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

Office of
Prevention, Pesticides and
Toxic Substances

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MEMORANDUM

Subject: Transmission of Background Materials for the August 14-15, 2007 FIFRA Scientific Advisory Panel entitled "Review of EPA/ORD/NERL's SHEDS-Multimedia Model, Aggregate Version 3". **PART 2 of 3.**

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Attached please find the first set of background materials (1 of 3) and related charge questions for the August 14-15, 2007 FIFRA Scientific Advisory Panel entitled "Review of EPA/ORD/NERL's SHEDS-Multimedia Model, Aggregate Version 3". This transmittal memo pertains only to ***Issue 2: Technical Aspects of Planned Methodologies to Extend SHEDS-Multimedia version 3 (aggregate) to version 4 (cumulative)***.

Three issues will be presented for the FIFRA SAP review of the SHEDS-Multimedia version 3. The materials and related charge questions for Issue 2 are detailed below. Separate materials and charge questions will be provided subsequently to the SAP (Part 3 of 3) for Issue 3 (SHEDS-dietary module).

I. Charge Questions

Issue 2: Technical Aspects of Planned Methodologies to Extend SHEDS-Multimedia version 3 (aggregate) to version 4 (cumulative)

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.

Question 2. SHEDS-Multimedia version 3 combines media concentration or residue data with simulated individuals’ contact rates (e.g., m³/hr for inhalation, cm²/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?

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- (σ_w^2) and between- variances (σ_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.

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 carefully 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.

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.

5a. 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.

5b. 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)?

II. List of Attachments for SHEDS-Multimedia version 3 Residential Module

Review:

1. Planned Methodologies for extending SHEDS-Multimedia version 3.0(aggregate) to SHEDS-Multimedia version 4.0 (cumulative or aggregate) (SHEDS_plans_for_version4_06-12.pdf)
2. Sobol I.M., 1990. Sensitivity Estimates for Nonlinear Mathematical Models (In Russian), *Matematicheskoe Modelirovanie* 2:112-118. Re-published in English (1993) in *Mathematical Modeling and Computational Experiment* 1:407-414.
3. Bennett D.H. and E.J Furtaw, Jr., 2004, Fugacity-Based Indoor Residential Pesticide Fate Model, *Environ. Sci. Technol.* 38:2142-2152.
4. Glen, G., L. Smith, K. Isaacs, T. McCurdy, and J. Langstaff, 2007, A New Method of Longitudinal Diary Assembly for Human Exposure Modeling, *Journal of Exposure Science and Environmental Epidemiology*, accepted article.

