

## AGENDA

### FIFRA SCIENTIFIC ADVISORY PANEL (SAP) OPEN MEETING

**August 14-15, 2007**

FIFRA SAP WEB SITE <http://www.epa.gov/scipoly/sap/>  
OPP Docket Telephone: (703) 305-5805  
Docket Number: EPA-HQ-OPP-2007-0388

U.S. Environmental Protection Agency  
Conference Center - Lobby Level  
One Potomac Yard (South Bldg.)  
2777 S. Crystal Drive, Arlington, VA 22202

### Review of EPA/ORD/NERL's SHEDS-Multimedia Model, Aggregate version 3

**Tuesday, August 14, 2007**

- 8:30 A.M.**    **Introduction and Identification of Panel Members** – Steven G. Heeringa, Ph.D. (FIFRA SAP Chair)
- 8:40 A.M.**    **Administrative Procedures by Designated Federal Official** – Mr. Steven Knott, Office of Science Coordination and Policy, EPA
- 8:45 A.M.**    **Welcome and Opening Remarks** – Debbie Edwards, Ph.D., Director, Office of Pesticide Programs, EPA
- 8:50 A.M.**    **Introduction** – Dana Vogel, Office of Pesticide Programs, EPA
- 9:00 A.M.**    **Overview of SHEDS-Multimedia Residential and Dietary Models, and Future Plans** – Valerie Zartarian, Ph.D., Office of Research and Development, EPA
- 9:15 A.M.**    **Public Comments**
- 10:15 A.M.**    **Break**
- 10:30 A.M.**    **SHEDS-Multimedia version 3, Residential Model Structure and Approach** – Valerie Zartarian, Ph.D., Office of Research and Development, and Jianping Xue, Ph.D., Office of Research and Development, EPA
- 12:00 P.M.**    **Lunch**
- 1:15 P.M.**    **Charge to Panel – Issue 1:** Documentation, completeness, and clarity of the technical aspects and usability of the SHEDS-Multimedia version 3 (aggregate residential) model

**Charge Question 1:** The SHEDS-Multimedia version 3 User's Manual provided to the SAP presents installation and operational instructions for the software.

**1(a): Were Panel members able to load the software on to their computers? What, if any, difficulties were encountered in loading or running the software?**

**1(b): The SHEDS-Multimedia version 3 graphical user interface (GUI) was designed to be user-friendly to exposure modelers and risk assessors. Please comment on the organization and usability of the GUI, any difficulties you encountered, which features and output capabilities were most useful, and whether any additional options would be helpful. Please also comment or offer suggestions for improving the GUI/model interface.**

**1(c): Please comment on the organization, clarity, completeness, and usefulness of the User Guide document and provide any suggestions for improvement.**

**Charge Question 2:** The SHEDS-Multimedia version 3 Technical Manual provided to the SAP provides an overview of the SHEDS-Multimedia version 3; presents detailed descriptions of key model components; and describes the model construct and algorithms, required inputs, and analysis/output capabilities.

**2(a): Please comment on whether the descriptions of specific model components are scientifically sound and whether the algorithms described in the Technical Manual represent the state of the science for performing exposure assessments. Please also comment or offer suggestions for improving or modifying these algorithms or other aspects of the model construct.**

**2(b): Please comment on the organization, clarity, completeness and usefulness of the Technical Manual and provide any suggestions for improvement.**

**Charge Question 3:** The Source Code Directory on the CD provided to the SAP includes annotated code for the exposure algorithms used in the SHEDS-Multimedia version 3.

**3(a): Please comment on whether the annotated code is sufficiently clear such that the algorithms can be followed and understood.**

**3(b): Please also comment on whether these algorithms are technically correct and consistent with the descriptions provided in the technical manual.**

**2:45 P.M.**

**Break**

**3:00 P.M.**

**Planned Methodologies to Extend version 3 to version 4 – Valerie Zartarian, Ph.D., Office of Research and Development, EPA; Jianping**

Xue, Ph.D., Office of Research and Development, EPA; and Graham Glen, Ph.D., Alion Science and Technology

**4:00 P.M. Charge to Panel – Issue 2** Technical Aspects of Planned Methodologies to Extend SHEDS-Multimedia version 3 (aggregate) to version 4 (cumulative)

**Charge Question 1:** SHEDS-Multimedia version 3 simulates exposures of individuals to one chemical at a time. As discussed in the Planned Methodologies document provided to the SAP, SHEDS-Multimedia version 4 will also allow tracking exposures of individuals to multiple chemicals at the same time. Unlike version 3, which has a single chemical focus, version 4 will have a “product formulation” orientation since a single product may contain multiple chemicals. A product-related co-occurrence priority system like the version 3 co-occurrence approach will be used to minimize the number of product combinations. In version 3, the running exposures of the chemical are tracked in three carriers (air, surface residues, and dust/soil), but the masses of the carriers themselves are not tracked. In version 4, the mass of each chemical and each carrier (soil, dust, residue, air, food, water) will be tracked. The basic operation of SHEDS-Multimedia will be unaffected by these changes, but the list of variables (vectors rather than single numbers for chemical-specific inputs, exposures, and doses) and model run time will be longer, and the GUI will need to be modified accordingly.

**Please comment on the technical aspects and usefulness of the planned methodology for extending SHEDS-Multimedia version 3 to address multiple chemicals in version 4.**

**Charge Question 2:** SHEDS-Multimedia version 3 combines media concentration or residue data with simulated individuals’ contact rates (e.g., m<sup>3</sup>/hr for inhalation, cm<sup>2</sup>/hr for dermal, or appropriate contact factors for ingestion via hand to mouth activity) to estimate exposure. The media (air, dust/soil, surfaces) concentrations or residue levels can be derived with a simple decay/dispersion model, from user-specified series of concentrations from either measurement studies or an external model, or from user-specified post-application distributions (as described in the Technical Manual). ORD intends to include a fugacity-based model as an added (fourth) option to SHEDS-Multimedia v 4. Fugacity can be considered the “escaping tendency” of a chemical from a given phase or compartment, and the fugacity-based model uses the thermodynamic, equilibrium, and physical-chemical properties of substances to model chemical transfers/movements of chemicals across these compartments. The proposed SHEDS v 4 fugacity model is more sophisticated and detailed than the other options currently available in SHED v3 and will require more extensive inputs on the part of the user. It divides a dwelling into treated and untreated areas, each having four compartments or

phases (vinyl or untextured surface, carpet or textured surface, air, and wall), and the output concentration time series for the different compartments will be used as contacted concentrations for simulated individuals in SHEDS v 4.

**Please comment on the technical aspects and usefulness of the planned methodology for incorporating a fugacity-based source-to-concentration module into SHEDS-Multimedia version 4. Does the Panel recommend additional efforts with the fugacity module (e.g., modeling more realistic multi-room dwellings) given available information?**

**5:00 P.M.    Adjournment**

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### Review of EPA/ORD/NERL's SHEDS-Multimedia Model, Aggregate version 3

**Wednesday, August 15, 2007**

- 8:30 A.M. Introduction and Identification of Panel Members -**  
Steven G. Heeringa, Ph.D. (FIFRA SAP Chair)
- 8:40 A.M. Administrative Procedures by Designated Federal Official -**  
Mr. Steven Knott, Office of Science Coordination and Policy, EPA
- 8:45 A.M. Follow-up from Previous Day's Discussion**
- 8:50 A.M. Charge to Panel - Issue 2 Continued**

**Charge Question 3:** SHEDS-Multimedia version 3 requires the construction of human activity diaries that cover the entire simulation period of a model run (e.g., several months, a year, or longer). The human activity diaries are drawn from EPA's Consolidated Human Activity Database (CHAD) and typically include just one day (24 hours) of activities from each person. SHEDS-Multimedia version 3 uses eight one-day diaries (one weekend and one weekday from each of four seasons) to assemble a longer-term activity profile for each simulated individual. A distinct and recognized disadvantage of this method is that any activity that happens at all will happen many times, since each diary is re-used many times and there is an absence of activities that happen only once or just a few times over the year.

Ideally, self-reported longitudinal diaries that cover the same person over a long period of time would exist for estimating longer-term exposures of days, weeks, or months; however, these studies are relatively rare and the data require substantial and sustained effort to collect, verify, and analyze.

As a result, EPA is developing a new approach for longitudinal diary assembly for SHEDS version 4 which allows for more control over the characteristics and longitudinal properties of the assembled diaries. The new diary assembly method requires the modeler to identify a diary property most relevant to exposure for the current application; to apportion the total variance for this selected property into within- ( $\sigma_w^2$ ) and between- variances ( $\sigma_b^2$ ); and to specify the relevant 1-day lag autocorrelation. The Panel has been provided with background material and a journal preprint entitled “A New Method of Longitudinal Diary Assembly for Human Exposure Modeling”.

**Please comment on the technical aspects, potential utility, and added value of the planned methodology for longitudinal diary assembly in SHEDS-Multimedia version 4. Does the Panel believe that this new method will create an assemblage of diaries that better simulates reality and provides more accurate estimates of exposures related to within-individual time-activity patterns? Please suggest procedures and/or longitudinal data which could be used to select factors (the “D” factor intra-class correlation coefficient, and the 1-day lag autocorrelation) or refine/ evaluate this method in SHEDS.**

**10:00 A.M. Break**

**10:15 A.M. Charge to Panel – Issue 2 continued**

**Charge Question 4:** SHEDS-Multimedia is sophisticated physically-based probabilistic model with numerous inputs. One of the unique advantages of SHEDS-Multimedia are sensitivity analysis methods that can be used to determine model inputs most influential on model output values. SHEDS-Multimedia version 3 utilizes “one-at-a-time” and “multivariate” sensitivity analysis methods, as described in the Technical Manual provided to the SAP. The Sobol multivariate method, described in the journal article provided in SAP background materials, provides significantly more information than current alternatives, but requires some reorganization of SHEDS code and redefining some inputs. The advantages of including the Sobol method as another option for SHEDS sensitivity analyses are: (1) it is capable of determining both direct and interaction influences for each input; (2) handles categorical, other non-numeric inputs; accounts for non-linear response; (3) can examine aspects (e.g., diary assembly) not easily handled by other methods; and (4) has not been used with a probabilistic model before SHEDS. Implementation of Sobol’s method in SHEDS requires two main alterations to model: all random determinations must be re-expressed as independent input variables; and random number seeds in SHEDS must be careful tracked. It requires that SHEDS be run a total of  $(2N+2)$  times.

**Please comment on the technical aspects and usefulness of the**

**planned methodology for utilizing Sobol's method for sensitivity analysis in SHEDS-Multimedia version 4, and whether Sobol's method would be a useful supplement to the existing sensitivity analysis methods used for the SHEDS-Multimedia version 3 model.**

**Charge Question 5:** Section 5 of the Background document entitled "Planned Methodologies for Extending SHEDS-Multimedia Version 3 (aggregate) to SHEDS Multimedia Version 4 (cumulative or aggregate)" describes some of the upcoming modifications and enhancements that are planned for SHEDS-Multimedia Version 4. The residential module of SHEDS-Multimedia Version 3 does not currently address cumulative exposures to multiple chemicals, does not utilize the MOE approach for aggregating exposures across routes, does not permit the user to repeat runs using the same random number seed, does not accept empirical input distributions, and does not allow outputs to be linked with PBPK models (e.g. ERDEM). These -- along with development and integration of the SHEDS dietary module -- are considered to be high priorities for SHEDS-Multimedia Version 4.

**Question 5(a): Please comment on (and prioritize, as appropriate) the technical aspects and usefulness of planned changes to the SAS code and GUI for SHEDS-Multimedia version 4 that are listed items in Section 5 of the above-referenced background document.**

**Question 5(b): Please comment on any additional modules, features, or capabilities that the Panel feels should also be high priorities for the next version of SHEDS including issues associated with the code, user interface/user friendliness, input, and output/output display. Are there modules, features, or capabilities of other human exposure models that should be considered for inclusion in SHEDS-Multimedia version 4 (e.g., simulation of individuals; longitudinal diary assembly)?**

**12:15 P.M. Lunch**

**1:15 P.M. SHEDS-Multimedia, Dietary Model Structure and Approach – Steve Nako, Ph.D., Office of Pesticide Programs, and Jianping Xue, Ph.D., Office of Research and Development, EPA**

**2:00 P.M. Charge to Panel - Issue 3: An Update on the Development of the SHEDS-Dietary Model**

**Charge Question 1:** Eating Occasion Analyses.

As described in the SHEDS dietary background document, the timing information available in CSFII can be used to model food and indirect water intake throughout the day. With the ability to incorporate the timing

of eating occasions in dietary exposure assessments, it is possible to assign either the same residue or a different residue to foods consumed on multiple eating occasions. In certain instances, the former seems logical (e.g, consumption of leftovers) while in other instances the latter appears appropriate (e.g, hash browns at home for breakfast and fried potatoes away from home for dinner).

**Please comment on developing simple decision rules - as described in the document - for assigning residues to commodities eaten on multiple eating occasions.**

**Charge Question 2:** Longitudinal Dietary Consumption

To estimate exposures associated with longer time periods than 1 day, SHEDS-Dietary draws from diary pools based on gender, age group, season and day-type (weekday, weekend). The 8-diary approach of SHEDS described in the background document limits each individual's diet to 2 per season, one of which corresponds to a weekday and the other corresponds to a weekend day.

**Please comment on the 8-record approach in SHEDS-dietary and the selection of age group, gender, season and day-type from which to create the "diary pools". What other approaches does the Panel recommend? Can the Panel suggest any "bounding approaches" that may - based on knowledge of actual eating patterns - provide upper and lower limits for longitudinal exposure estimates (e.g., yearlong consumption of the same diary throughout the year vs. random daily selection of CSFII diaries).**

**Charge Question 3:** Bayer Drinking Water Consumption Survey Data

The CSFII data does not contain information on the time and amounts of direct drinking water consumption. Bayer CropScience sponsored a study, Drinking Water Consumption Survey (DWCS) that was designed to obtain a distribution of water intake for a 24-hour time period from a representative sample of the US population. Participants recorded their water consumption (time of day and amount consumed) over a one-week (7 consecutive day) period. The authors, Barraj et.al. (2004) suggested that it may be possible to "allocate the total daily water consumption amount reported in the CSFII into various drinking occasions" using information from the DWCS. In addition to offering a fixed option for allocating direct drinking water throughout the day, the Agency is planning to include in SHEDS-Multimedia v. 4 the option to allocate direct drinking water consumption throughout the day through empirical use of the Bayer DWCS data.

**Please comment on the advantages and disadvantages of providing an option to use the Bayer DWCS data in SHEDS-Multimedia v. 4.**

**Please include in your comments any statistical concerns or issues associated with the design and conduct of the DWCS study.**

**3:15 P.M.**

**Break**

**3:30 P.M.**

**Charge to Panel - Issue 3 Continued**

**Charge Question 4:** Bootstrap Approach to Uncertainty Analysis  
Sensitivity and contribution analyses are a routine part of OPP risk assessments. These analyses help inform the risk manager how exposures may change when certain model inputs are modified. These modifications to the model inputs are typically performed “one at a time” to permit isolation of the effect. In a typical risk assessment, all the dietary consumption data (i.e., reported CSFII diaries) are used along with the best available pesticide residue data. OPP risk assessors specify a sufficiently large number of Monte-Carlo iterations such that exposure estimates are stable with respect to the random seed. The Agency has not conducted formal quantitative uncertainty analyses. The Agency presented a simple bootstrapping procedure for conducting uncertainty analyses, utilizing only a subset of the consumption and residue data inputs. That procedure was designed to provide some insight into the question ‘How much better would our exposure estimates be if we had more data’ by conducting the uncertainty analysis in the other direction.

**Please comment on the scientific soundness and utility of the proposed bootstrap uncertainty approach.**

**Can the Panel recommend alternative approaches - and how they might be interpreted and used - for conducting uncertainty analyses of dietary exposure estimates?**

**Charge Question 5:** NHANES Dietary Consumption Survey

The SHEDS-Dietary paper noted that the NHANES 1999-2006 dietary consumption data does not contain information on season nor region.

**Please suggest statistical or other methods that might be used to determine the extent to which region- and season- specific dietary consumption amounts and patterns might be important in developing dietary exposure estimates. Please consider in your response whether and how quantitative uncertainty methods could be used in addressing this issue.**

**5:00 P.M.**

**Adjournment**

Please be advised that agenda times are approximate; when the discussion for one topic is completed, discussions for the next topic will begin. For further information, please contact the Designated Federal Official for

this meeting, Mr. Steven Knott, via telephone: (202) 564-0103; fax: (202) 564-8382; or email: [knott.steven@epa.gov](mailto:knott.steven@epa.gov)