will take place via telephone  
only. The public face-to-face meeting will be held at the SAB  
Conference Center, 1025 F Street, NW., Suite 3700, Washington, DC 20004.

FOR FURTHER INFORMATION CONTACT: General information concerning the SAB  
can be found on the SAB Web Site at: <http://www.epa.gov/sab>. Members of

the public who wish to obtain the call-in number and access code for the teleconferences, or further information concerning the public face-to-face meeting may contact Ms. Kathleen White, Designated Federal Officer (DFO), by mail at EPA SAB Staff Office (1400F), U.S. EPA, 1200 Pennsylvania Avenue, NW., Washington, DC 20460; by telephone at (202) 343-9878; by fax at (202) 233-0643; or by e-mail at: [white.kathleen@epa.gov](mailto:white.kathleen@epa.gov)  
Technical Contact: For questions and information concerning the software being reviewed, please contact Dr. Robert Boethling, U.S. Environmental Protection Agency, by telephone (202) 564-8533; or by e-mail at [boethling.bob@epa.gov](mailto:boethling.bob@epa.gov)

**SUPPLEMENTARY INFORMATION:** The SAB was established by 42 U.S.C. 4365 to provide independent scientific and technical advice, consultation, and recommendations to the EPA

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Administrator on the technical basis for Agency positions and regulations. The SAB has been asked to review software developed by the Office of Pollution Prevention and Toxics known as the Estimation Programs Interface (EPI) Suite and has formed a specialized EPI Suite Review Panel for this purpose as previously announced (70 FR 4846, January 31, 2005).

The Panel will comply with the provisions of the Federal Advisory Committee Act (FACA) and all appropriate SAB procedural policies. EPI Suite is routinely used in evaluating new chemicals under EPA's Premanufacture Notices (PMNs) for new chemicals under section 5 of the Toxic Substances Control Act, and is widely used for predicting physical/chemical properties and environmental fate and transport properties for chemicals already in commerce. A more extensive description of EPI Suite can be found at:

"<http://www.epa.gov/opptintr/exposure/docs/episuite.htm>

EPI Suite can be downloaded from

<http://www.epa.gov/opptintr/exposure/docs/EPISuitedl.htm>

The purpose of the teleconference on February 22, 2006, is to prepare the Panel for the review through briefings and a discussion and clarification of the charge. The purpose of the March 1, 2006, teleconference is to prepare the Panel and the Agency for the face-to-face meeting by responding to panelists' preliminary questions and identifying areas where additional information is needed. The purpose of the March 7-9, 2006, face-to-face meeting is for the Panel to reach consensus on the content of their response to the charge questions, to capture that consensus in writing, to brief the Agency on the major findings and conclusions, and to respond to Agency questions. The

purpose of the April 5, 2006, teleconference is to provide the panelists with an opportunity to discuss their draft report and agree to final language. Subsequently, the Panel's report will be considered by the Board and transmitted to the Administrator.

**Procedures for Providing Public Input:** Members of the public may submit relevant written or oral information for the EPI Suite Review Panel to consider during the advisory process.

**Oral Statements:** In general, individuals or groups requesting an oral presentation at a public teleconference will be limited to three minutes per speaker with no more than a total of thirty minutes for all speakers. In general, individuals or groups requesting an oral presentation at a face-to-face meeting will be limited to five to ten minutes with no more than two hours for all speakers. Those interested should contact Ms. White (preferably via e-mail) no later than seven days before the meeting date to be placed on the public speaker list.

**Written Statements:** Written statements should be received in the SAB Staff Office at least seven days before the meeting so that the comments may be made available to the Panel for timely consideration. Comments should be supplied to the DFO in the following formats: One hard copy with original signature by mail, and one electronic copy by e-mail (acceptable file format: Adobe Acrobat PDF, WordPerfect, MSWord, MSPowerPoint or Rich Text files in IBM-PC/Windows 98/2000/XP format).

**Accessibility:** For information on access or services for people with disabilities, please contact Ms. Kathleen White at 202-343-9878 or [white.kathleen@epa.gov](mailto:white.kathleen@epa.gov) . To request accommodation of a disability, please contact Ms. White, preferably at least ten business days prior to the meeting, to give EPA as much time as possible to process your request.

Dated: January 26, 2006.  
Anthony F. Maciorowski,  
Associate Director for Science, EPA Science Advisory Board Staff Office.

**EPA SCIENCE ADVISORY BOARD  
EPI SUITE REVIEW PANEL  
PUBLIC TELECONFERENCE  
FEBRUARY 22, 2006  
1:00 - 3:00 Eastern Time**

The purpose of this teleconference is to prepare the Panel for the review through briefings and a discussion and clarification of the charge

1:00	Opening, Introductions and Practicalities	Kathleen White Designated Federal Officer
	Welcome	Anthony Maciorowski Associate Director for Science, SABSO
	Review of Agenda	Michael McFarland, Chair
	Overview	OPPT
	Introduction to EPI Suite	OPPT
	Charge to the Panel	Michael McFarland
	Discussion	Panel and OPPT
	Public Comment	None requested as of February 16
	Discussion of Next Steps	Chair and Panel
3:00	Adjourn	Kathleen White

**U.S. Environmental Protection Agency  
Science Advisory Board  
EPI Suite Review Panel**

**CHAIR**

**Dr. Michael J. McFarland**, Associate Professor, Department of Civil and Environmental Engineering, Utah State University, Logan, UT

**MEMBERS**

**Dr. Deborah H. Bennett**, Assistant Professor, Department of Public Health Sciences, University of California, Davis, Davis, CA

**Dr. Robert L. Chinery**, Research Scientist, Environmental Protection Bureau, New York State Department of Law, Albany, NY

**Dr. Christina E. Cowan-Ellsberry**, Professional Staff, Risk Science, Policy and Regulatory Sciences Department, The Procter & Gamble Company, Cincinnati, OH

**Dr. Miriam L. Diamond**, Professor, Department of Geography, University of Toronto, Toronto, Ontario, CANADA

**Dr. William J. Doucette**, Professor, Department of Civil and Environmental Engineering in the Utah Water Research Laboratory and, Center for Environmental Toxicology, Utah State University, Logan, UT

**Dr. David A. Dzombak**, Professor, Department of Civil and Environmental Engineering, Carnegie-Mellon University, Pittsburgh, PA

**Dr. Anton J. Hopfinger**, Research Professor, Deans Office Administration, University of New Mexico, NM.

**Dr. Michael W. Murray**, Staff Scientist, Great Lakes Field Office, National Wildlife Federation, Ann Arbor, MI

**Dr. Thomas F. Parkerton**, Advanced Sci Assoc, Toxicology & Environmental Sciences, ExxonMobil Biomedical Sciences, Annandale, NJ

**Dr. Kevin H. Reinert**, Principal Toxicologist, AMEC Earth and Environmental, Plymouth Meeting, PA

**Dr. Daniel T. Salvito**, Manager - Environmental Program, Research Institute for Fragrance Materials, Woodcliff Lake, NJ

**Dr. Hans Sanderson**, Director, Environmental Safety, International and Regulatory Affairs, Soap and Detergent Association, Washington, DC

**Dr. Louis J. Thibodeaux**, Jesse Coates Professor, Gordon A. & Mary Cain Department of Chemical Engineering, College of Engineering, Louisiana State University, Baton Rouge, LA

#### **SCIENCE ADVISORY BOARD STAFF**

**Ms Kathleen E. White**, Designated Federal Officer, Science Advisory Board Staff Office, Washington, DC

## BioSketches

Deborah H. Bennett, Ph.D. is Assistant Professor of Environmental and Occupational Health in the Department of Public Health Sciences at the University of California Davis. She received an M.S. and Ph.D. in Mechanical Engineering from the University of California, Berkely and a B.S. in Mechanical Engineering from the University of California, Los Angeles. Her research focuses on the fate, transport, and exposure to chemicals in a multimedia environment within the context of environmental risk assessment. Current research interests fall into three areas: development of an indoor fugacity model to assess exposures resulting from indoor releases of pesticides and other organic compounds; exposure to Hazardous Air Pollutants (HAPs) in various indoor microenvironments through modeling and monitoring; and methods for quantifying, and uses for, the Intake Fraction of compounds. The Intake Fraction is the integrated incremental intake of a pollutant released from a source or source category and summed over all exposed individual per unit of emitted pollutant. She has also developed methods for quantifying the spatial range and temporal persistence of organic pollutants in a multimedia environment, a classification system for persistent pollutants and evaluated the use of long range transport models in the context of regulatory decisions through a model comparison. A list of Dr. Bennett's publications may be found at <http://phs.ucdavis.edu/Faculty/Bennett.php>.

Robert L. Chinery is a Environmental Research Scientist in the Environmental Protection Bureau in the New York State Department of Law. Mr. Chinery is licensed as a professional engineer in the state of New York and holds a M.S. in environmental engineering from Rensselaer Polytechnic Institute. Mr. Chinery's research includes carbon dioxide removal technology, fate and toxicity testing requirements of pesticides, and geospatial analysis of environmental data.

Christina E. Cowan-Ellsberry, Ph.D. is a Principal Scientist in the Environmental Sciences Department of Procter & Gamble Company in Cincinnati, OH. Dr. Cowan-Ellsberry has worked in the area of environmental fate and risk assessment for over 25 years. She has conducted fate studies and developed models for predicting the fate of both inorganic and organic chemicals in the environment. Most recently, she has been involved in conducting and participating in workshops focusing on the use of multi-media models in environmental fate assessment, the development of environmental risk assessment guidelines, the application of uncertainty analysis in ecological risk assessment, the use of monitoring data in environmental risk assessment, and the evaluation of persistence and long-range transport potential for chemicals. Dr. Cowan-Ellsberry has also served as a technical representative for industry to the US-EPA's Endocrine Disrupter's Priority Setting workshop, Environment Canada's "Categorization and Screening of the DSL" project, and numerous

international panels including the OECD's Environmental Exposure Task Force, the OECD working group for developing an internationally harmonized classification scheme for hazardous to the Aquatic environment, and both the NAFTA Commission for Environmental Cooperation and the UNEP Criteria Expert Groups for developing the criteria and process for identifying candidate persistent, bioaccumulative and toxic substances for international management. Dr. Cowan-Ellsberry hold one U.S. patent and has authored or co-authored over 50 scientific papers, 3 book chapters and 2 books.

Miriam Diamond, Ph.D. is a Professor in the Department of Geography at the University of Toronto. Dr. Diamond received her Ph.D. in chemical engineering at the University of Toronto. Dr. Diamond's work involves mathematical modelling, analytical chemistry, lab studies, field studies, and information management. Her research is motivated by the need to develop defensible strategies to improve environmental quality in systems subject to anthropogenically elevated contaminant inputs. Dr. Diamond focuses on aquatic systems (air, water and sediment) and multimedia movement (air, water, soil, sediment, vegetation and impervious surfaces), specifically, in urban areas. Selected publications of Dr. Diamond's may be found at <http://www.geog.utoronto.ca/info/faculty/Diamond.htm>.

William J. Doucette, Ph.D. is a professor at Utah State University with appointments in the Department of Civil and Environmental Engineering, Utah Water Research Laboratory, and Center for Environmental Toxicology. He has BS and MS degrees in chemistry and a PhD in Aquatic Chemistry from the University of Wisconsin-Madison. Dr. Doucette has been an Environmental Chemistry Editor for the *Journal of Environmental Toxicology and Chemistry* since 1999 and serves on the Solid and Hazardous Waste Control Board for the State of Utah. He has also worked as an environmental chemist for Eli Lilly in Greenfield, IN and at the US EPA's Environmental Research Laboratory in Duluth, MN. Dr. Doucette's research has focused on the fate and behavior of organic contaminants in the environment, with emphasis on phytoremediation, the uptake of industrial chemicals into edible plants, the measurement and prediction physical-chemical properties using Quantitative Structure Property Relationships (QSPRs), and the environmental fate of pharmaceuticals. A list of recent publications of Dr. Doucette's may be found at <http://www.engineering.usu.edu/uwrl/www/faculty/doucette.html>.

David A. Dzombak, Ph.D. is professor of civil and environmental engineering at Carnegie Mellon University, a registered professional engineer in Pennsylvania, and a diplomate of the American Academy of Environmental Engineers. He holds a Ph.D. in civil-environmental engineering from the Massachusetts Institute of Technology. The emphasis of his research is on water and soil quality engineering, especially the fate and transport of chemicals in subsurface systems and sediments, wastewater

treatment, in situ and ex situ soil/sediment treatment, hazardous waste site remediation, and abandoned mine drainage remediation. Dr. Dzombak has served on the National Research Council Committee on Bioavailability of Contaminants in Soils and Sediments and on various research review panels for the Department of Defense, Environmental Protection Agency, National Institute of Environmental Health Sciences, and the National Science Foundation. He has also served on the Board of Directors and as an officer of the Association of Environmental Engineering and Science Professors; as chair of committees for the American Academy of Environmental Engineers, American Society of Civil Engineers, and Water Environment Federation; and on advisory committees for various community and local government organizations and for the Commonwealth of Pennsylvania. Dr. Dzombak was elected a fellow of the American Society of Civil Engineers in 2002. Other recent awards and honors include the Professional Research Award from the Water Environment Association of Pennsylvania in 2002, an Aldo Leopold Leadership Program Fellowship by the Ecological Society of America and the David and Lucile Packard Foundation in 2000, and the Jack Edward McKee Medal from the Water Environment Foundation in 2000. Dr. Dzombak's publications are listed in <http://www.ce.cmu.edu/~dzombak/pubs.html>.

Anton Hopfinger, Ph.D. is a Professor of Medicinal Chemistry at the University of Illinois at Chicago. Dr. Hopfinger holds a Ph.D. in Biophysical Chemistry from Case Western Reserve University. Dr. Hopfinger's areas of expertise include methods of computational chemistry, computer-assisted molecular design, quantitative structure-activity relationships, modeling chemical mechanisms of toxicity, and computer graphics in molecular property representation. Dr. Hopfinger is Associate Editor of the *Journal of Chemical Information and Modeling*. Dr. Hopfinger has held numerous grants and contracts, most recently as Principal Investigator for "Cellular and Molecular Targets of General Anesthetics – Modeling and QSAR" Subcontract to National Institutes of Health Program Project. A list of Dr. Hopfinger's selected publications may be found at [http://www.uic.edu/pharmacy/depts/pmch/faculty\\_sites/Hopfinger.htm](http://www.uic.edu/pharmacy/depts/pmch/faculty_sites/Hopfinger.htm).

Dr. Michael McFarland, Ph.D. is currently an associate professor in the Department of Civil and Environmental Engineering at Utah State University where his research interests are focused in the areas of biosolids engineering, industrial waste management and pollution prevention. Dr. McFarland received his Bachelors' degree in Engineering and Applied Science from Yale University, his Masters' degree in Chemical Engineering from Cornell University, his Ph.D. in Agricultural Engineering from Cornell University and completed his postdoctoral research program in the Dept. of Civil and Environmental Engineering at the University of Texas at Austin. Dr. McFarland has served on numerous federal, state and local environmental engineering and public health advisory committees for the U.S. Dept. of Defense, U.S. Environmental

Protection Agency, U.S Dept. of Energy, National Science Foundation and the state of Utah.

Michael Murray, Ph.D. joined the Great Lakes office of the National Wildlife Federation (NWF) as Staff Scientist in 1997. His work has focused on the scientific and policy aspects of toxic chemicals in the Great Lakes region, particularly with regard to mercury sources, fate and transport, ecological and human health effects, and control options. Dr. Murray has worked on water quality criteria and fish consumption advisories. Mike received M.S. and Ph.D. degrees in Water Chemistry from the University of Wisconsin-Madison, where his research addressed several aspects of the environmental chemistry of polychlorinated biphenyls. He has authored or co-authored six peer-reviewed papers and book chapters as well as numerous reports. In addition to current duties with NWF, Dr. Murray is an adjunct lecturer in Environmental Health Sciences at the University of Michigan's School of Public Health, where he has taught courses in environmental chemistry and water quality management. Funding support has been from U.S. EPA and several private foundations, including the Garfield Foundation, Beldon Fund, George Gund Foundation, and the C.S. Mott Foundation. In addition to serving as peer-reviewer for EPA and state agency reports, Dr. Murray has served on a number of technical review, advisory group, and steering committees, including Michigan Quantification Level Advisory Group, Michigan Mercury Electric Utility Workgroup, and committees of the Society of Environmental Toxicology and Chemistry.

Thomas F. Parkerton, Ph.D. is an Associate for Exxon Mobile Biomedical Services. Dr. Parkerton received his Ph.D. in Exposure Assessment from Rutgers University in 1993. Dr. Parkerton has conducted research in multimedia exposure modeling, data and QSAR models, and risk assessment of complex hydrocarbon substances. Dr. Parkerton's publications cover environmental chemistry and engineering; development of estimation models for fate/effect assessment; and evaluation/application of EPI Suite models. Dr. Parkerton is a Member of European Centre for Ecotoxicology and Toxicology of Chemicals QSAR Task Force and co-author on recent technical report providing industry evaluation of commercially available QSAR software tools. Dr. Parkerton has completed a major project funded by the European oil industry that involved multimedia exposure modeling and risk assessment of gasoline

Kevin H. Reinert, Ph.D. is Principal Toxicologist at AMEC Earth and Environmental. He received his Ph.D. in biological sciences at the University of North Texas, his M.S. in environmental science at Rutgers University, and his B.S. in natural science at Muhlenberg College. Dr. Reinert has more than 20 years of experience in environmental fate and effects assessment, environmental modeling, ecological and human health risk assessments, litigation support, groundwater, and hazardous waste projects. Dr. Reinert serves as Chair of the Pennsylvania Department of Environmental Protection Cleanup Standards Scientific Advisory Board. He is a member of the Society of

Environmental Toxicology and Chemistry (SETAC), Sigma Xi, and the American Association for the Advancement of Science (AAAS).

Daniel Salvito, Ph.D. is the Manager of the Environmental Program for The Research Institute for Fragrance Materials, Inc. (RIFM). Dr. Salvito is responsible for overseeing the planning, conduct and completion of the environmental research and testing program at RIFM. These activities include the development and use of models to predict the properties, fate and effects of organic chemicals in the environment. Dr. Salvito holds a Bachelor of Science degree in chemistry from Adelphi University and a Masters of Science degree in chemistry from the State University of New York at Stony Brook. He completed his Ph.D. in environmental science from Rutgers University. Among his professional affiliations, Dr. Salvito is a member of the American Chemical Society, the Society of Environmental Toxicology and Chemistry, and the New York Academy of Sciences. He has authored over 20 scientific publications and presentations. He presently serves on ECETOC's Task Force on the Risk Assessment of Persistent, Bioaccumulative and Toxic Chemicals, chairing the Effects sub-group. He was served on the scientific advisory committee for the joint TNO/Wildlife International Workshop on Simulation Testing and Environmental Persistence. Dr. Salvito leads the fragrance industry's support of the pilot PBT Profiler program on a case study of personal care ingredients with SC Johnson.

Hans Sanderson, Ph.D. is Director of Environmental Safety for the Soap and Detergent Association. Dr. Sanderson received his Ph.D. in Ecotoxicology from Roskilde University in Denmark. Dr. Sanderson has focused on pharmaceuticals and personal care products (PPCPs) at the lowest tier (QSAR) and the highest tier (mesocosm) of risk assessment. Current areas of expertise include responsibilities for nine global High Production Volume Chemical categories (PPCP ingredients) under the EPA HPV challenge and the OECD HPV program. Dr. Sanderson has co-authored a chapter on global extrapolation techniques and practices for QSAR (SETAC press); a book on risk screening and exposure methodologies for HPVs (internal and external peer-review), and published several papers on QSARs. Dr. Sanderson chairs a workgroup under Society of Environmental Toxicology and Chemistry (SETAC) on PPCPs and modeling.

Louis J. Thibodeaux, Ph.D. is currently the Jesse Coates Professor in the College of Engineering at Louisiana State University. His terminal degree is a Ph.D. in chemical engineering and presently his teaching, research and service is dominated by the field of chemical fate and transport in multimedia compartments of the natural environment. Current areas of research expertise include chemical release processes to water from sediment beds and to air from soil-like dredged materials as well as chemical releases to water and air from environmental dredging activities. Although Dr. Thibodeaux is the Emeritus Director of the USEPA funded South and Southwest Hazardous Substance Research Center, head quartered at LSU and Directed by Danny D. Reible. Professor

Thibodeaux has served on advisory committees for the USEPA, USACE, DOD, DOE, NRC and the private sector, all related to environmental chemodynamic issues. Further details on Dr. Thibodeaux's projects and publications may be found at <http://www.che.lsu.edu/faculty/thibodeaux/>

Preliminary Draft Charge Distributed to EPI Suite Review Panel January 13, 2006

### **General charge to the Science Advisory Board**

The Agency is primarily interested in the SAB's review of the supporting science, functionality, and appropriate use of EPI Suite. While SAB should feel free to comment broadly, specific responses to the following technical questions would be welcomed.

1. Supporting Science

A. Comprehensiveness

- i. Are there additional properties which should be included in upgrades to EPI Suite for its various specified uses (PMN, P2, ???)? (An example might be Characteristic Travel Distance.) Can any be dropped?
- ii. Are there additional sets of existing measured data which should be included in upgrades to EPI Suite? Are there specific measurements with the potential to improve EPI Suite estimates so much that an effort should be made to collect them?
- iii. Are there other capabilities that should be included in upgrades to EPI Suite? The Agency is especially interested in the SAB's views on uncertainty analysis and if/how information on how good the estimates are can be conveyed to users.

B. Method accuracy and validation

- i. Is the accuracy of the modules in the EPI Suite sufficient for its various specified uses?
- ii. Have the modules been adequately validated, and have they been published in the peer-reviewed technical literature or elsewhere?
- iii. Are some modules more accurate/better validated than others, and if so, which need more work?
- iv. To the extent that modules work together to generate estimates, do they do so correctly?

- C. Estimation Methods and Alternates
  - i. Are the estimation methods in EPI Suite up-to-date and generally accepted by the scientific community for its various specified uses?
  - ii. Are there other estimation methods which should be considered in upgrading EPI Suite?
  
- 2. Functionality (Program documentation; user interface; convenience features)
  - A. How convenient is the software and does it have all the necessary features?
  - B. Are there places where EPI Suite user's guide (and other program documentation) does not clearly explain EPI's design and use? How can these be improved?
  - C. Are there aspects of the user interface (i.e., the initial, structure/data entry screen; and the results screens) that need to be corrected, redesigned, or otherwise improved? Do the results screens display all the desired information?
  - D. Currently one enters EPI Suite using SMILES and CAS; are there other ways to describe the structure (e.g., ability to input a structure by drawing it), that should be added?
  - E. The EPI Suite has many convenience features, such as the ability to accept batchwise entry of chemical structures, and automatic display of measured values for some (but not all) properties. Are there other features that could enhance convenience and overall utility for users?
  - F. Are property estimates expressed in units that are easily understood by a broad cross section of potential users, not just scientists and engineers with advanced technical training?
  - G. Is adequate information on accuracy/validation conveyed to the user by the program documentation and/or the program itself?
  
- 3. Appropriate Use

- A. Currently Identified Uses: review of PMNs, P2 decisions, predicting physical/chemical properties and environmental fate and transport properties for HPV Challenge chemicals, to begin the assessment of exposure, and other routine OPPT uses. It is important to understand that EPI Suite is intended to be used in the absence of measured data and not take their place.
- i. Is the science incorporated into EPI Suite adequate for each of these current uses?
  - ii. If not, what improvements are needed to make EPI Suite adequate and what alternate approach could be used in the interim?
- B. Potential Additional Uses

To: White.Kathleen@epamail.epa.gov  
From: .farlandm@msn.com  
DeliveredDate: 07/26/2007 03:13:19 PM

Hello Kathleen,

These minutes look very familiar. At any rate, they do reflect the discussions that took place regarding EPI Suite. I approve them as written.

Thanks

Mike

-----Original Message-----

From: White.Kathleen@epamail.epa.gov  
[mailto:White.Kathleen@epamail.epa.gov]

Sent: Thursday, July 26, 2007 12:39 PM  
To: farlandm@msn.com  
Subject: Old Minutes: EPI Suite (1 of 4) February 22 2006 EPI Suite  
Conference Call Minutes for Your Review, Correction, Approval

I'm not sure whether you responded to these or not, but they've gotten lost in the shuffle one way or another. Can you look them over and let me know?

K

----- Forwarded by Kathleen White/DC/USEPA/US on 07/26/2007 02:37 PM

Kathleen White/DC/USEPA/US  
To McFarland  
05/01/2007 03:26 PM  
Subject: February 22 2006 EPI Suite Conference Call Minutes for Your  
Review, Correction, Approval

I'm happy to make any changes you suggest. Once you are satisfied with the minutes, will you send me an email to that effect so that I can support signing them for you?

Thanks!

K