



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

January 24, 2006

OFFICE OF THE ADMINISTRATOR
SCIENCE ADVISORY BOARD

MEMORANDUM

SUBJECT: Determination for U.S. EPA Science Advisory Board (SAB) EPI Suite Review Panel

FROM: Kathleen E. White /Signed/
EPA Science Advisory Board Staff Office (1400F)

THRU: Daniel Fort /Signed/
SAB Ethics and FACA Policy Officer
EPA Science Advisory Board Staff Office (1400F)

TO: Vanessa Vu, Ph.D.
Director
EPA Science Advisory Board Staff Office (1400F)

This memorandum summarizes steps taken in regard to the request from EPA's Office of Pollution Prevention and Toxic Substances (OPPTS) for an SAB review on the Estimation Programs Interface (EPI) Suite (Project No. 04-09). This memorandum documents the determinations for selecting members for the EPI Suite Review Panel.

A. Background

A mission of the U.S. EPA's Office of Pollution Prevention and Toxics (OPPT) is to evaluate potential risks of commercial chemical substances that are or will be released to the environment. OPPT also has the primary responsibility for implementing Agency policy on pollution prevention (P2), and in this role is a critical provider of information and guidance to risk assessors and risk managers. The understanding of and ability to predict the behavior of a chemical substance in a biological or environmental system depends upon knowledge of the physical, chemical and environmental properties of that substance. Accordingly, OPPT has supported the development of software for estimating these properties from chemical structure known as the Estimation Programs Interface (EPI) suite. 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 related to the potential fate and transport behavior of chemicals already in commerce.

Because of its importance in the PMN program and widespread use, OPPT requested that the SAB review the EPI Suite software. The charge for the review is attached to this memo.

B. Formation of the EPI Suite Review Panel

The SAB Staff Office announced to the public through a *Federal Register* notice 70 (FR 4846, January 31, 2005) that an *ad hoc* panel would be formed to review the EPI Suite. The Panel, which will be chaired by chartered SAB member, Dr. Michael J. McFarland of Utah State University, will provide advice regarding the comprehensiveness and soundness of the science supporting EPI Suite. The SAB Staff Office was seeking nominations of recognized scientists and engineers with expertise in one or more of the following areas:

- (1) Environmental chemistry and engineering;
- (2) Pollution prevention, especially experience deciding whether or not to go into production with a chemical;
- (3) Development of estimation models, such as QSARs that predict properties, effects and fate of chemicals from structure; and
- (4) Application of EPI Suite or similar tools.

The SAB Staff Office considered 45 candidates for the panel, including 16 whose nominations were received electronically. Due to the relevancy of the candidates' expertise and willingness to serve, the SAB Staff Office placed all 45 candidates on the "short list." On September 21, 2005, the SAB Staff Office posted a notice on the SAB website inviting public comments on the "short list" of prospective candidates for the Panel. The SAB Staff Office received three comments on the "short list" of candidates for the EPI Suite Review Panel. The commenters were: Michael E. Johnson, CH2M HILL Hanford Group, Inc., Richland, Washington; Walter Tamosaitis and Fred Damerow, Bechtel National, Inc.; Richland, Washington; and James H. Southerland, NC Dept. of Environment and Natural Resources, Raleigh, NC.

After the availability of prospective candidates for potential meeting dates was determined, the Staff Office identified a subset of candidates from which a balanced Panel could be formed and these candidates were asked to provide information that would allow the SAB Alternate Deputy Ethics Official to determine whether a conflict or interest or an appearance of a lack of impartiality might exist of the individual were to serve on the Panel. (These considerations are described more fully in the next section.)

C. Conflict of Interest Considerations

18 U.S.C. 208 provision states that:

"An employee is prohibited from participating personally and substantially in an official capacity in any particular matter in which he, to his knowledge, or any person whose interests are imputed to him under this statute has a financial interest, if the particular matter will have a direct and predictable effect on that interest [emphasis added]."

For a conflict of interest to be present, all elements in the above provision must be present. If an element is missing, the issue does not involve a formal conflict of interest. However, the general provisions in the "appearance of a lack of impartiality guidelines" may still apply and need to be considered.

Personal and Substantial Participation:

Participating personally means participating directly. Participating substantially refers to involvement that is of significance to the matter [5C.F.R. 2640.103(a)(2)]. For this review, panel members will be participating personally in the matter through attendance at meetings, teleconferences and other means.

Direct and Predictable Effect:

A direct effect on a participant's financial interest exists if, "... a close causal link exists between any decision or action to be taken in the matter and any expected effect of the matter on the financial interest...A particular matter does not have a direct effect...if the chain of causation is attenuated or is contingent upon the occurrence of events that are speculative or that are independent of, and unrelated to, the matter. A particular matter that has an effect on a financial interest only as a consequence of its effects on the general economy is not considered to have a direct effect." [5 C.F.R. 2640.103(a)(i)]. A predictable effect exists if, "...there is an actual, as opposed to a speculative, possibility that the matter will affect the financial interest." [5 C.F.R. 2640.103(a) (ii)].

Particular Matter:

A "particular matter" refers to matters that "...will involve deliberation, decision, or action that is focused upon the interests of specific people, or a discrete and identifiable class of people." It does not refer to "...consideration or adoption of broad policy options directed to the interests of a large and diverse group of people." [5 C.F.R. 2640.103 (a)(1)].

The EPI Suite is used so broadly that the EPI Suite Review Panel's activity cannot be said to be **particular matter of general applicability** because the resulting advice will involve neither the interests of a discrete and identifiable class of people nor specific parties.

Appearance of a Lack of Impartiality Considerations:

The Code of Federal Regulations [5 C.F.R. 2635.502(a)] states that:

"Where an employee knows that a particular matter involving specific parties is likely to have a direct and predictable effect on the financial interest of a member of his household, or knows that a person with whom he has a covered relationship is or represents a party to such matter, and where the person determines that the circumstances would cause a reasonable person with knowledge of the relevant facts to question his impartiality in the matter, the employee should not participate in the matter unless he has informed the agency designee of the appearance problem and received authorization from the agency designee."

Further, 5 C.F.R. 2635.502(a)(2) states that:

"An employee who is concerned that circumstances other than those specifically described in this section would raise a question regarding his impartiality should use the process described in this section to determine whether he should or should not participate in a particular matter."

Each potential advisory panel member was evaluated against the 5 C.F.R. 2635.502(a) general requirements for considering an appearance of a lack of impartiality. Information used in this evaluation has come from information provided by potential advisory panel members (including, but not limited to, EPA 3110-48 confidential financial disclosure forms) and public comment.

To further evaluate any potential appearance of a lack of impartiality, the following five questions were posed to all prospective advisory panel members:

- 1) Do you know of any reason that you might be unable to provide impartial advice on the matter to come before the Panel or any reason that your impartiality in the matter might be questioned?
- 2) Have you had any previous involvement with the issue(s) or document(s) under consideration, including authorship, collaboration with the authors, or previous peer review functions? If so, please identify those activities.
- 3) Have you served on previous advisory panels or committees that have addressed the topic under consideration? If so, please identify those activities.
- 4) Have you made any public statements (written or oral) on the issue? If so, please identify those statements.
- 5) Have you made any public statements that would indicate to an observer that you have taken a position on the issue under consideration? If so, please identify those statements.

As a result of a review of these forms and the responses to the five questions above provided by each prospective panel member, the SAB Alternate Deputy Ethics Official of the

Science Advisory Board determined that there are no conflicts of interest or appearances of a lack of impartiality for the members of this panel.

The SAB Staff Office makes the final decision about who serves on the Panel. Selection criteria included: scientific and technical credentials and expertise; the need to maintain a balance with respect to members' qualifying expertise background and perspectives; willingness to serve on the Panel, and availability to meet during the proposed time period; the absence of conflict of interest; and absence of any appearance of lack of impartiality. The final panel was selected from candidates on the "short list."

Accordingly, based on the above-specified criteria, a EPI Suite Review Panel of the following experts was selected:

1. Dr. Michael J. McFarland, Utah State University, Chair
2. Dr. Deborah H. Bennett, University of California - Davis
3. Mr. Robert L. Chinery P.E., Environmental Protection Bureau, New York State Department of Law
4. Dr. Christina E. Cowan-Ellsberry, The Procter & Gamble Company
5. Dr. Miriam L. Diamond, University of Toronto
6. Dr. William J. Doucette, Utah State University
7. Dr. David A. Dzombak, Carnegie-Mellon University
8. Dr. Anton J. Hopfinger, University of New Mexico
- 9.. Dr. Michael W. Murray, National Wildlife Federation,
10. Dr. Thomas Parkerton, ExxonMobil Biomedical Sciences
11. Dr. Kevin H. Reinert, AMEC Earth and Environmenta
12. Dr. Daniel T. Salvito, Research Institute for Fragrance Materials, Inc.
13. Dr. Hans Sanderson, The Soap & Detergent Association
14. Dr. Louis J. Thibodeaux, Louisiana State University

Concurred,

/Signed/

Vanessa Vu, Ph.D.
Director
EPA Science Advisory Board Staff Office (1400F)

25 January 2006

Date

Charge Distributed for 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