
**WORK ASSIGNMENT 5-18 UNDER**
**CONTRACT EP-W-10-014**

# PEER REVIEW OF EPA'S CONSUMER EXPOSURE MODEL AND DRAFT USER GUIDE

## FINAL PEER REVIEW REPORT

## September 2, 2016

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## CONTENTS

**1.0 INTRODUCTION ..... 1**

**2.0 PEER REVIEW PROCESS ..... 1**

2.1 Reviewer Search and Selection ..... 1

2.2 Conducting the Review ..... 1

**3.0 REVIEWER COMMENTS ORGANIZED BY CHARGE QUESTION ..... 2**

**Part 1. Equations Used in Models and Exposure Defaults ..... 2**

3.1 Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies. ..... 2

3.2 Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios". ..... 15

3.3 Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered. ..... 20

3.4 CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways ..... 22

3.5 There are several items listed in the "Areas for Future Enhancement" section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term. ..... 25

**Part 2. User Interface ..... 31**

3.6 Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface. ..... 31

3.7 Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful. ..... 36

**Part 3. Documentation and User Guide ..... 38**

3.8 Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited. ..... 38

3.9 Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear. ..... 40

3.10 Additional Comments Provided ..... 43

**APPENDIX A CHARGE TO REVIEWERS ..... A-1**

**APPENDIX B INDIVIDUAL REVIEWER COMMENTS ..... B-1**

Alesia C. Ferguson, Ph.D. ..... B-3
Gary L. Ginsberg, Ph.D. ..... B-21
P. Barry Ryan, Ph.D. ..... B-31
Woodhall Stopford, M.D. ..... B-45
Stephen T. Washburn, M.S. ..... B-55

## 1.0 INTRODUCTION

This report documents the results of an independent letter peer review of the U.S. Environmental Protection Agency's (EPA's) *Consumer Exposure Model (CEM) and Draft User Guide*. Eastern Research Group, Inc. (ERG, a contractor to EPA) organized this review and developed this report. Section 2 of this report describes the reviewer search and selection process; and Section 3 provides the individual reviewer comments organized by charge question. Appendix A provides the charge to reviewers, and Appendix B provides the complete set of comments submitted by each reviewer.

## 2.0 PEER REVIEW PROCESS

### 2.1 Reviewer Search and Selection

For this review, ERG identified, contacted, and screened qualified experts, and then proposed a pool of seven candidate reviewers who had no conflict of interest (COI) in performing the review and who collectively met the technical selection criteria provided by EPA. EPA specified expertise in the following technical areas:

- Exposure assessment;
- Use patterns of consumer products (frequency, duration, amount) and methods to obtain or estimate such data;
- Product emission and migration testing;
- Material science;
- Environmental chemistry;
- Model development and coding;
- Inhalation exposure to vapors and particulates;
- Ingestion exposure to dust, soil, and mouthing; and
- Dermal exposure from liquids and vapor.

EPA verified that the experts in the candidate pool were appropriately qualified. From among the qualified candidates, ERG then selected the following five final reviewers who collectively best met the selection criteria and could meet the review schedule.

- **Alesia C. Ferguson, MPH, Ph.D.:** Associate Professor, Department of Environmental and Occupational Health, College of Public Health, University of Arkansas Medical Sciences.
- **Gary L. Ginsberg, Ph.D.**: Senior Toxicologist, Connecticut Department of Public Health.
- **P. Barry Ryan, Ph.D.:** Professor, Rollins School of Public Health, Emory University.
- **Woodhall Stopford, M.D., MSPH**: Clinical Assistant Professor, Department of Community and Family Medicine, Duke University Medical Center.
- **Stephen T. Washburn, M.S.:** Principal, Ramboll ENVIRON.

### 2.2 Conducting the Review

ERG provided reviewers with instructions, the CEM, User Guide, and the charge to reviewers prepared by EPA (Appendix A). To kick off the review, ERG organized a 1-hour briefing call. During this call, which was facilitated by ERG, EPA provided background about the purpose and development of the CEM, and reviewers had the opportunity to ask questions of clarification regarding the charge and review process.

After this call, reviewers worked individually (i.e., without further contact with other reviewers or EPA) to prepare written comments in response to the charge questions. ERG collected reviewers' preliminary comments in response to the charge questions and then organized and facilitated a teleconference for reviewers to discuss their comments as a group. EPA attended the teleconference as an observer of the discussions, and provide clarification on the CEM where requested by the reviewers.

Reviewers then submitted their final written comments to ERG, and ERG forwarded them to EPA. Both ERG and EPA checked the comments to ensure that reviewers had responded clearly to all charge questions. EPA indicated that no clarifications were needed on the reviewers' comments. Section 3 of this report presents reviewer comments organized by charge question, and Appendix B provides the comments by individual reviewer. In both cases, comments are presented exactly as submitted, without editing, summarizing, or correction of typographical errors (if any).

## 3.0 REVIEWER COMMENTS ORGANIZED BY CHARGE QUESTION

This section presents reviewer comments organized by charge question. Individual comments are provided exactly as submitted by reviewers (see Appendix B for individual reviewer submissions).

### Part 1. Equations Used in Models and Exposure Defaults

### 3.1 Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies.

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| **Ferguson** | There are a few areas where improvements can be made (also please note that some of these comments are related to understanding the modules better but also improving the content of the user guide which pertains to Question 9 below-ERG may choose to arrange parts of my response under that question):<br><br>a) I see equation numbers in CEM for equations. The user guide needs equations numbers that match CEM equation numbers.<br><br>b) In some areas, where an equation is repeated, remove this repetition and refer to the equation number. For example, the equation for mass of product used (g) is at least repeated 4 times, starting on page 23 of the user guide. The equation does not change, and so use the equation number (when assigned) to refer back to it.<br><br>c) The naming pattern for models and equations should be better explained. INHO1, INH02 for example are concentration determination models, but ING01 and all DER models are exposure and dose models. Consider a renaming format for those models that only determine an environmental concentration and those that determine an exposure and dose. Some inhalation and some dose exposure/dose models use the concentration determination models.<br><br>Some additional point related this: |

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| | - Page 29: Calculation of Inhalation Dose from Product Use really should be a separate numbered model and stand out to the reader. This model can utilize INO1, IN02, INH03, IN04, the emissions models, which I believe should be named differently from exposure and dose models.<br><br>- In Section 2 (page 17): Insert an overall explanation of the various models in this summary section (you have some of that content at the beginning of Section 3). I would also suggest a schematic of models and equations and how they can feed into each other, after a renaming has occurred. The schematic would answer the questions, "what concentrations models can feed into what exposure and dose models by route and based on whether the chemical is found in an article or product?"<br><br>- For a model when naming, it should be clear what this model will do? So as an example in your current naming format: INHO2: Product Applied to a Surface Indoors Double Exponential Model", would be better called: INH02: Air Concentration Determined from a Product Applied to a Surface Indoors Using a Double Exponential Model". Consider a renaming scheme for models.<br><br>d) The user guide often goes back and forth between the terms algorithm (e.g., page 15), equation and model. I suggest sticking to equation and models. Also when does an equation rise to the level of a model (when it is a series of equations)?<br><br>e) In the Introduction (Page 16), after describing the contents for the user guide, please list all secondary models utilized in CEM (e.g., PARAMS, E-FAST and so forth). Also describe their function in CEM. This would be very useful to the user and will demonstrate the utility and parameter estimation functions in CEM.<br><br>f) Section 3 (page 20): When the two Zone model is explained (Figure 1), Q12 and Q21 is confusing. Just use one Q for a bidirectional flow or interzonal flow, like the figure on page 22 (Figure 2). It may have been a typo.<br><br>g) At first I had a hard time understanding the parameter H in the IH01 model on page 24. The term H helps to determine which part of the model is being applied; When H is zero, this is the first use or application period. Maybe just a couple words on this parameter and the user will better envision the different aspects or phases of this equation.<br><br>h) E(t) on page 24 is the same as E(t2) on page 27, because in the model INH03 a product sprayed has INH01 emissions as one component. You can eliminate this equation being repeated by numbering and referring to it and then users can see the relationship between models, where there is an extension of INHO3 over INHO1. Or at least point this out to the user, and use consistent terms and equation numbering.<br><br>i) Page 27: Product added to water: Evaporation might depend on whether it is added to a container that is then closed, such as a washing machine. The chemical's 90 percent evaporation time might not be relevant to dynamics in a washing machine. This is an empirical equation, please say the reference for this equation for "EvapTime" here and how it was determined by Chinn 1981. In other words provide |

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| | some further explanation on "EvapTimes" used to reduce the emission rate for a chemical added to water and how it might vary based on a closed container versus an open container. Once the container is closed, should emissions be truncated? Right now it says truncation will occur when everything is washed down the drain.<br><br>j) Page 30, LADC is mentioned for the first time without a definition as "Because of this iterative process CADD cannot be calculated directly from the LADC presented in the model results." Please note, the definition for LADC "Potential Lifetime Average Daily Concentration (mg/kg-day)" is first defined on page 32. Therefore this section needs some re-organization to perhaps present the various air concentrations that are actually determined and presented to the user (i.e., LADC, Peak Concentration, time integrated concentration) before then presenting time integrated dose over 60 days used for ADR and time integrated dose over one year used for calculating CADD. Some smaller section label or titles are also needed for this very important inhalation exposure and dose section.<br><br>k) Page 41, "Inhalation Dose of from Article Exposure" uses InhalAfter as a parameter. The glossary defines these "Inhalafter" and "InhalBefore" as use during and use after a product. Please clarify in all these inhalation models when these parameters would be used and why we assume breathing rates would be different during the use of a product and after the use of a product. In addition, this parameter "Inhalafter" is first mentioned with inhalation for article exposure, page 41 and a "inhal" parameter was used for inhalation after product use on page 30. Glossary also needs to match these definitions. "Inhalbefore" is not used in any of the equations. I see "InhalBefore" use as a selection in the CEM model but not in the equations of the model in the User Guide.<br><br>l) Page 43, D is used for Density of Formulation in the AR equation for DER01. Den is used for Density of formulation on the next page and D is used for Duration of use on page 50. Please check these equations for consistency and ensure actual CEM model is using the right parameters. Please also note earlier that Den is used for density of product. I suggest two separate terms for density of product and density of formulation where formulation is intended for a product applied directly skin like a cosmetic.<br><br>m) Page 51, DER03, the Factor says "weight fraction of chemical in product". DER03 model is for article where skin contact occurs. Change to "weight fraction of chemical in article" or explain the "product". This also occurs in the ADR equation on Page 52.<br><br>n) Although I think in most cases the dose will be far lower than the exposure or the chemical concentration in the environment, is there an underlying mass balance check on the chemical mass that is released from product and article uses. So if a product is assigned three routes of exposures, is the final dose amount (chemical mass) experienced by all receptors added to ensure that they total does not exceed total product mass released from product use. Can the model also report total dose as a function original chemical mass? |

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| | o) Some clarity needed here. Dermal exposure from use of product outside on soil is actually considered. Currently ingestion exposure is considered in CEM (ING02) from product used on ground, but the product user is more likely experience dermal exposure during use or a child playing on grass outside is likely to experience dermal exposure for days after the product use. This was not well explained. I choose fertilizers and ING02 and DER01 are used for product used outside. This was not explained in the user guide. DER01 is suggested as product applied to skin, but was used for product accidently applied to skin (where the percent retained is key). Again, does the model keep track between the DER01 and ING02 for such a scenario. If I choose 90% retained on skin, what restrictions are placed in the mass available for the ING02 model.<br><br>p) Another note: I ran a test with fertilizers and it allowed me to change the use environment to Residence-Whole House from Yard, but on the input page CEM still asked for the Yard Area and soil properties, so although it appears the model flexible on use environments, it is not. This needs to be explained. |
| **Ginsberg** | Article Equation (Page 36):<br><br>This equation focuses on the release of SVOC from the article into the gas phase with partitioning into suspended particles and deposited house dust. Separate tracking of suspended particle and house dust concentrations, with their own mass transfer coefficients makes the modeling more complex and may be of questionable value depending upon whether TSP contribution to house dust (for oral exposure) and influence on inhalation exposures is sufficient to warrant this level of detail. The main portion of the equation shows a steady state mass balance partitioning of SVOC between the article and gas phase with an exponential term apparently used to represent the back pressure of built up gaseous SVOC to partition back into the article over time. While this appears to be a reasonable mathematical representation, one potential issue is that the equation predicts the change in air SVOC mass (dNair/dt) by subtracting out the existing air amount (-Q*Nair/V). However, the incremental change over time may be best modeled by adding not subtracting what is already in air, which could allow the inclusion of background sources of Nair from other indoor and outdoor sources of the SVOC. By subtracting the baseline of Nair that exists from the previous time step it is worth asking whether the model has the potential to underestimate indoor concentrations. Further, the set of model equations for this scenario (pp 36-39) do not show how the model gets from the differential (change in Nair per time) to what is needed in the next set of equations (the consumer dose equations) and that is a concentration of SVOC in gas for inhalation. I would assume that the mass balance equations which produce mass of SVOC in air are fed into an equation which divides this quantity by Q*V, but I didn't see this described. Further, the mass balance equations which partition SVOC into TSP and dust on a mass basis must be fed into equations which dilute this mass into a total amount of house dust and TSP in the room or house. However, these equations are not shown and the way to estimate how dusty is the interior space is also not shown. Finally, there is no effort given to relate predicted TSP and house dust concentrations to actual data for these quantities in homes. Given the importance of dust loading levels on the release of |

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| | SVOCs from flooring, it would be comforting if USEPA provided a comparison between predicted loading levels and measured loading in homes that showed that the CEM estimates are reasonable.<br><br>The Page 36 equation shows SVOC partitioning into dust and TSP. The definitions and abbreviations for dust and TSP parameters are somewhat confusing, for example $A_{TSP}$ is "Mass of TSP suspended in the floor" – it would make more sense if that were "suspended above the floor" to distinguish it from $F_{TSP}$, which is "Mass of TSP settled on the floor".<br><br>$L_{art}$ is part of the exponential term on Page 36 but is not defined. The exponential appears to remove chemical from gas phase by partitioning back into article over time based upon the partition coefficient and $L_{art}$? Is that length of article? If so, shouldn't it be surface area of article instead of length of article?<br><br>The description of chemical specific mass transfer coefficient on Page 37 suggests that there are 3 ways to calculate it but then decides to use one of the methods (thermal convection) based upon a 2007 EPA modeling document. This decision should be better documented, and if there are substantial differences between the 3 methods, this parameter uncertainty should be discussed given the importance of this parameter. Further Equation 11 shows H to be a simple function of chemical molecular weight. It is worth describing whether other physical and chemical properties of the SVOC might impact H.<br><br>$K_{TSP}$, Page 38, Equation 12: this partitioning is based solely on octanol/air partition coefficient and the percent organic matter in the TSP or dust. As stated in this section, it is also possible to parameterize this partitioning based upon SVOC vapor pressure but this is suggested to be more complicated. However, SVOC vapor pressure may be more easily obtained from the literature for a wide range of chemicals than Koa, and in fact Page 38 did not say how Koa is derived (I assume it's the oct/water divided by the water/air (Henry's Law coeff?)). Further complicating the chosen approach (Koa based) is that the organic carbon matter percent of TSP and dust may vary and is not known but assumed to be 0.4, without further reference. It would be helpful to have further explanation about the possible differences between these two approaches and further justification for selecting the Koa approach.<br><br>Kart, Page 38, Equation 13: this partition coefficient is said to be based upon SVOC vapor pressure. However, when I ran the article model for vinyl flooring using DINP as SVOC, I tried a wide range of vapor pressures and found the model completely insensitive to this chemical parameter. The fact that Equation 13 is a log-log function should not prevent the model being responsive to VP if in fact it is used to create Kart and Kint. Further, it is conceptually inconsistent to base one partition coefficient, $K_{TSP}$, on Koa while a similar partition coefficient, Kart, is based upon vapor pressure.<br><br>Overall impression of the Article/SVOC Model (pp 36-39)<br><br>Model equations and parameterization appear reasonable except as noted above. However, the modeling is complex with chemical released from the article and ending up |

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| | in air, dust or TSP based upon a few chemical specific properties (concentration in article, Koa, VP, MW) and the eventual concentration in dust or TSP based upon some undescribed estimate of the dustiness of the interior space, or in the gas phase based upon some undescribed estimate of the volume of air the SVOC mass is diluted within. Given the various extrapolations and uncertainties, it would be very helpful for model results to be cross-checked against actual data. I exercised the article model for flooring using DINP as SVOC since it was a chemical already in the modeling parameterization database and since there are interior air and dust measurements for DINP in the literature to cross-check against. This exercise yielded an indoor air concentration of DINP of 93 ug/m3 and a TSP concentration of 3.59 ppm, while the model output did not report the house dust concentration. In contrast, Cousins et al. 2014 modeled indoor air and dust concentrations of DINP from Swedish flooring based upon actual emission tests of the flooring, with their model output estimating DINP in indoor air at approximately 0.003 ug/m3 and in indoor dust at approximately 10 ppm. Actual measurements of DINP in interior dust from a range of studies reported in Cousins et al. 2014 are in the 50-100 ppm range. These studies did not report on DINP in indoor air. However, the implication is that because of the low volatility of DINP, whatever is released from flooring and other household products will tend to be in particles and dust, not in the gas phase. This is not what the CEM article model predicts for DINP. Compared to a predicted indoor air concentration of 93 ug/m3 for DINP by CEM, Cousins et al. predict much lower levels in indoor air as mentioned above. Another point of comparison is the California Prop 65 review of DINP in vinyl flooring in which they estimated a gas phase indoor air concentration of 0.207 ug/m3 and a house dust concentration of 3416 ppm ( Cal OEHHA, 2016, available at: http://oehha.ca.gov/media/ downloads/crnr/ sud1supportingmaterials06212016.pdf). Again this is a much different air to dust ratio than what my trial run of the CEM flooring model yielded.<br><br>There are more data for DEHP, another large molecular weight phthalate with similar chemical properties as DINP. Modeling of DEHP emission from vinyl flooring and indoor measurements in homes from several studies involving hundreds of samples (summarized in Xu et al. 2012) show that DEHP in indoor air is uniformly well below 1 ug/m3 while in house dust its concentrations are routinely above 100 ppm. I suggest the CEM article model be revisited by EPA to explore how it can better simulate patterns for phthalates and perhaps over SVOCs that appear in the modeling literature as emanating from household articles and consumer products (e.g., flame retardants). Further, it was somewhat surprising that a commonly studied chemical such as DEHP was not included in the CEM database. Even if many uses of DEHP have been phased out, it is not banned in household articles and still appears to be at substantial levels in house dust. Given all the experimental data for DEHP, it would be helpful if the CEM contained DEHP to directly compare model results with empirical data and other modeling efforts.<br><br>A further indication of differences between CEM vinyl flooring results and that reported by others is with respect to the apportionment of doses to different routes. The DINP CEM run showed house dust ingestion for young children at 0.1x the inhalation dose to gas phase DINP. This is opposite to what was forecast by Little et al. 2012 for DEHP emanating from vinyl flooring and taken up by young children (ingestion of house dust = |

| Reviewer | Comments |
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| | 700 times more dose than inhalation of gas phase DEHP). An interesting feature of the CEM results with DINP for vinyl flooring is that the childhood mouthing dose was 25 times the house dust ingestion dose. This would appear to be a highly uncertain estimate as it would appear to require a child's direct mouthing of the floor for sustained periods and appears to be based upon a mouthing methodology developed by CPSC (2014) for toys. The CEM documentation (Page 55) states the numerous uncertainties in the mouthing modeling.<br><br>I attempted to run a second CEM model, this one for an indoor crack and crevice treatment of a pesticide. Since there are several chlorpyrifos studies in test rooms and houses, my first goal was to simulate those experiments with the CEM. However, the CEM does not have chlorpyrifos as a chemical ingredient. Rather than import parameters for this pesticide, I scrolled through the list and found that diazinon is in the CEM database and so looked for studies which tested or modeled diazinon in indoor applications. A pesticide indoor modeling paper by Bennett and Furtaw (2004) provided fugacity model estimates for chlorpyrifos and diazinon air concentrations after a test application with actual data provided for chlorpyrifos. Their fugacity model was able to simulate the chlorpyrifos air concentrations in the test house. In trying to use their diazinon application parameters in the CEM I quickly found that there was no pesticide indoor scenario. The closest scenario I could find was "one component sealants and caulks", within which I ran Inh01: Product Applied to a Surface, Incremental Source. Applying the diazinon application information (amount applied, application area and house size) from the Bennett and Furtaw paper to this CEM scenario and running INH01 yielded a peak exposure concentration of 7.7 ug/m3 which was within 2 fold of the reported peak of the fugacity based model from a single application (4.5 ug/m3) (Bennett and Furtaw, 2004). Thus, based upon this one attempt at checking CEM product application results against the literature yielded a confidence-building good fit. However, this is a limited cross-check as the CEM report only provides peak and chronic air concentrations instead of the full temporal pattern as reported in the literature. Further, the CEM does not provide a pesticide indoor application scenario so the user has to improvise which creates uncertainties in whether this is really an appropriate use of the model. It would be helpful for CEM to describe how to adjust the existing scenarios for products and applications not contained within the default array of scenarios.<br><br>On Page 25 of the user's manual, Wilkes et al. 1996 is used to support an estimate of 25% in one place and 10% in another for the fraction of applied product that rapidly vaporizes in the double exponential model. This apparent inconsistency should be fixed.<br><br>Additional comments post review group teleconference: The comments made by Dr. Ferguson regarding renaming of type of equations as environmental concentration prediction vs dose prediction I think would help, together with a flow chart of how one goes from product or article to contamination of media contacted by humans and then to dose in those humans. I agree with Dr. Ryan especially when he talks about the need for better documentation of models and parameter values, and in fact it would be very helpful to include a bit of mechanistic text to introduce the equations for a given pathway so that the reader knows whats going on physically and knows what the key assumptions |

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| | are (e.g., boundary layer conditions, diffusional flux in different media, sorption/ partitioning based upon organic carbon content of particles and other properties, etc.) |
| **Ryan** | Overview - Two-Zone Model<br><br>The Section entitled: 3. Detailed Description of Models and Equations used within CEM, as the title might suggest, lays out the models used in CEM. The two-zone model diagram and differential equations are clear and represent a standard two-compartment approach affording different concentrations for materials in the near-field and the far-field. At the bottom of Page 20, there are a pair of empirical expressions relating inter-zone exchange for two scenarios- Closed Rooms and Open Rooms. One must assume that the data used to develop these empirical models is sufficiently generalizable to account for most situation, at least at the level of a screening tool, but a reference to the work that developed this empirical expression would be of interest. The variables in the differential equations are defined sufficiently to enable the user to identify them clearly. By and large, the equations used appear sound and rely on fundamental physics. The coupled differential equations will be used extensively as they will determine the air concentration, and consequently the inhalation exposure and dose, in later models.<br><br>General Overview of Specific Models<br><br>As a general overview of the specific models, the equations, with some exceptions, rely primarily on typical combinations of variable, e.g., concentration, contact time, volumes, etc., that are manifestations of fundamental physics. These are not in question. However, many rely on specific data or specific manuscripts and reports. These need to be made available for users. One might envision a repository or compendium of documents that would be maintained by EPA for this project. As noted in the text, some of the key references are not generally available and it would be useful for the reader to have easy access.<br><br>INH01: Product Applied to a Surface Indoors Incremental Source Model Pages 22-24.<br>What is questionable is the reliance on certain empirical relationships that appear to be based on regression models of data not readily available. For example, in the Section entitled: INH02: Product Applied to a Surface Indoors Double Exponential Model, the emission rate is determined using an exponential decay of emissions with time. The total time for evaporation is given by an empirical relationship developed by Chinn in a DOD reference, i.e., Chinn 1981 reference given as: Chinn, KSK. (1981). A simple model for predicting chemical agent evaporation. Alexandria, VA: U.S. Department of Defense, Defense Technical Information Center, Cameron Station. http://www.epa.gov/opptintr/exposure/presentations/efast/chinn_1981_a_simple_method for_predicting.pdf<br><br>The link is dead and thus the expression cannot be evaluated. As this is an important reference, the link must be refreshed. I cannot understand the physics that leads to a product of molecular weight and vapor pressure without his work, which appears to be the results of a regression model relating the log of evaporation time with the log of this product. This evaporation times is then used to determine the time over which 90% of |

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| | the material has evaporated. This seems feasible from a physical point of view, but difficult to assess.<br><br>The next equation references Evans (1994), which will be discussed presently. However, this is a relatively straightforward look at the time dependent emission rate and does not require a reference.<br><br>The equation at the top of page 24 has a constant in it, namely $1.33x10^5$. It would be useful to describe this constant, which I believe is a conversion among torr, g/mol, and perhaps other units in order to make the saturation concentration come out to the correct units.<br><br>INH02: Product Applied to a Surface Indoors Double Exponential Model<br>I have no particular problems with the initial set of equations in this section, but have questions regarding the statements made and the references called. The equation at the bottom of Page 24, appears soundly based, however, the parameters that go into it, most notably, the fraction of material emitted and the exponential constants are less well developed.<br><br>The first paragraph contains the text:<br><br>Only 25% of the applied chemical mass is released, because a substantial fraction of the mass becomes trapped in the painted substrate when it dries. Empirical studies reported by (Wilkes et al., 1996) support the assumption of 25% mass released and have estimated a relationship between the fast rate of decline ($k_1$) and vapor pressure ($VP$), and between the slow rate of decline ($k_2$) and molecular weight ($MW$), leading to the equation below for the time-varying emission rate (Evans, 1994).<br><br>The references are repeated here to illustrate a problem:<br><br>Wilkes, C; Koontz, M; Ryan, C; Cinalli, C. (1996). Estimation of emission profiles for interior latex paints. Paper from proceedings of Indoor Air '96.<br><br>Evans, WC. (1994). Development of continuous application source terms and analytical solutions for one- and two-compartment systems. In Characterizing Sources of Indoor Air Pollution and Related Sink Effects (pp. 279-293). ASTM STP 1287, American Society for Testing and Materials. http://www.astm.org/DIGITAL_LIBRARY/STP/PAGES/STP15627S.htm.<br><br>The Wilkes reference is to a Proceedings paper from 20 years ago. It cannot be found anywhere online. The Evans reference is behind a pay wall requiring a payment of $25 in order to get a copy of the paper and an additional $109 for the "Complete Source (pdf)." Yet these two references are essential to the understanding where the empirical emission constants came from in the equation on Page 24 as well as the assumption that 25% of the mass is released while the rest is bound up in the matrix of the surface. This is not satisfactory. These two papers should be distributed as an appendix or kept online with simple access for users of the model. The quality of the modeling equation cannot be determined without them. |

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| | While I agree that the concentration must be limited to the saturation vapor pressure of the compound under investigation, one must still ascertain the inflow and outflow concentrations, and the inter-zone flow rates in order to determine rates of evaporation well. We blow on soup to increase evaporation and thereby cool the hot soup and such an analogy might be included here to explain the process. This is the basic physics of two-zone concentrations here.<br><br>INH03: Product Sprayed<br>I have no specific comments on this model. I was able to find the Delmaar reference, but not able to find the appropriate version of the EPA 2007 reference. A reference to page and pargagraph in this large document would help. The equations for emission rates are similar to INH01 equations.<br><br>INH04: Product Added to Water<br>While not directly called, this model also makes use of the Chinn empirical equation for Evaporation Time, which cannot be assessed. This model also uses the method of fixing the maximum concentration in air at the saturation vapor pressure and reducing the emission rate so that, when coupled with the inter-zone and overall exchange rate, that the concentration does not exceed saturation. Under some conditions, evaporation would cease. I believe that this is accounterd for in the model, but it is a bit unclear.<br><br>INH05: Product Placed in Environment<br>I have no new comments in this section. This model also makes use of Chinn's empirical formulation of evaporation time and the same treatment of saturation concentration.<br><br>Calculation of Inhalation Dose from Product Usage<br>The CADD calculation is a standard application used in screening risk assessment. I do have one comment regarding the adaptive time step: there is a big jump that occurs after 24 hours of exposure. In the first 24 hours, the time increment is 30 seconds. This is increased to one hour for the next 59 days. This is a two-order-of-magnitude increase in time step, which seems large. I believe the assumptions is that emission characteristics should be stabilized and flat after this after 24 hours. For a screening tools, this may be adequate, but I think caution is a watchword here as some substances or Articles may require a more adaptive time course. An adaptive time-step algorithm could be invoked here, but it is not my purview to tell the modelers how to do their work.<br><br>It is noteworthy that the authors have elected to determine the Potential Acute Dose using the maximum one-hour concentrations observed during the 60-day period. While this is a conservative estimate, I think it is appropriate for this screening tool. In our meeting discussions, this component was addressed. There is some concern about using this approach. I still think it is a valid conservative approach.<br><br>INH06: Article Placed in Environment<br>Figure 3 on Page 33 gives is a good depiction of the components affecting concentration and dose under these conditions. One might ask for more discussion of the figure for clarifying purposes. |

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| | A small point- the use of TSP as nomenclature for particles <10 µm in diameter is not quite standard notation. TSP, when EPA regulated it, included larger particles, perhaps as large as 100 µm. The <10µm particles were referred to as "respirable" particles, or RSP.<br><br>The 50% figure for settled particle mass transfer area can be readily seen, but might require a reference or a figure depicting the action.<br><br>On page 35 is the first equation in this Section. It relates surface area to volume ratio of the zone. This is an empirical relationship, not a physical one. It requires a reference or a model indicating why the number 2.08, which has units of inverse length, assumed to be meters, is appropriate. At this point, it seems completely arbitrary.<br><br>On Pages 36 and 37, there is a series of differential equations giving emission rates, denoted as change in particle number, for various emission surfaces. These are difficult to understand and would be quite a bit more transparent if there were explanations of the terms. For example, the very first equation includes a term:<br><br>$$\frac{A_{TSP}}{\rho_{TSP}} \text{ X } \frac{3}{r_{TSP}}$$<br><br>I looked at this, and the equations that followed trying to figure out where the constants 3 and 1. 5 came from; is the physics appropriate? After some manipulation, I realized that the term is conversion of volume to area assuming a spherical particle. The equation would have been much clearer if the Area had been put in and a notation used that effected the conversion, e.g.<br><br>$$\frac{\text{Mass of TSP}}{\text{Density of TSP}} = \text{Volume of TSP}$$<br><br>$$\text{Surface Area of a Sphere} = \text{Volume of a Sphere X } \frac{3}{\text{Radius of a Sphere}}$$<br><br>The concept is simple, but not at all transparent when one skips the steps. The 1.5 constant indicates particles on a settled surface that then emits only in the upward direction. This is also appropriate, but there is no need to make the equations so opaque. The equation is appropriate, as are all of them others with "3" in them as the surface area is the appropriate variable for emission of SVOCs bound to the surface of particles. But why make is so difficult to understand, especially in light of the central nature of these equations to the model?<br><br>At the bottom of Page 38 is the equation:<br><br>$$D_s = \frac{0.00000000003}{(MW \div 292)^{0.65}}$$<br><br>Why do the authors choose to use the long decimal number instead of scientific notation, i.e., 3 x $10^{-11}$? I found myself counting zeroes, for no good reason, again obfuscating the use of the equation. I do note the use of scientific notation for the same number on Page 39 and the definition of the value as the diffusion coefficient of PCP-52, the reference compound, which has a MW of 292 g/mol. At least in this section, the EPA document |

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| | references as USEPA 2005, is readily available for download. Note that this relationship probably came from a regression model as well. A simple Graham's Law of Diffusion approach would have the exponent on the denominator as 0.5. The last sentence on page 39 gives the default assumption for surface diffusion thickness as 0.005 m, and supports this with three references. It would be nice to get an assessment of the variability in this parameter and perhaps a sense of the sensitivity of results to this assumption. However, for a screening tool, this is likely accurate enough.<br><br>Calculation of Inhalation Dose from Article Exposure<br>I have no comments in this section; the equations seem quite appropriate given the correct values for input.<br><br>ING01: Product Applied to Ground Outdoors<br>The first reference in this section, USEPA 2012b, is readily accessible for download. In addition, the equations appear appropriate from a physical point of view. I have no additional comments.<br><br>ING02: Product Ingested via Swallowing<br>The first reference in this section, ACI 2010, is readily accessible for download. In addition, the equations appear appropriate from a physical point of view. They are typical of screening equations used in risk assessment for other types of exposures. I have no additional comments.<br><br>ING03: Article Ingested via Mouthing (Migration Rate Method)<br>The primary reference for this section USCPSC 2014, is readily downloadable. However, the reference focuses on phthalates for baby toys and similar items. One may question the validity of the application to other materials. Can the authors justify the leap from phthalate exposure to other exposures? Further, the so-called "migration method" may be operable on some materials, while a "bound-to-surface approach" maybe more valid on others. I would speculate that the user would select one or the other of these and evaluate the differences noted. Nonetheless, I believe the model to me adequate for the purposes of screening and offer no further comments. The dose equations are typical of screening equations used in risk assessment for other types of exposures.<br><br>ING04: Incidental Dust Ingestion (Article Model)<br>This model presents no new modeling approaches. It is similar to the other ingestion models discussed just above. I believe the model to me adequate for the purposes of screening and offer no further comments. The dose equations are typical of screening equations used in risk assessment for other types of exposures.<br><br>ING05: Ingestion after Inhalation (Article Model)<br>This model is modestly more complex in that it includes an inhalation component. However, it is relatively straightforward and similar to other models used in risk assessment for exposure and dose. I have no further comments.<br><br>DER01: Product Applied to Skin (Fraction Absorbed Method)<br>Dr. Ferguson is the expert on the panel in dermal exposures. I defer my comments to her extensive review. |

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| | The primary reference for this section is, again USEPA 2007. I was unable to download the appropriate version of this reference and thus cannot fully evaluate the model. However, see below.<br><br>The equation at the bottom of Page 47, uses the term D, which is confusing given equations above that use D as a diffusion coefficient. In the legend for this equation "Dens" is used and it is defined as "density." Density is usually symbolized as ρ (Greek letter rho), in is, in fact, symbolized this way in other parts of the manual. Others commented on this problem as well, further suggesting editing the document for symbol consistency throughout. The rest of the equations used in this model are fairly straightforward and similar to those used in other exposure/dose screening models. I have no further comments.<br><br>DER02: Product Applied to Skin (Permeability Method)<br>I was not able to find the expression for Kp in the first reference in this section, USEPA 1992, despite the reference being relatively easy to download. Hence I cannot fully evaluate the model. However, the expressions used are fairly straightforward and similar to those used in other exposure/dose screening models. I have no further comments.<br><br>DER03: Article where Skin Contact Occurs<br>There are three references cited in the first sentence of this section. ECETOC 2012 requires membership. As I am not a member, I cannot evaluate it. USEPA 2012b is readily downloadable from EPA. Delmaar 2005 is readily available from RIVM. Regardless, the equations used are fairly straightforward and similar to those used in other exposure/dose screening models. I have no further comments.<br><br>DER04: Article with Direct Transfer from Vapor Phase to Skin<br>The principal reference for this model is a paper by Weschler and Nazaroff obtainable from Environmental Science and Technology. Their equation for penetration the stratum corneum is a regression model they have developed. It is well described in their paper. This is the type of reference the modeling section needs, i.e., one that is readily available and can readily be evaluated. The remainder of the equations are standard flux equations based on relatively straightforward physics. I have no further comments. |
| **Stopford** | Outside my area of expertise. |
| **Washburn** | In general, the equations used in the CEM are well explained, appropriate for the purposes of this model, and accurately executed. Note that I have not had the time to check to make sure that each equation in the CEM user guide is correct or agrees with the cited reference.<br><br>For modules that estimate volatilization of organic chemicals from water (e.g., INH03), I recommend that EPA consider models based on Henry's Law (using Henry's Law Constants) instead of Raoult's Law (using Vapor Pressure) when evaluating relatively low contaminant concentrations. While both Henry's Law and Raoult's Law are ideal vapor-liquid equilibrium relationships that are relevant to dilute component mixtures, Henry's Law tends to better approximate volatilization of the solute (i.e., lower concentration |

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| | component) and Raoult's Law tends to better approximate volatilization of the solvent (i.e., higher concentration component). Raoult's Law assumes an ideal mixture and can result in much less accurate results than Henry's Law for dilute solutions of a contaminant (e.g., aqueous solutions of a chemical susceptible to hydrogen bonding).<br><br>Additional comments regarding inputs to the models are provided below. |

**3.2 Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios".**

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| **Ferguson** | a) There is a wide range of scenarios available to the user. If the user guide is rearranged and ordered more clearly according to some of my earlier suggestions to Question 2, this may be more apparent to the user.<br><br>b) On page 4, can you give example of when to use near field for product. Meaning how stationary is near-field. Would painting a room and moving around slowly be considered near field? Would walking through two rooms and spraying to be rid of "stinky teenager boy" smells be near field? In other words you have the product in your hands, but you are leaving the immediate vicinity of some of the air concentration. Maybe suggest to the user examples of product usage in near field. This may be a more trivial point, but it might help the user.<br><br>c) The percent retained on skin (Ret) in DER01 (page 43) is an extremely important factor. After searching a while I see that Table B-2 has this for products. Please indicate the references for these values and refer to this table in Section 3. Do these values consider wash and wipe events within a certain time period or consider the maximum loading possible on a skin surface over the time period? The implications of this factor may need to be further explained to the user, because heavily weighted factor for determining exposure and dose estimates. For some cosmetics applied to the skin (which I believe this model could also be used-although no cosmetics are listed as products) estimates could made on the mass of the product and expected use period of the product. For example, is facial cream expected to last 30 to 60 days and therefore daily exposure is just chemical mass divided by the number of days? So, ultimately however this model for CADD just means the person is exposed to all the chemical in certain fully used products, and the dilution factor is all that matters. This would be an assumption of no wash or removal event.<br><br>d) On page 24 for INH02, a study from Wilkes et al., 1996 is quoted as determining the 25% of mass is released typically. On page 26, f is described as the fraction of mass emitted from first exponential as 0.1. This f should be allowed to vary from 0.1 to 1.0 by the user, and should be dependent on volatility of chemical and product. However, |

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| | why is it described as 25%, but 0.1 is used in description. Again 10% is mentioned in the write-up on page 25. I may be confused and 10% what is released at first but overall only 25% mass of the chemical mass is ever released. Also combine the explanation of 25% and 10% release into the same paragraph for clarity.<br><br>e) Page 49, for DER02, please clarify to the user that the Kp is a permeability coefficient through the stratum corneum only (actually derived from Potts and Guy 1992 and then used by EPA in their dermal document-I gave reference for the EPA document below). Kp also exist for permeability through the hydrophilic epidermis (other 4 layers beneath SC). Models that consider movement through the two layers might be better predictors (Bunge 1995). At least let the user know this as this might be confusing, especially since DER04 uses a more complex and more recent model from Weschler and Nazaroff, 2012 that does consider a Kp for SC/viable epidermis composite and even permeability all the way through to blood (i.e., dermal capillaries). Explain that one model may be more complex than the other (many assumptions made also for partition coefficients). DER04 considers more barriers to movement. Really CEM is pulling different models together with varying levels of complexity and the reader needs to know this. Again there is consideration for volatiles and semi-volatiles, but once and if they cross the air-skin or liquid-skin barrier it is their solubility and molecular weight in both layers that will determine movement through layers and uptake into the bloodstream. The lipophilic and hydrophilic properties of all chemicals will need to be considered consistently in all layers or one layer.<br><br>f) Related to my point above, the "transfer coefficient" in DER03 is no more than a permeability coefficient through the skin. Please explain if the user determines this transfer coefficient and if it is different than kp in DER 02. Please note that the "transfer coefficient" in DER01 has units of cm/hr (length-time). The "transfer coefficient" in the glossary is $cm^2$/hr (area-time). Terminology for permeability coefficient and transfer coefficients need to be clarified. It gets further confusing when table –B13 has diffusion coefficients through a materials in units of m2/s (area-time). If differences in these models are dependent on the phase of the chemical (VOC versus SVOC) or media (air, versus liquid) that the chemical is housed in a better explanation is needed for the user for these dermal models and their considerations of movement of the chemical through the skin. Merging models from different sources can pose the additional challenge of establishing parameter terms consistently. In the exposure field transfer coefficients are also used to denote the mass of a chemical that transfer from a surface to the skin following one or multiple contacts ($mg/cm^2$). In DER03, you use fraction of chemical on surface that is dislodgeable as a proxy for mass transfer coefficients along with the mass of the chemical on the article in the contact layer.<br><br>g) Equations for INH05 and INH04 are identical on page 27 and page 28. So will a product placed in the environment will have the same emissions as the product placed in water? The only difference explained as I understand it, is that when the product goes down the drain or Csat is exceeded for INH04 the emissions is truncated then, while for INH05 emissions is truncated at the end of the product use or when |

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| | Csat is exceeded. I do have a hard time seeing that "EvapTime" the chemical product poured into water is the same as the "Evaptime" of the chemical from only the product. What might be different is the weight fraction of the chemical in the product. For INH04, it may now be weight fraction of the chemical in the mixture of water and product (not while pouring the product into the water-but for some time of exposure after). There must be some variable difference between the models, aside from emissions truncation time. In fact one model could be presented for both scenarios and just the truncation difference explained then. |
| **Ginsberg** | The scenarios represent an impressive array of product uses and household articles, with these scenarios appropriately tied to inhalation, oral and dermal exposure models. The scenario depictions of size of area treated, size of room and house, frequency of application, near and well mixed model, ventilation rates, etc. appear to be what is necessary to simulate a real world consumer exposure. As described above, the range of scenarios could be expanded to include pesticide crack and crevice treatment given the variety of studies with empirical data to ground-truth the model, mouthing of fabric to become exposed to dyes and flame retardants, and emission of phthalates from additional plastics such as shower curtains and Christmas trees. However, there will always be additional scenarios and products one may encounter that merit consumer exposure modeling. Therefore, it would be helpful if there was a general discussion of how the existing modules could be adapted to unique scenarios and product uses or articles in the home.<br><br>Near field modeling is mentioned repeatedly as an option and yet no guidance is given as to when it should be used. I would think that if exposures to young children are being modeled one may want to use the well mixed room model assuming that most cleaning, painting, stripping, pesticidal, etc. products would be applied by an adult and the young child would be somewhere else in the room (or house) rather than in the near field. However, such an assumption is not health protective of children. Guidance on when near field modeling is appropriate would be helpful.<br><br>Product Sprayed (Page 17) – would the overspray that is available for direct inhalation differ between aerosol cans and pump bottles used for cleaning chemicals?<br><br>DOES THE MODEL COVER PRESSED WOOD OFFGASING? COOKING EXPOSURES? RELEASE OF PERFLUORINATEDS? |
| **Ryan** | The scenarios available are extensive and range throughout typical activities encountered by individuals in their daily activities. I did not explore each and every scenario, activity, and default values, as that would have required modeling runs numbering in the thousands. However, the ones I did explore appeared to have default values that were, at least, reasonable, and quite adequate for the screening tool design of the CEM. Data sources appeared quite complete, given the caveat that not everyone could be explored in the allotted time.<br><br>As is the case with the models themselves, I am concerned that some of the data may be from sources not easily evaluated such as reports, proceedings presentations not later |

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| | published in the peer-reviewed, etc. USEPA should strive to document these as well as can be done and develop a library of such data in readable format for downloading and evaluation.<br><br>The MSExcel spreadsheet includes an extensive list of Products, Articles, and Functional Use Categories, with 88, 79, and 123 items listed respectively. The worksheet labeled "Product cat_Sceanrio Overlap" offers a useful compendium of cross-referenced Product Categorist and usage that should aid the user in selecting appropriate scenario, activities, articles, etc.<br><br>The discussion in the meeting requested both more scenarios and fewer scenarios, which is obviously contradictory. Personally, I think a simpler approach- one with a limited number of scenarios- is the way to go, but some of my colleagues thought otherwise. I am just putting my vote in. |
| **Stopford** | A major oversight in the scenarios is for exposures to dusty materials or solid aerosols such as ceramic clays and glazes. Exposures to such products have been associated with lead exposures and/or poisoning in homes, schools, work places and nursing homes as well as exposures to crystalline silica and fibrous talc in studios and schools. Data on exposures can be found as follows:<br><br>Roth WR, Stopford W. Classroom Contamination from Lead Bearing Ceramic Art Glaze. 2007. http://duketox.mc.duke.edu/EIA_Rev_4.doc<br><br>Stopford W, Turner J, Cappellini D. Determination of the Magnitude of Ceramic Glaze to Skin and Skin to Mouth Transfer. August, 2007 http://duketox.mc.duke.edu//ceramicglazetransfer.doc<br><br>Stopford W. Aerosol Production During the Use of Art & Craft Materials. Submitted to Consumer Product Safety Commission. 2003. http://www.duketox.mc.duke.edu/recenttoxiissues.htm<br><br>Stopford W, Stanion C. Potential for Lead Dust Exposure During the Operation of Contemporary Ceramic Studios. Research Report Submitted to the American Society for Testing and Materials in Support of Test Method C1023, Labeling of Ceramic Materials for Chronic Health Hazards, 1998. http://duketox.mc.duke.edu/CERAMICSlead.rtf<br><br>An alternate model for assessing peak exposure and average exposure over time is the general dilutional ventilation equation:<br><br>$C_t = C_i e^{-Qt/V}$<br><br>Where: $C_t$ = concentration (mg/m$^3$) at time t<br>$C_i$ = initial concentration<br>Q = Ventilation rate (m$^3$/min)<br>V = room volume (m$^3$) |

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| | This model has been used to determine peak exposure and average exposures to a number of aerosols and solvent vapors as summarized in the following article:<br><br>Stopford W. Aerosol Production During the Use of Art & Craft Materials. Submitted to Consumer Product Safety Commission. 2003. http://www.duketox.mc.duke.edu/recenttoxiissues.htm.<br><br>This model was confirmed for exposure to marker solvents in the following paper:<br><br>Stopford W. Solvent Exposure from use of Whiteboard Markers. Submitted to CPSC. http://www.duketox.mc.duke.edu/recenttoxiissues.htm. 2003 |
| **Washburn** | The breadth of scenarios contained within the CEM is impressive and actually a bit overwhelming, particularly given the large number of products and articles that are also included. While I have not tested all combinations of chemicals, products, articles and scenarios, some clearly represent relatively lower potential for exposure, are less common, and/or are based on less established modeling approaches. I recommend that EPA strongly focus the initial version of the CEM on a smaller number of scenarios, articles and products that under most exposure conditions are likely to be the most significant or most common, and put effort into refining those scenarios rather than attempting to be as exhaustive as the version release for peer review.<br><br>Although the current list of products is relatively exhaustive, cosmetics is conspicuously absent. Unless cosmetics are being addressed separately by EPA, I recommend that they be included in the current CEM or, at a minimum, be a top priority future enhancement.<br><br>Regarding the scenarios that are included in the CEM:<br><br>– Products appear to be limited to "consumable liquids, aerosols or semi-solids". What about powders, such as dishwashing powder or abrasive cleaners?<br><br>– Explain why SVOC emissions, but not VOC emissions, are evaluated for articles while presumably both VOCs and SVOCs are evaluated for products.<br><br>– Why are metals and other essentially non-volatile chemicals not included for any products or articles? They could be particularly important when evaluating exposure to particulates.<br><br>In most instances, references are provided for default values or approaches. Some exceptions appear to include the following:<br><br>– p.19, Section 3. Reference or basis for 60 day emission period needed.<br><br>– p. 33. Reference or basis needed for assuming that 100% of the area is available for suspended particulates and 50% is available for settled particulates<br><br>– Table B-2. Reference or basis needed for film thickness values. |

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| | – Appendix B should provide all default physical-chemical property data with references. While some physical-chemical data are provided (e.g., diffusion coefficient), others are not (e.g., vapor pressure).<br><br>How frequently will the database of physical-chemical data for individual compounds be reviewed and, as necessary, updated? Who will be responsible for making sure that the physical-chemical database is maintained and reflects the current scientific literature? |

### 3.3 Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered.

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| **Ferguson** | a) This model is <u>not</u> geared for probabilistic calculations, where a number of calculations could be run by varying multiple parameters to look at worst case (i.e., Monte Carlo simulations using distributions). The user could carefully select an input for each parameter to get to worst case, with an understanding of parameter's influence in the equation. But the range of values and exposure possibilities cannot be determined using this model. This statement is made in the user guide on page 6, and could be moved into an executive summary since this is very important to understand. The model allows the user to enter their own parameters for a particular scenario to offer flexibility in the model and in the case of the user to capture the variability using a unique set of parameters in a single run.<br><br>b) A product user could become a receptor during the duration of use of the product. I just experienced this. I painted for a while, allowed my partner to paint for a couple hours, but I stayed close to source. The CEM could allow the user to add exposure for the two scenarios to a total exposure. The first scenario entails "near field" exposures, and later a far field with the time frame of the acute or chronic dose calculations.<br><br>c) The user is required to enter air exchange rates and ventilation rates. These largely depend on type of building, layout of building (upstairs/downstairs), use of building and type/performance of HVAC system (room HVAC and central HVAC). The user can be referred to a few references to determine this. ASHRAE recommended ventilation rate is 50 cfm and changes for house size. ASHRAE has a formula for recommended ventilation rates dependent on the number of bedrooms in the building. See: https://resaveguide.lbl.gov/step-3-whole-building-ventilation-rate<br><br>d) The "60-day modeling period is used to calculate the total exposure associated with a single use of a product". Can this be flexible, and more dependent on mass of product and ultimately environmental concentration of some significance over time?<br><br>e) Model can ask if other receptors in in the same room as product user or a different room during the use period. This would increase the exposures for some receptors |

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| | and offer some flexibility in the model. Right now on page 14 of the user guide it is not clear to me where the receptors are located (zone 1 or zone 2 when at home)?<br><br>f) For Activity Patterns, currently only one type of activity pattern (i.e., full time or part) will be calculated all receptors in the user guide. This is an area of flexibility the model can consider changing later.<br><br>g) User has to choose between DER01 and DER02 (absorption fraction or permeability method) on the Scenario tab. Allow user to also select both for comparison. |
| **Ginsberg** | The CEM modules are populated by many different equations and parameters. In most cases the uncertainty and variability associated with a model parameter is not described. The product usage modules do contain a low, medium and high range of default estimates for product content and use rate which is helpful to bound estimates. But for many other parameters such ranges are not provided. As described above under Charge Question #1, the uncertainty with using Koa instead of VP-based partition coefficients is not described and the uncertainty of matrix interference with release of SVOCs from articles is also not described, although some of the data presented in Appendix tables B12 and B13 show the potential effect of matrix on diffusivity and emission. Further, the uncertainty and possible alternative values for other parameter defaults (e.g., percent organic carbon in TSP of 0.4) is not described. Finally, the large range in human activity patterns, breathing rates, body weights, dust ingestion rates, dermal parameters, etc. is captured to some extent in the modeling options but a better description of intra-human variability related to age groups and activity patterns would be helpful.<br><br>It appears that the low/medium/high scenarios are not necessarily representative of low, medium or high exposure rate as is implied by the labels. For example, App Table B-12, top of Page 87, shows that the high scenario has greater TSP and house dust generation rates than the low scenario. These higher particle generation rates will likely dilute the emitted chemical into a greater mass and thus reduce the concentration in the particle. Further, the high scenario is associated with a higher frequency of cleaning and efficiency of cleaning which would tend to lower TSP and house dust levels. The net effect on chemical concentration mean for these inhalation models.<br><br>Seasonality is not considered in the modeling. This could affect temperature, humidity and building ventilation. Phthalate emissions from plastic surfaces and flooring is known to be affected by humidity and temperature. Discussion of such sources of variability would be a helpful addition.<br><br>The lack of model calibration and validation against actual data is a source of considerable uncertainty. Greater confidence could be obtained by cross-checking model output for TSP levels, house dust levels, and chemical concentrations in various media, against actual studies from test houses. Under charge question number 1 I provide two such modeling cross-checks, one which did not provide very comforting results (vinyl flooring) and another which did (pesticide application). Other such cross-checks are recommended in an iterative process to improve model reliability and confidence. |

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| **Ryan** | The approaches presented in the CEM are deterministic in nature and thus contain no information on variability and uncertainty. I saw no way of implementing such beyond the brute-force method of varying input parameters by hand to assess the impact of such. I think the approach followed here is appropriate for a screening method. It could, perhaps, be modified to reflect calculations of uncertainty and variability, but the CEM is complicated enough as it is and would be complicated substantially by further modification to include this type of analysis. I think that most users of CEM would be interested in measures of central tendency or high/screening values that could be modeled directly. The CEM does have the ability modify the input parameters to simulate variability and uncertainty through direct changes in input parameters, but I do not think that this is essential to the utility of the system. The system is meant to be a screening tool and I think uncertainty and variability in a screening tool may be misplaced. More sophisticated models may be required as the uncertainty introduced by taking conservative parameter estimates and models is large and would likely dominate. |
| **Stopford** | Outside my area of expertise. |
| **Washburn** | Overall, the CEM does an acceptable job of considering variability and uncertainty – especially and primarily because it allows the user to readily conduct his or her own sensitivity and uncertainty analyses by entering alternatives to the defaults. I believe this is one of the chief values of the CEM. I do not believe that we have sufficient data to conduct reliable probabilistic (Monte Carlo) simulations for most components of the model and thus do not recommend that additional level of complexity. However, I think the User Guide should include a separate sections that emphasizes the variability and uncertainty in the models and their inputs, and the results summaries should also distinguish between default, model-calculated and user-supplied inputs. |

### 3.4 CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc.). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways.

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| **Ferguson** | a) The exposure/dose metric to consider might also be relevant to the toxicity of the chemical, the question the user might want to ask is….is it likely to cause an acute effect or a chronic effect to a particular user, and is it based on how the product or article is used. However in the home setting, odd use patterns can occur and all exposure metrics should be available for every product and article. However as a start, in the excel sheet of product and article functional use categories, you might consider adding columns for product and articles on likely use patterns in terms of weekly, month, and yearly. When additional dose metrics are added, it will guide the user on |

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| | selecting what dose metrics are suitable. Naturally you would allow lifetime measures for those articles and products that are used quite commonly over very long periods (e.g., cleaners, cosmetics).<br><br>b) Many products cause a dermal/skin local effect equation (e.g., harsh cleaning agents like bleach). Allow the dermal dose equation to focus on determining what remains on the skin surface over the exposure period. In model DER01 for example this is more appropriate for the Acute Dose Rate equation, FRabs would not be needed. The model in CEM should ask if a skin exposure or a dose is needed. Likewise DER02, DER03, and DER04 can be adjusted also to accommodate this extra feature. |
| **Ginsberg** | It is helpful that the modules provide both an acute peak exposure profile as well as a chronic dose. However, the CADD doses on Page 30 are calculated based upon 1 year of exposure. How does this relate to the chronic averaging of dose needed in risk assessment to compare against an RfD or CPF? If basing exposure upon only 1 year, which year of life for children – the maximal year of exposure? It would also be advantageous for the model to provide dose estimates that are more in line with what is needed in risk assessment to calculate risk for chronic cancer and non-cancer endpoints. |
| **Ryan** | All of these exposure metrics are important depending on the context. Specific activities of the various age groups influence which are considered most important. Since these are commercial products, most would be used by Adults. However, the Child and Youth categories are also important. I will express concern that the latter two categories may be too broad. Activity patterns for the Child category differ widely over the age range (1-10 years) with differential skin contact for many compounds varying substantially. In the Youth category, the older ages may actually experience activities similar to Adults in that they will be using some of the same Articles and Products, as Adults in the same way. Further, Adults, themselves, may experience use of Commercial Products differently as they age- particularly after age 65. All of these shortcomings may be overcome by using user-inputted data, but more flexibility on the scenarios, activity patterns, etc., including default values for other categories may be of utility, especially in screening scenarios. But see my updated comments on increasing the number of scenarios.<br><br>One may reasonably argue that the screening nature of CEM precludes the need for more detailed scenarios as outlined above. This argument has some merit as long as the default values selected represent, if not worst-case scenarios, at least high-end exposure scenarios for all classification of individuals. Under this umbrella, the screening tool can give results that, if shown protective, are sufficient. Potentially, however, they may give "false positive" results that require further exploration. Balance must be maintained and such balance is precarious. |
| **Stopford** | We are currently looking at skin exposure from the use of pastels, spray paints and airbrush paints. To assess risk of dermal effects (allergy and irritation), we are specifically looking at skin exposure in terms of micrograms of toxicant per $cm^2$ of skin. This approach is documented in the following article: |

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| | Stopford W. Protocol for the assessing dermal exposures while using pressurized aerosol sprays, airbrushing and drawing with pastels. 2014. http://duketox.mc.duke.edu/dermal%20exposure%20to%20aerosols%20protocol9.doc<br><br>We have used both surveys of populations representative of the US both geographically and economically as well as user questionnaires to determine use patterns for various types of art materials. For spray aerosols use by artists, see:<br><br>Stopford W, Miller JS, Smith KN, Bosserman W. Solvent Exposure to Graphic Artists. Submitted to CPSC. http://www.duketox.mc.duke.edu/recenttoxiissues.htm. 2002<br><br>For pastel use by artists, see:<br><br>Brock T, Stopford W. Bioaccessibility of metals in human health risk assessment: Evaluating risk from exposure to cobalt compounds. J Environ Management. 2003; 3(5):71N-76N. |
| **Washburn** | As discussed below, the CEM should include Lifetime Average Daily Dose (LADD), rather than leave it for a "future enhancement", given the importance of cancer as an endpoint. Calculation of the LADD should be a fairly simple matter for the CEM given that I believe that the model already includes all of the information needed for such a calculation. I note that, in the "Calculation of Inhalation Dose from Product Usage" (p. 32), CEM already calculated Lifetime Average Daily Concentration (LADC).<br><br>I believe that the calculation of chronic average daily dose is misleading (and probably not scientifically defensible) in those instances where exposures are relatively infrequent. For an exposure to be considered chronic, it usually should be continuous (or at least relatively continuous) over time. In a number of the exposure scenarios in the CEM, the exposures occur only a few days a year, and then a default averaging period of 1 year is used to calculate the chronic exposure. (For example, for "whole appliance cleaners", "anti-freeze liquids", and "interior car care cleaning and maintenance products", the default "medium" exposure frequency is 3 days per year and the default "low" exposure frequency is 1 day per year. The default exposure frequencies for "fertilizers" are even lower – 4 days for "high" exposure, 2 days for "medium" exposure and 1 day for "low" exposure. I believe that such exposures, when averaged over a year, do not really represent chronic exposure and are generally best characterized as either separate acute exposures or subchronic exposures depending on the chemical and scenario, and should be handled as such.<br><br>The appropriate averaging time for chronic exposures will depend on the chemical. The 1 year default for averaging time is likely quite conservative in many instances. In any case, the CEM should prohibit the user from specifying an exposure duration (ED) that is longer than the chronic averaging time or automatically adjust the chronic averaging time to be equal to the ED if an ED of greater than 1 year is specified – otherwise the calculation will be incorrect (see related comment below). |

**3.5 There are several items listed in the "Areas for Future Enhancement" section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term.**

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| **Ferguson** | a) **For exposure metrics for Short_Term, Chronic and Lifetime Exposures:** Yes, these additions would be important for certain classes of chemicals, and in part would depend on the toxicity of the chemical. Chronic and Lifetime exposures would be important where people use products on a very regular basis. Cosmetics, cleaning products, and air fresheners would fall into that category. The acute use rate would be used with a multiple to calculate some reasonable use patterns. Cosmetics are used daily and cleaning products can have a use rate of 52 (once a week), twice a week (104) or once a month. These could be set a low, medium and high use rates. I would think that short term exposure can be easily determined in the model to reflect just the time of product use. Instead of averaging over a day, just determine the exposure for dose for the use period and report as such.<br><br>Please reorganize this section for better flow. Move the second paragraph below the third.<br><br>b) **For Products intended to go down the drain**: I am not understanding how this concentration equation relates to a residential or public environmental exposure in CEM. What do you mean by the concentration in the river water? We need concentrations in media that the residential or office building receptor would contact. This scenario is either not explained well or irrelevant to what CEM is trying to do. Perhaps, concentration in river water needs to be related to concentration in a media in or around the home. If the approach or intent is how this concentration helps to account for mass loss of product in the home, this potential scenario needs to be explained as such.<br><br>c) **For Vector-facilitated Releases from Articles Not intended to go Down the Drain**: Here you describe movement of additives from articles to vectors, where in fact vectors are still articles (e.g., clothing and this is confusing to the reader). Again why are we concerned about the greywater being a source of exposure, or are we considering chemical are being lost from articles in this manner from the home environment. Is this a consideration of a mass balance equation accounting for all losses? Keeping track of all exposure to a chemical that is moving from one article to the next will be complicated without a type of detailed human activity pattern. So please clarify whether the vector is a source of exposure, an exposure pathway, or a consideration of mass balance for the chemical of concern. Please also clarify CEM as a residential or building exposure model for exposures. These are losses to the larger environment and then we also have to trace removal at a wastewater facility.<br><br>d) **Products that Spill or Leak over Time**: The description needs to clarify if this would affect exposure for the product user or other receptors. Or would this decrease or |

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| | increase the exposure for the product user from one route vs. the other route and how would models would keep track of overall product and chemical mass balance between routes. Because I do not think that there are standards for product percent spills in the residential and office setting (a person clumsiness might help dictate that on any given day), the model can just have the user enter variable spill rates to see how it affects product mass, chemical mass and route exposures. Route exposure will depend on the volatility of the chemical and product formulation and likely use patterns.<br><br>e) **Elevated Temperatures During Application and After**: The user can be reminded in the user guide that emission rates (i.e., fate and transport) of the chemical are affected by temperature. Likewise ventilation rates are affected by temperature.<br><br>f) **Consideration of chemical or material specifics**: Currently, the ingestion model ING03 only uses a migration rate not a mouthing transfer efficiency (i.e., % or fraction removed during mouthing) found in Table B-5 of the appendix. These are not separate factors but are related, yet listed together in B-5, and might confuse the user about which is used. Mouthing activity (intensity) and acidity of saliva can indeed affect the migration rate of a chemical through and from the article. For models where articles are placed in the environment (e.g., INH06-one of the most detailed models), migration rates of the chemical is not a term used for the chemical as it moves from the bulk article to the air and then partitions to TSP and dust particles. Diffusion and mass transfer coefficients are utilized in those models (from Table B-12 and B-13). To some extent migration rates are related to diffusion or mass transfer coefficients (a chemical migrates because it diffuses and partitions). But to ensure the user does not get confused Table B-5 for "migration rates" needs to say "migration rate from saliva". Again when we are merging models from different sources, terms and concepts overlap or get confusing. Also please note the "product matrix" in Table B-13 and B-12 are articles by CEM definition not products (e.g., density board, vinyl flooring). For CEM "product matric may need to be changed to 'article matrix" for clarity. Vinyl floor for example is an article in Table B-1. If I am confused, someone else might be.<br><br>g) **Other scenarios**:<br><br>- Please consider a child in a bath. A dermal exposure model that considers water immersion is possible, where exposure can occur to soap products but also residual cleaning products in a bath. The EPA child specific exposure factors book has equations for exposure to chlorine products while swimming. This can be adapted for the CEM model.<br><br>- Consider adding exposures to chemicals in cosmetics. Some of my comments on considering local skin effects and percent retained on skin are relevant for exposures to cosmetics. But I notice under products that cosmetics are not included. Soaps and shampoos are considered, and for women exposures to harsh cosmetics that remain on the skin for many hours every day are of concern. When cosmetics are considered and if the chemicals are volatile or semi volatiles, then evaporation can be considered from the skin surface. This can already be done for |

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| | DER01 and DER02 (product applied to skin). I suggest an article by Frasch et al., 2014 (found at http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3868874/ with some reluctance because I believe all the dermal models needs to be consistent in considering movement through layers or skin, evaporation from the skin surface and finite versus infinite skin loading conditions. But it is still a good read with some suggested model equations. |
| **Ginsberg** | In the above responses I have already made a variety of recommendations for enhancements to the models themselves (iterative calibrations against actual data, cross-comparison to other modeling efforts), to the CEM user's guide, to the computer interface and to variability and uncertainty descriptions. I agree with EPA that enhancements are also possible with respect to shorter term averaging times for products used sporadically and briefly (eg. paint stripping scenario), calculation of LADD to better match up with risk assessment needs, and a variety of other scenarios mentioned by EPA in this section. I also believe it imperative that models include leaching of chemicals from consumer products in relation to food and water uses (e.g., phthalate release into water from plastic tea pots). In terms of chemicals to add, flame retardants, perfluorinated compounds, pesticides, DEHP, dyes, and a variety of other ingredients (aside from phthalate) present in plastic would be helpful. |
| **Ryan** | Several Areas for Future Enhancements are presented in the User's Manual. Essentially all are feasible and their implementation is based on the needs and expectations of future utility by USEPA. I will comment on them individually and give my assessment of the need and utility of each. Data sources are varied for the enhancements. I have no special knowledge of specific sources for the data needed to develop the specific enhancement, however.<br><br>My personal preference, not discussed here, is the ability to perform variability assessments and uncertainty evaluations before implementing any of these modifications of CEM. However, this must be tempered by the increasing complexity of such a system. Even implementing the strategies suggested below in a deterministic fashion will complicate an already-complicated system to a significant degree. Such modifications should be evaluated cautiously. It would be easy for this system to become complicated enough to overwhelm the typical user and reduce its usefulness in the field.<br><br>Exposure Metrics for Short-term, Chronic, and Lifetime Exposure<br>It would seem that this is the next logical step in the development of CEM. Estimates of shorter- and longer-term metrics would be a relatively straightforward modification and could be of interest to many users. Implementation would not result in substantial complication of the model as viewed by the user as it would simply be a few more boxes that could be checked in the Input section. This would be a useful addition. Further, I believe the implementation would not be overly difficult, which would clearly be a desirable trait. However, USEPA has "carved in stone" the acute, sub-chronic, and chronic temporal exposure regimes, and modification may not be possible at this time for USEPA use. But other Agencies and researchers may find other temporal regimes of interest. |

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| | Articles in Routine Contact with Water<br>While certainly of interest, I believe this component would be of lower priority than some others as the number of Articles that fit under this rubric would likely be limited and not commonly implemented. Further, data may not be ready available to develop the modeling approaches. I would give this lower priority.<br><br>Products Intended to go Down the Drain<br>Again, this could be an interesting addition to the CEM and is receiving interest in, for example, medical waste and endocrine disrupting chemicals. However, as pointed out in the text, while the model addition as shown in the text, is straightforward, the data to support some of the parameters is lacking. Given this, I would place this at lower priority as well.<br><br>Vector-Facilitated Releases from Articles Not Intended to go Down the Drain<br>As reported in the text, data are emerging on this subject. Further this may be tied in with para-occupational exposures in the home and elsewhere. There was lively discussion of para-occupational exposures on our conference call. This may be an important additional scenario, at least it light of that discussion. Such an implementation is of intermediate priority, but it is my opinion that the data are not yet available to develop the modeling parameters. However, they are likely to become available in the next few years upon which time implementations could be done. I suggest developing the modeling components- equations, data reduction methods, etc., but wait for better data prior to implementation.<br><br>Products that Spill or Leak Over Time<br>Implementation of this component should be of lower priority as it requires an unusual set of circumstances to be operational. I recommend waiting on this one. Data may become more available with time and, if it is deemed an appropriate measure, a set of modeling equations could be developed. I do not think such a system is currently available.<br><br>Elevated Temperatures During Application and Use<br>I had not considered this aspect at all in evaluating the models used in CEM. Essentially all of the approaches may want to consider these temperature-related effects in some fashion. Such an implementation would be quite difficulty, however, as one would need to develop, for example, a temperature profile over seasons for the application of materials and subsequent volatilization. Changes in vapor pressure and Henry's law constants as a function of temperature are notoriously difficult to model. At least one reviewer expressed the need for Henry's law approaches as opposed to Raoult's law (vapor pressure) approaches. Regardless, both have temperature dependence that is not well characterized for most compounds of interest. Further, emissions associated with personal care products must take into account interaction with body-cooling mechanisms such as sweating. This is quite complicated and I am not at all sure on what data exist. I think this is a higher-priority item, but that implementations would be especially difficult and may require substantial work to ascertain their utility.<br><br>Consideration of Multiple Zones in the SVOC Article Model<br>Multiple zone models are relatively easy to design but require substantially more data to |

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| | implement than single-zone or two-zone models as one must ascertain the zones that are interacting. Implementation is straightforward, but the data to support such implementation is not readily available. I agree with the statement made in the text, that such a system should be implemented when data become available but the complexity goes up like the square of the number of zones. I do not see such data becoming general available for multiple locations in the near future and even if it does, the applicability goes down quickly as they models become more focused on a single scenario rather than generally applicable. This observation places the implementation of such a modeling system on a lower priority.<br><br>Consideration of Chemical and/or Age-Specific Transfer Efficiencies from Surface-to-Hand, Hand-to Mouth, and Object-to-Mouth<br>Again, Dr. Ferguson is the expert and I defer to her judgement. I discussed this in a general sense early in my review. Generally, I think that there is substantial variability in age groups on any of the parameters in CEM. The Child age group is too wide, and the Youth age group needs further examination. Toddlers are very efficient in transferring materials from hand to mouth and the system CEM should make use of such knowledge. This may be the first priority of modification of CEM.<br><br>Consideration of Chemical or Material-Specific Migration Rates<br>Implementation of this rubric may open an extremely large can of worms as I can see no place to stop. Materials, Articles, etc., may have to be considered almost on a unit by unit basis increasing the complexity of the model exponentially. I would punt on this one as CEM is a screening tool, not the be-all and end-all model. It may be possible to increase complexity in a manageable fashion by classifying Articles and Materials into general categories to keep the complexity manageable, but the categorization itself would be problematic. I would put this at low priority not because of its perceived lack of importance, but rather because of the difficulty of implementation.<br><br>Consideration of Total Ingestion Rates of Indoor Dust and Particles<br>There is consideration in the text of variability and uncertainty in implementing this component. I do not think data exist to look at variability and uncertainty in this parameter or many others. I would not consider implementing this at this time. Should more data become available, one could reconsider.<br><br>Absorbed Dermal Dose<br>Again, Dr. Ferguson is the expert and I defer to her judgement. This approach could be readily implemented by offering a different check box in the input section. Data are available for many of the needed parameters and are already stored in the chemical compound section. Assuming that models of dermal dose are good, the implementation is relatively straightforward, then it becomes a higher priority. This is a simple, deterministic alternative to what is already available for implementation.<br><br>Consideration of Additional Exposure Scenarios and Exposure Defaults<br>There is little to add to what has been said in the text. As more data are gathered, more scenarios can be implemented. Further, more Articles, compounds, and activities could be implemented as well. This should be an ongoing activity with modifications of CEM occurring on a regular basis. The priority is high and continuing for this modification. But |

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| | caution due to increasing complexity is important. Maybe develop a simpler model with limited scenarios that account for much of the population exposure and reserving additional scenarios to a larger model is an appropriate strategy. |
| **Stopford** | *Exposure metrics*<br><br>For consumer exposures it is very important to know the peak inhalation exposure. Peak exposures to some sensitizers, such as diisocyanates, are the expected inducer of a sensitization reaction. Once sensitized, however, determination of acute, daily exposure will provide data on the likelihood of a reaction to the environment.<br><br>For assessing cancer risk, determination of both a working lifetime (usually 40 or 45 years) and lifetime exposure would be needed.<br><br>*Vector-facilitated releases*<br><br>Skin or clothing contamination with materials that vaporize, such as solvents or mercury, can be the primary source of exposure both in the workplace and home. For one example of this type of exposure, see:<br><br>Stopford W, Bundy SD, Goldwater LJ, Bittikofer JA. Microenvironmental exposure to mercury vapor. Am. Industr. Hygiene Assoc. J. 1978; 39:378-384.<br><br>*Hand-to-mouth and object-to-mouth transfers*<br><br>We have collected data of the efficiency of hand to mouth transfer of the following:<br><br>Solid film (phthalates)<br><br>Pastes (polymer clays), see:<br><br>Stopford W, Turner J, Cappellini D. Determination of the Magnitude of Clay to Skin and Skin to Mouth Transfer of Phthalates Associated with the Use of Polymer Clays. 2003. Submitted to CPSC. http://duketox.mc.duke.edu/polymerclayresults2.pdf<br><br>Liquids (glazes), see:<br><br>Stopford W, Turner J, Cappellini D. Determination of the Magnitude of Ceramic Glaze to Skin and Skin to Mouth Transfer. August, 2007 http://duketox.mc.duke.edu//ceramicglazetransfer.doc<br><br>We have also looked at metal exposures from mouthing in the following paper:<br><br>Stopford W, Cappellini D. Bioaccessibility of Lead in Metal Pen Tips. Submitted to CPSC, 2009. http://duketox.mc.duke.edu/recenttoxissues.htm |
| **Washburn** | As discussed above, the current version of the CEM should include Lifetime Average Daily Dose (LADD), rather than leave it for a "future enhancement". Calculation of the LADD should be a fairly simple matter for the CEM given that I believe that the model already includes all of the information needed for such a calculation. I note that, in the |

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| | "Calculation of Inhalation Dose from Product Usage" (p. 32), CEM already calculated Lifetime Average Daily Concentration (LADC).<br><br>Of the other identified "Areas for Further Enhancement", I recommend that the focus be on the following as being the most significant:<br><br>– Products that Spill or Leak Over Time", particularly in occupational settings.<br>– Elevated Temperatures During Application and Use".<br><br>As previously discussed, if exposure to cosmetics is not incorporated into the current version of the CEM, I recommend that they be included as a top priority future enhancement. |

## Part 2. User Interface

### 3.6 Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface.

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| **Ferguson** | Please note that some of these responses are very related to Part 3 (l) and refinement of the user guide, but it also affects the understanding and functionality of the graphical user interface.<br><br>a) Helpful to tell the user to put the software program on "Full Screen", then the five tabs of CEM can always be seen. You advise the user on page 9 to use the scroll button to the right to move up and see these tabs.<br><br>b) It would be more useful to move "New Analysis" Button to the left of View Analysis. This button will be the most commonly used button and needs to be in immediate line of sight.<br><br>c) Please separate the product list from the article list in the CEM model on the scenario tab. If the user selects a product then the rest of the interface only list "product". Therefore combination such like "product/article" goes away for the use environment and we know what we selected through the entire run and data screens. This might take a bit more programming and it would be like creating two clear paths in CEM, one for product and one for article. Right now when you select a product or article, the popup box always mentions "Do you want to use the defaults use environments for this product (RubberArticles:Toy). CEM and use guide need to remove any confusion between article and model for a better understanding of models applied and assumptions and defaults assigned.<br><br>d) The user should be given practice problem to run the CEM, if this was not in the plan. Reviewers had some training sets in the first Phone call with EPA and ERG. |

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| | e) I had problems trying to enter my own CAS or chemical string. It would not then find the chemical on the list. I have to select a chemical from the list. This may be code issue running on my computer. Can someone please check this?<br><br>f) Can any chemical be matched with any product or article? I tried fooling around and it appears so. Some combinations are highly unlikely. Let the user be aware that although every combination is possible in CEM, they need to check the ingredient lists (if available on the product or article label).<br><br>g) Consider some more direct statements in the introduction on the limitations of CEM per run, such as…. "Automated is the environment for a product or articles based on likely use environments and patterns. The product or article is then linked to the relevant exposure route and therefore relevant exposure models for in CEM. These likely scenarios, use patterns and exposure routes are shown in Table B-1. CEM determines one use environment at a time for a chemical in a product or article."<br><br>h) Page 10 of user guide, when product user and receptor are defined, description is misleading at first. It suggests the model can be run for more than one product user at a time, "CEM may be run for multiple users and receptors". However, it can only be run for one product user at a time, and will automatically be run for 7 age groups of receptors (where one of those receptors is a product user). Of the 7 possible receptors, one of 3 can be a product user. I suggest refining the definition here for clarity.<br><br>i) For Activity Patterns please on page 10, also indicate clearly that only one type of activity pattern (i.e., full time or part) will be calculated all receptors in the user guide. This is an area of flexibility the model can consider changing later.<br><br>j) On the activity pattern tab of the CEM model, to the right is an explanation that activity patterns can be changed. It suggests you can go into the file and change the patterns by the hour. But this is not possible. You can only change from full time to part time, across all receptors. At least my version of the model does not allow these changes. However, if possible it would add great flexibility.<br><br>k) Page 10 for background Air and Dust concentrations, is it true that Products asks for background air concentrations and articles asks for background dust concentration? Can you include a better explanation of why here? This has to do with volatiles associated with products vaporizing to the air and articles associated with semi-volatiles attaching to dust and TSP particles? This would also help to explain how the models works.<br><br>l) Page 9: Modeling Options says that models that are not available are grayed out. I think in this version, they just do not show models that are not used.<br><br>m) Page 9 and page 10, I am not sure all the Help buttons are necessary if they did not add any more details than the label. So? button for "Product/Article Environment" adds no additional detail. |

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| | n) Page 12: for "2.a Chemical Properties" tab: Put all acronyms besides the parameters. I also found that this was not consistent in the glossary. Some parameters have the acronym as used in the model listed and some do not.<br><br>o) Page 12: Define QSAR when first used and explain what you mean by "training sets". These are the sets you used to develop and test the CEM model. This is confusing here.<br><br>p) Sections describing the input tabs are not balanced in the details they contain. 2.b. and 2.c. The 2.b tab describing the product/article properties tab on page 13 could further say: "Under this tab the user is required to enter use data for the product or article, and exposure factor information (e.g., mouth transfer, percent retained on skin). The model also has use inputs for acute and chronic assessment….." or something more to that effect.<br><br>q) Page 13 under the 2.d. If incidentally exposed humans are the 7 age groups defined as "receptors" please say "receptors" instead of incidentally exposed humans.<br><br>r) I think on page 13-14, under the 2.Receptor Exposure factors Tab, # 4 you mention surface areas. I think it is okay to say here that a table exists (what table?) for likely surface areas for each product type or article type. CEM uses that as the default, but the user can adjust. Is this correct?<br><br>s) Under the model selection tab, page 14, and throughout the document, I find that there are some key facts such as the "60-day modeling period is used to calculate the total exposure associated with a single use of a product" that is crucial in understanding how CEM operates and might need to be moved to a summary or overview.<br><br>t) In CEM, some inputs/parameters under the "model" tab are bolded and some are not. |
| **Ginsberg** | The CEM is cumbersome to use because of the many scenario-specific and chemical-specific parameters needed to run models. In trying to execute a model it was common to get an error message that some parameter not particularly germaine to what I was seeking to learn (e.g., film thickness on skin) was missing. It would be helpful if there were simplified ways to run the model, e.g., without all the exposure dose calculations, so that one might focus on the difference between chemicals or use rates on indoor air concentrations.<br><br>While the user's manual is helpful, it is not detailed enough for a casual user (e.g., an average risk assessor) to use the model in default mode or to make adjustments to the model with confidence. A bit more background on how the model works in terms of diffusion, boundary layer conditions, partitioning, and exponential decay would help with understanding of what is going on with chemical release, fate and availability for exposure.<br><br>The user's manual refers to USEPA's EPI-Suite Version 4.11 to obtain chemical-specific parameter values. However, it is not obvious what information must be known about a |

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| | chemical (e.g., MW only?) to get the rest of the information needed to run the CEM scenarios. A table of chemical-specific information needed to extrapolate to other higher order information would be helpful. A direct interface with EPI-suite would be an advance so that it would be easy to bring additional chemicals into the modeling with confidence.<br><br>In terms of the user interface, I found it disappointing that some parameter values input for a scenario were not saved the next time that scenario was opened, but other parameters were saved. Further, it is unclear why some parameters are automatically provided with a default value and others require one to hit a button requesting an estimated value (essentially a default).<br><br>The report produced from a model run is limited, focusing mostly on dose estimates for different pathways and acute vs chronic scenario. Information such as house dust concentration or chemical loading on surfaces would be excellent to have to compare to literature values. Additionally, graphic representation of the time course of air concentrations after a product use would be useful to present. |
| **Ryan** | The user interface is complicated and, at times, proved difficult to use. I found myself often having to readjust the screen so I could see the top row. Admittedly, there are explicit instructions to do this, but it was annoying. There are a large number of input lines on multiple screens. It is quite easy to miss one (or more) of these. Fortunately, when the "Run CEM Models" button is hit, the system does a quick scan and tells you what you have left out. As I became more familiar with the interface, I was able to navigate more quickly to the correct location, but at the beginning this was cumbersome and frustrating. If one runs the model a few dozen times, it becomes more intuitive, but the "intuition" must be learned.<br><br>I have no real ideas on how to improve the interface. There is a lot going on, and a lot of things must be done to get useful information out. The menu of compounds, activities, articles, scenarios, etc., is extensive. Thus it is difficult to see how the process could be streamlined without eliminating the flexibility. The authors have made an excellent effort in dividing tabs up into related areas so that the user, if s/he is systematic in the approach to the CEM system, can streamline the process her/himself.<br><br>One thing that may be of use is, when the scan for missing data is done, categories that require additional input could be highlighted somehow. The system tells you which model is problematic, and which parameters are missing, but when you go to that model, you have to hunt around for the parameter of interest, often re-running the model to get the error back up and follow it through. I would really like to see this implemented - and it should be pretty simple to do so as the items missing have already been identified. |
| **Stopford** | The user interface is excellent. I particularly like the following:<br><br>– notices of what was overlooked during entry<br>– quick explanations for input parameters<br>– estimate tool |

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| **Washburn** | Overall, I found the user interface relatively easy to use although I did run into a number of problems. However, I obviously did not have time to run all combinations of scenarios/ products/articles, so there may be other issues/problems in combinations I did not attempt. To illustrate the types of problems that I did encounter, I refer to an example I ran for bubble solution product for two chemicals with very different properties (formaldehyde and a zinc formulation, CAS #4259158), for a number of different combinations of inputs and different sensitivity analyses:<br>• No controls on impossible/incorrect inputs<br>– Entered an exposure duration (ED) of 30 years, without changing default averaging time (AT) of 1 year. This mistake could easily be made by a non-expert. Model accepted input of a 30 year ED and calculated the CADD result with an ED of 30 years and an AT of 1 year, which is clearly incorrect (ED must be =< AT).<br>– Entered a film thickness on skin (FT) of 100cm (1m) which is clearly impossible. Model accepted 100cm FT when using the "estimate" button to calculate the amount retained on skin (AR).<br>– I also noted that once an FT valued was entered, it was impossible to recalculate the AR value by correcting/changing the FT value. In other words, once I had entered a 100cm value for FT and used the "estimate" feature to calculate AR, the model would not change the AR value after I changed the FT value to 0.1cm.<br>– In addition, I was able to enter both an AR value and an FT value, which should not be allowed, since the FT value is used only to estimate the AR value. In other words, if I specify the AR value, then I should not be able to also enter a film thickness value since they may be inconsistent. In fact, if I enter an AR value, I am actually still required to enter an FT value in order to run the model even though the FT value is not used.<br>• Report Format<br>– The "Full Analysis" report does not appear to include all inputs. For example, for the bubble solution test described above, I was not able to find the ED value on any page of the report.<br>– The "Full Analysis" report does not appear to properly present all inputs entered. For example, for the bubble solution test described above, the film thickness on skin was always presented as "0" no matter what value I entered into the input screen.<br>– For some sensitivity tests on the bubble solution test described above, the report did not show the scenario name or chemical, although other inputs were shown. I was not able to determine what caused the scenario name or chemical to be shown in the report – the problem was difficult to duplicate.<br>• I found the "View/Save Report" process after producing a report to be confusing. Also, I found it very unclear what the "Access" and "PDF" buttons are for, or how they are |

| Reviewer | Comments |
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| | related to "View/Save Report". I think this should be made much clearer when working within the CEM (without having to refer back to the User Guide).<br>• I had a difficult time trying to save report files outside the CEM model (e.g., to another file folder). This is something I think all users would want to do so that, for example, they could send a Full Analysis report to a colleague. Eventually, I tried printing a Full Analysis report to a PDF but after waiting 10 minutes while the Adobe program said it was "creating" the PDF file, I gave up. There should be an obvious and easy way to save report files outside CEM (unless I missed it).<br>• Notification that required inputs are missing<br>– When leaving the "Scenarios" page, I am immediately notified which required inputs are missing. However, this feature doesn't seem to be incorporated for the other pages.<br>– For example, if required inputs for the "Inputs" page are missing, I do not find out until I try to run the CEM model itself. I suggest that the user be notified upon leaving each page if any required inputs are missing. |

### 3.7 Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful.

| Reviewer | Comments |
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| **Ferguson** | a) Exposures to chemical having the same toxicological endpoint would be useful, as would the ability to estimate exposures to multiple chemicals from one product or article. Can your software initially ask if the client with be making any such calculation, and return to start each time, while retaining the information from the calculation from before. It is currently feasible for the user to download each report on one chemical at a time into access, but future versions of the this software could have an extra data entry screen to ask a series of relevant questions that would determine how many sets of calculations to perform and save into one report.<br>b) Multiple zone referred to in the "Future Enhancement" will facilitate the idea of distance from source in a room. This statement can be placed in this section to better explain when this would be used.<br>c) For the statement. "Consideration of Chemical and/or Age-Specific Transfer Efficiencies from Surface-to-Hand, Hand-to-Mouth, and Object-to-Mouth" The transfer efficiencies might depend more on article or product type, how it is used and pressure of contact, and whether skin is wet or dry. There are limitations however for maximum transfer. |

| Reviewer | Comments |
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| | d) Does the user have access to the excel files describing product category, article category and functional use categories from the CEM model interface?<br><br>e) Under the result tab, can the results remind you who you choose as the product user, even though you might be able to tell by the higher exposure results? |
| **Ginsberg** | This is already covered in my response to other questions but I think the main points are reporting of additional data from model runs such as shorter term peak exposures (<24 hr), house dust concentrations of SVOCs and a time course for indoor air concentrations after a product use. |
| **Ryan** | Batch mode would be useful as the number of input values is large and one would like to evaluate the effect of certain changes. This can be accomplished by building upon an existing scenario, but the batch approach would be useful a well. I am not familiar with the capabilities of MSAccess in this regard, but if it would be relatively easy to implement. This could be a way of assessing uncertainty in the model a well by affording a method of quick entry of data varying an input parameter. Variability might also be assessed most easily with a batch mode method but one would have to know about distributions of parameters.<br><br>Operating in batch mode or even "inline," it could be useful to be able to direct the Save commands to a directory at the beginning of a session and have all the Report files show up there.<br><br>Although I am not sure what the format would look like, a graphical output system would be useful a well. A sheet containing appropriate input data and, perhaps, bar graphs of the output of various run scenarios in graphical form would be a nice package to have. This may not be implementable as I do not have any idea that a graphical input would be short of bar charts instead of numbers. |
| **Stopford** | One change that needs to be considered is defining the following in the report on exposure factors:<br><br>BW<br>Past_ing<br>Inhal_after<br>SABW_body<br>TC |
| **Washburn** | The "Full Analysis" report should highlight when default or model-calculated input values have been used, and when user-specified values are used.<br><br>The user should be required to provide reference or source for user-specified values, or denote that they are based on professional judgement and this information should be included in the "Full Analysis" report. |

## Part 3. Documentation and User Guide

### 3.8 Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited.

| Reviewer | Comments |
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| **Ferguson** | a) I recommended referring to tables in the appendices when the parameters are presented in the user guide. I mentioned an example above for the parameter "percent retained on skin for product usage" refer to table B-2.<br><br>b) Recommended formula for ventilation rate dependent on number of bedrooms: See: https://resaveguide.lbl.gov/step-3-whole-building-ventilation-rate.<br><br>c) Readings on deposition of particles in Lungs (portion swallowed)<br><br>1) http://www.archbronconeumol.org/en/deposition-inhaled-particles-in-lungs/articulo/S1579212912000845/ … Ana Fernández Tena, Pere Casan Clara, 2012.<br><br>2) Also see http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.275.9282&rep=rep1&type=pdf,<br><br>3) Also see www.mass.gov/eea/docs/dep/cleanup/laws/inh0708.do for the following more precise information<br><br>i. 100% of respirable particulate mass is equal to or less than 30 microns in diameter (≤ PM-30) (ORS 1994, MassDEP 1997)<br><br>ii. 50% of total respiratory particulate mass is equal to or less than 10 microns in diameter (≤ PM-10) (ORS 1994; Weidner et al.; ORS 2006).<br><br>iii. **100% of inhaled particulates greater than 10 microns but less than or equal to 30 microns are swallowed (ORS 1994).**<br><br>iv. **50% of inhaled particulates equal to or less than 10 microns are swallowed, and the remaining 50% enter the lungs (MassDEP, 1997).**<br><br>d. Use EPA's own simple dermal exposure model to suggest consistency in the complexity of the dermal models, Kp values and other terms used: Refer to EPA/600/R-07/040F. Also use this document to look at skin loading from various media and specifically for my suggestion for dermal exposure for "treated surfaces" for dermal exposure to pesticides applied to grass (Eq. 6 of this document). One of the existing DER models in CEM can also be adjusted.<br><br>e. See http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3868874/ for evaporation from skin surface, especially when cosmetics that might have some more volatile compounds are considered (things like nail polish remover for example). Frasch et al. "Analysis of finite dose dermal absorption data: Implications for dermal exposure assessment", J Expo Sci. Environ Epidemiol. 2014, 24 (1): 65-73. |

| Reviewer | Comments |
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| | f. EPA child specific factors handbook for children in pools and exposures to chlorinated products (EPA/600/R-)8/135). Ingestion of water while swimming find in Chapter 3). A dermal model can be adapted for dermal exposure while swimming. |
| **Ginsberg** | References that I cite above are:<br><br>Cousins et al., 2014, Sci Tot Env 470-471: 527-535.<br><br>Little et al., 2012 – already cited in CEM user manual.<br><br>Bennett and Furtaw (2004) Environ. Sci. Technol. 38, 2142-2152.<br><br>Xu et al., 2012, ES&T 46: 12534-12541. |
| **Ryan** | See discussion under Charge Question 1.<br><br>I have identified at least one broken link and a couple of instances of references being behind a (substantial) pay wall. I think that EPA should obtain a "fair use" license to distribute these references and others from a website at EPA. As an academic, I have access to most journal references. However, others not affiliated with a large University may have a much more difficult time getting references and evaluating the appropriateness of the various equations used. If USEPA is the sole target for this model, then it would be easy to have a private website for EPA staff only. But such a restriction would limit the use of the CEM and diminish its worth.<br><br>Other than the broken links, I did not identify any references that were inaccurately identified.<br><br>It would be useful in the models description section to identify where in the specific reference, e.g., page number, the given equation might be found. Some of the USEPA references are a couple of hundred page long and identifying the specific section and page number associated with a given equation was, at times, impossible. This is less critical when a particular published paper is referenced as such papers are typically 10 pages long rather than 200. |
| **Stopford** | Although USEPA (2007) E-Fast documentation manual is no longer available on line, the current manual (2014) is available at https://www.epa.gov/tsca-screening-tools/e-fast-exposure-and-fate-assessment-screening-tool-2014-documentation-manual<br><br>I am unable to find ECETOC's targeted risk assessment user's guide, though their model is readily available. |
| **Washburn** | p. 19, Section 3. Why are indoor sinks not considered for SVOC emissions from products?<br><br>p. 35. Reference for highlighted equation for interior area.<br><br>p. 41. Must user specify half-life in soil? If unknown, how does CEM address? |

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| | p. 43. How in migration rate from article to saliva (MR) estimated? This factor is identified as an "Area for Future Enhancement" but it is not clear to me what is being done in the current version of CEM. |

### 3.9 Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear.

| Reviewer | Comments |
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| **Ferguson** | a) Be sure to include and executive summary with an overview of model for the user. This can be similar to "Note to Peer Reviewers" section but can omit the 9 list of changes made in last version. This can be incorporated into other model capabilities.<br>b) On page 8 of user guide it indicates a tab for Lookup Table, but not a tab for Reports.<br>c) Page 10: Indicate briefly how many different product and article categories, and chemicals are currently available in CEM.<br>d) In the Introduction to Reviewers the following statement occurs. "Product use categories define various kinds of products. Examples include aerosol spray paints, laundry detergent, foam-based furniture, hard-plastic toys, and motor oil." I might be confused. Are certain types of furniture defined as products? Check all documents for consistency in definition of products and articles.<br>e) I consider this suggestion very optional. The glossary can be moved up under a description of the user interface. It helps the reader get familiar with terms and acronyms very quickly and they can understand Section 3 more effectively. Make sure to not include equations in the glossary and move all equation to descriptions of models and equations, in Section 2 and Section 3 (this last part of the suggestions should be done anyway).<br>f) Delete Button: Does not allow you to unselect a selection, once you select. It asks if you are sure about deleting. If you say no, it needs to go back to screen and un-highlight all choices automatically, please check. Or explain that "Done", closes the screen without deleting anything. Just in case this makes someone nervous.<br>g) Can the user download or view the entire user guide from CEM. Currently CEM generates short descriptions from a search now.<br>h) Appendix A says "Output from INH06-ING05-DER04 and Conversion to Dose. The first part describes assumptions for SVOC concentrations then used to estimate inhalation and ingestion doses. Four doses are described, one for the ingestion route and three for the inhalation route. Please explain how DER04 is involved here. DER04 is "Article with Direct Transfer from Vapor Phase to Skin". There is no SVOC parameter or ingestion or inhalation parameter used for this DER04 model, or the relationship is not clear for reference to this vapor phase model here. |

| Reviewer | Comments |
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| | i) For Table B-12, please put material-air partition coefficient in the table title.<br><br>j) For table B-11, please include a reference or state assumptions for these near-field assumptions.<br><br>**Specific Glossary suggestions:**<br><br>a. The zone one concentration can be called Cff or CR1 depending on whether a near field is selected or not? We need to check all equations and stick to one term that might not be confusing to the reader. This comment also applies to near and far field volumes versus Zone 1 and Zone 2 volumes and also for air exchange rates? Check glossary and equations.<br><br>b. What does the word "harmonized" when referring to the SHEDS-HT model in the definition of "Amount Retained on skin" is the SHEDS-HT model the reference for the 'mount retained on skin" in table B-2. Then this reference needs to be added to this table for clarity.<br><br>c. For some definitions in the glossary or guide-parameters the reference is given to where the defaults for the parameter were taken, but for some not.<br><br>d. In the definitions for chronic average daily dose and from acute average daily dose please again mention the averaging time for exposure and for the product concentrations for clarity (daily and yearly, 60 days, etc.).<br><br>e. Cleaning frequency: Cleanings per hour applied to an acute dose rate calculation will likely underestimate exposure where particulate exposure is concerned. Check if the models allow this cleaning frequency can be set to zero for these short term exposures and an explanation be provided to user.<br><br>f. Degradation half-life in soil. Most of the product mentioned for outdoor ingestion exposures are applied to grass (e.g., fertilizers and pesticides-both herbicide and insecticides) are applied to grass. This exposure pathway needs to be reconsidered or better explained to users, or that a soil half-life is used as a proxy<br><br>g. Earlier on it should be explained that soil exist outside, dust refers to large particles that settles inside and TSP refers to finer particles in air inside as media of exposures.<br><br>h. Diffusion coefficient models used here refer to Fickian law of diffusion assuming steady state concentration. Fickian second law of diffusion would account for time changing variation of concentration on the surface. Page 39, a solid-phase diffusion coefficient is mentioned to determine mass transfer for the complex" IN06 model: Inhalation Article placed in Environment." Diffusion coefficients are not used for the dermal models (permeability and transfer coefficient related terms are used), should we just call this the solid-phase diffusion coefficient determined in the PRAMS model for IN06 here in the glossary. Again the user guide may need to take some care in defining transfer coefficients, permeability |

| Reviewer | Comments |
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| | coefficients and diffusion coefficients for what and through what as used in various models.<br><br>i. Under the First Order Emissions Decline you have a couple of equations in the glossary. To be consistent move this to Section 3 where extended descriptions of models and parameters are found. Also a 25% mass release is mentioned but 10% is used in the model.<br><br>j. Fraction of Contact (unitless) is described as "fraction of touches of all surfaces that are in contact with the article of interest", took me a few times to understand. Would it be better to say "fraction of all contacts with surfaces in the environmental that are with the article of interest?"<br><br>k. Fraction Ingested. The default is 1. It would mean everything inhaled is ingested. The default should really be 0 unless you have other information. The primary route is inhalation originally. How are the inhalation and ingestion model matched here for mass balance. There are size recommendations for what portion of particles are ingested after inhalation. See my included references above.<br><br>l. HVAC penetration, mention the range of value used from Creech et al., 1996. |
| **Ginsberg** | My previous responses go into some detail on how the user's manual could be more comprehensive and accessible to a risk assessor. |
| **Ryan** | I found no problems in this area. The User Guide presented all the equations for the models and these are repeated in the help screens that I encountered. As I did not open each and every possible help screen, there may be some that were not covered, but they were quite complete in what I saw.<br><br>As outlined in my response the Charge Question 1, certain of the model presentations were cryptic and could be improved markedly with a bit more explanation, and perhaps partitioning equations into parts then putting the parts together. This would add to the clarity of the presentation substantially and reduce frustration on the part of the novice user. However, I believe that many users would simply assume that USEPA had "done it right" and not dive into the equations at the level of a reviewer of the CEM might. This may be a dangerous assumption and many users would like the details before relying on the model for any specific purpose.<br><br>A suggestion for presentation of the User's Manual might include separating the section describing the details of the models into an appendix but including a brief description of each model where it is now but leaving out the detailed equations. That is, use a text description of the model and refer the User to the appendix for details. I am not clear on how this might best be done, however. |
| **Stopford** | On page 15 of the Draft User Guide, the authors note that: |

| Reviewer | Comments |
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| | "Primary sources of data methods or assumptions: Please see the "Product Properties Sources" look up table on the lookup tables and VBA Code tab for further information on parameter source information specific to each product."<br><br>The version we are reviewing has no such VBA Code tab or lookup tables. The appendices, however, are excellent giving the documentation for sources of mass data, duration data, frequency data and aerosol fraction data used in the models.<br><br>It would be nice to see similar documentation for environmental inputs, particularly for:<br><br>Building volume<br>Use environmental volume<br>Default air exchange rates (by zone and near field boundary) |
| **Washburn** | The User Guide properly characterizes the models within CEM as appropriate for screening level assessments. However, I believe that the CEM should more clearly discuss the intended purpose of the CEM and target user profile, and emphasize its limitations in estimated actual exposures, particularly in site-specific and individual-specific analyses. While the CEM represents a noteworthy accomplishment in compiling models and information that allow for a characterization of potential exposures, there are generally very significant uncertainties in the results. This does not mean that the CEM does not have true value, but it does mean that EPA should be very careful to emphasize that the results cannot be assumed to represent reality. When EPA issues a model like the CEM, there is often a tendency for users (and those who receive the user's reports based on the models) to accept the output as "gospel" when in this case, in particular, there are very limited data for confirming the accuracy of models in predicting potential human exposures. It is my opinion that the CEM is most useful as a range-finding tool, in evaluating the likely sensitivity of exposure estimates to changes in exposure conditions or assumptions, in assessing the relative importance of different exposure pathways and scenarios, and in identifying what data would be most valuable to collect so that we can improve our understanding of potential exposures – in other words, as a risk management tool rather than in evaluating absolute magnitude of dose. |

### 3.10 Additional Comments Provided

| Reviewer | Comments |
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| **Ferguson** | Additional note: I did not thoroughly review INH06, because this type of fate, transport is less my area of expertise but I hope one of the reviewers did review. It is a complex model and separate runs/beta testing hopefully were performed on the standalone with various chemicals to see if it makes sense based on chemical parameters and time.<br><br>**Post Comments:** |

| Reviewer | Comments |
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| | After discussion with other reviewers and EPA, I wish to keep my comments as is. I believe they are valid areas of concern and areas for improvements. Some comments are minor and some more major. I suggest in the future that EPA be allowed a time to review our responses and indicate where perhaps we had a misunderstanding and also indicate what might be easy changes versus more difficult changes. Or why perhaps certain functionalities or models were not considered at the time. It is easy for reviewers to come along and suggest everything, but we may not understand the original intention of the model or certain difficulties encountered. This should occur before the conference call. In general I felt that there was an overall concern that current models needed to be further validated and verified to ensure models were working as expected according to algorithms as presented and against data in the field. In addition, although some reviewers felt mass balance checks might be difficult, I think further effort can be made to create subroutines that indicate the exposure and dose for all receptors as a function of the original mass (this ensures at least some impossibility does not occur although exposure and dose may be magnitudes of order less).<br><br>I overall felt there was great variability in the complexity of models that needed to be explained to the user, and later improved (e.g., evaporation of products applied to a surface but no evaporation of product from a skin or diffusion through one layer of the skin but through multiple layers for the dermal models). There are areas for future enhancements, suggested by reviewers, that involve developing models for other exposure scenarios, but I suggest that EPA fully focus on improving current models in the current CEM and adding explanations on the functionality of these models where they reveal to the user what is and is not considered at this time.<br><br>I am looking forward to the release of the improved model over time. |
| **Ginsburg** | **<u>General Comments</u>**<br><br>It is excellent that USEPA is developing an integrated set of peer reviewed consumer exposure models suitable for understanding exposures from the use of products and from household articles for a range of human receptors and scenarios. There are 15 different models and each has a variety of elements (e.g., migration of chemical, estimation of chemical concentration in exposure medium, estimate of human contact rate, estimate of human intake dose). Further, there are a wide variety of potential chemicals that could be involved in these scenarios. Thus, there are many aspects to review. Given time constraints I have decided to focus on one article (vinyl flooring) and one product (pesticide indoor application) and have reviewed each of the 3 pathways considered in these models (inhalation, oral, dermal).<br><br>My overall finding is that model parameterization could be more thoughtful in certain places and that opportunities for calibration and validation of model output have not been fully utilized. A sensitivity analysis and reality check of the article (flooring) model suggests that the output does not match what is anticipated based upon the literature while the product (pesticide) model appears to provide reasonable inhalation estimates. |

<table>
<tr><th>Reviewer</th><th>Comments</th></tr>
<tr><td>Stopford</td><td>
<u>Background</u><br><br>
Markers<br><br>
I have completed an in depth study of exposures to solvents from the use of solvent-based whiteboard markers to address a concern raised by CPSC of the potential for excessive exposures with use of this type of consumer product either at home or in the classroom Stopford, 2003). Studies were done with up to 5 users in an unventilated room (0.4 air changes per hour) and with up to 4 users in a school room with a recirculating ventilation system (0.5 air changes per hour). The solvent system in these markers was a mixture of methyl isobutyl ketone (MIBK) and n-butyl acetate (NBA). Solvent consumption was determined by measuring marker weight loss. Exposures were measured in the breathing zone and at a background site with 3M Model 3500 samplers. Users drew for 30 minutes and then the sampler was moved to the background site for an additional 3.5 hours.<br><br>
Measured personal exposures to MIBK for one user (30 minutes use plus 3.5 hours background) were 1.8 mg/m3 for classroom exposures and 3.8 mg/m3 for exposures in an unventilated room. For NBA, personal MIBK exposures were 0.67 mg/m3 for classroom exposures and 1.1 mg/m3 for exposures in an unventilated room. Modeling using the general dilutional ventilation equation was done to determine peak and average exposures. The highest average individual solvent consumption rate per user (424 mg for MIBK and 193 mg NBA per user) was used to determine exposures. For MIBK peak exposures using this model were found to be 1.69 mg/m3 in the ventilated classroom and 1.58 mg/m3 in the unventilated room. 4 hour average exposures were found to be as follows:<br><br>
<table>
<tr><td></td><td>MIBK (mg/m3, measured)</td><td>MIBK (mg/m3, model)</td><td>NBA (mg/m3, measured)</td><td>NBA (mg/m3, model)</td></tr>
<tr><td>Classroom</td><td>0.45</td><td>0.75</td><td>0.33</td><td>0.34</td></tr>
<tr><td>Unventilated room</td><td>1.52</td><td>0.94</td><td>0.28</td><td>0.43</td></tr>
</table>
<br>
Assuming a workplace inhalation exposure rate of 1.25 m3/hour for 40 hours a week and a body weight of 80 kg, the above would result in exposures of:<br><br>
<table>
<tr><td></td><td>MIBK (mg/kg/d, measured)</td><td>MIBK (mg/kg/d, model)</td><td>NBA (mg/kg/d, measured)</td><td>NBA (mg/kg/d, model)</td></tr>
<tr><td>Classroom</td><td>0.040</td><td>0.067</td><td>0.029</td><td>0.030</td></tr>
<tr><td>Unventilated room</td><td>0.136</td><td>0.084</td><td>0.025</td><td>0.038</td></tr>
</table>
<br><br>
Spray Paints<br><br>
I have looked at exposure to spray paints using the following parameters: 47 m3 room with 1.1 air change/hour; measurement of exposures after filling out 6-12 sheets of artist paper per session with a total of 6 sessions; measurement of skin exposure using Ti as a marker with testing of Tyvek suits and nitrile gloves; measurement of air exposures using 10 micron personal exposure monitor, a PMA 10 in room monitor and a total particulate monitor in the
</td></tr>
</table>

| Reviewer | Comments |
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| | room exhaust. Skin exposures to hands averaged 326 micrograms/cm2 and to total body (minus hands) 45.5 microgrms/cm2. No inhalation exposure was measured with the personal samplers or the PM10 monitor. The average total paint particulate levels released to the room were 37.3 mg/session. Each session lasted 30 minutes. Each session consumed 26 gm of paint of which 5.7 gm was solvent.<br><br>Consumer exposure models<br><br>Markers<br><br>The above maximum highest average solvent consumption figures were used to test each consumer exposure model. The input parameters do not include markers or writing instruments. I used SOLVENT-BASED WALL PAINT as a default. Additional parameters used were as follows:<br><br>Environment of use: school/office<br><br>Users: adult<br><br>Background 0 mg/m3<br><br>User defined emission rate: 53 mg/hr (424 mg/8 hr)<br><br>Duration of use per event: 30 min<br><br>Mass of product used per event: 0.424 g<br><br>General comment: the chemical look up is very difficult to use by chemical name. It would be quite useful to allow look up by CAS# as well.<br><br>Spray Paints<br><br>For the solvent exposure, I used the Aerosol Spray Paints product type. I assumed an adult was using the product in a utility for a 30 minute interval and then stayed in utility room for 8 hours. 5700 mg of solvent was emitted in 30 minutes.<br><br>Results<br><br>INH02 (markers)<br><br>No near field area in zone 1: adult acute inhalation: 4.33-5.05 mg/kg/d.<br><br>Comment: these results are a factor of 100 fold greater than would be expected from exposure to solvent-based markers. It would appear that it would be prudent to develop a consumer product category for markers and writing instruments.<br><br>INH03 (spray paints)<br><br>There is no option to run this model for just for paint aerosols (no chemical identified). I added titanium dioxide (the marker in our studies) as a chemical for testing this model. All inhalation and dermal exposure parameters were 0.00E+00. |

| Reviewer | Comments |
|---|---|
| | For solvent exposure, using the general dilutional ventilation equation (Brock and Stopford, 2003), the peak exposure was found to be 94 mcg/m3, the 8 hour average exposure was found to be 13.8 mcg/m3. Using the INHO3 model, and a garage with typed in values for duration of use (30 min) and mass of product used, the acute and chronic inhalation results were 0.00E+00., When using drop down values (45 min and 200 g/use with a dilution fraction of 0.22 inhalation exposures were calculated to be as follows:<br><br>Peak exposure: 595 mg/m3 (program defined emission rate)<br><br>2790 mg/m3 (user defined emission rate)<br><br>Comment: The peak exposure is a factor of 6000-30000 greater than expected<br><br>DER-01 (markers)<br><br>Acute dermal: 132-184 mg/kg/d, limited to hands<br><br>SA-BW ratio limited to both hands in youth (11-20 yo) in cm2/kg. youth 16-20 yo 71.6 kg, 11-15 yo 56.8 kg.<br><br>Comment: using a two hand skin area of 820 cm2 (Stopford, 2014), the above exposure would result in a dermal exposure to hands of 2.8-3.1 mcg/cm2.<br><br>DER-02 (spray paints)<br><br>There is no option to run this model for just for paint aerosols (no chemical identified). I added titanium dioxide (the marker in our studies) as a chemical for testing this model. All inhalation and dermal exposure parameters were 0.00E+00.<br><br>For solvent exposure, acute dermal exposure was 0.16 mcg/kg/d. For an adult, the SA/BW ratio was 12.4 cm2/kg for both hands. For an 80 kg adult, skin exposure to the hands would be expected to be 59 mcg/cm2.<br><br>Overall Assessment<br><br>The CEM models I evaluated were deficient in the following areas:<br><br>1. Lacking exposure scenario for markers writing instruments, pastels and chalks and ceramic clays and glazes.<br><br>2. Inability to enter non-volatile chemicals under chemical of interest. There is the ability to enter dust parameters for models INH06-ING04. I suspect this input could be modified to include dusts/aerosols where there is indoor exposures.<br><br>An alternate would be to develop the general dilutional ventilation equation as a CEM model. This model could be used for determining peak exposures as well as exposures over time to both volatile chemicals as well as respirable particles.<br><br>References |

| Reviewer | Comments |
|---|---|
| | Brock T, Stopford W. Bioaccessibility of metals in human health risk assessment: Evaluating risk from exposure to cobalt compounds. J Environ Management. 2003; 3(5):71N-76N.<br><br>Stopford W. Solvent Exposure during use of Solvent-Based Whiteboard Markers. 2003. http://duketox.mc.duke.edu/mibkmarkerstudy.pdf<br><br>Stopford W. Protocol for the assessing dermal exposures while using pressurized aerosol sprays, airbrushing and drawing with pastels. 2014. http://duketox.mc.duke.edu/dermal%20exposure%20to%20aerosols%20protocol9.doc |

# APPENDIX A

# CHARGE TO REVIEWERS

# Technical Charge to External Peer Reviewers

**Contract No. EP-W-10-014**
**Work Assignment 5-18**
**July 2016**

## External Letter Peer Review of EPA's Consumer Exposure Model and Draft User Guide

### BACKGROUND

The Office of Pollution Prevention and Toxics (OPPT) estimates inhalation, dermal, and oral exposure to chemicals emitted from products or materials used indoors. Estimating consumer exposures involves integrating age-specific exposure factors and activity patterns with media-specific environmental concentrations encountered by individuals. The exposure is used by OPPT along with hazard and dose-response information to estimate potential risks from consumer products. If insufficient monitoring data are available to describe measured concentrations or personal exposures for the consumer exposure scenario of interest, then some means of estimating or predicting concentrations is needed. OPPT has updated its Consumer Exposure Model (CEM) to assist in estimating human exposure for a wide variety of consumer scenarios. Table 1-1 provides a list of the individual modules within CEM.

**Table 1-1. Overview of Modules within the CEM**

| Model Number | Model Description |
|---|---|
| INH01 | Product Applied to a Surface (that evaporates): Incremental Source Model |
| INH02 | Product Applied to a Surface (that cures): Double Exponential Model |
| INH03 | Product Sprayed (indoors and outdoors) |
| INH04 | Product Added to Water |
| INH05 | Product Placed in Environment |
| INH06 | Article Placed in Environment |
| ING01 | Product Applied to Ground Outdoors |
| ING02 | Product Swallowed |
| ING03 | Article Mouthed |
| ING04 | Incidental Dust Ingestion |
| ING05 | Particle Ingestion After Inhalation |
| DER01 | Product Applied to Skin (Fraction Absorbed Method) |
| DER02 | Product Applied to Skin (Permeability Method) |
| DER03 | Article where Skin Contact Occurs |
| DER04 | Direct Transport from Air to Skin |

These models will be used by OPPT to estimate exposures and doses from a wide variety of consumer products and materials. These modules are available as applications within Microsoft Access that call executable programs developed in Python. The front-end graphical user interface in Microsoft Access is used

to enter required model inputs and run the models. Accompanying help screens and user guides are contained within the model interface.

CEM estimates human exposure to chemicals contained in consumer products and articles:

- **Products** are generally consumable liquids, aerosols, or semi-solids that are used a given number of times before they are exhausted.

- **Articles** are generally materials such as polymers, foams, metals, or woods which are always present within indoor environments for the duration of their useful life which may be several years.

Although there are existing definitions of consumer products and articles, they are distinguished from each other in a more general way in CEM. Certain chemicals may only be added to articles, others only used to formulate products, and others could be used for both. For the purposes of consumer exposure assessment, products and articles are treated differently. Formulations, anticipated use patterns, and available approaches to estimate exposure are different**. Note that the excel file "Use Categories and Descriptions for CEM Scenarios" is related to Charge Question 2 and further elaborates on definitions of consumer product, article, and functional use categories.**

## CHARGE QUESTIONS

For each question, please provide an appropriate explanation. When discussing or presenting specific data, please justify your response and qualify the data to indicate acceptability and quality. In your review, consider data and approaches that are currently available rather than data and approaches that may be available in the future. Please provide any other comments that you feel will improve the models.

### Part 1. Equations Used in Models and Exposure Defaults

1. Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies.

2. Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios".

3. Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered.

4. CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways.

5. There are several items listed in the "Areas for Future Enhancement" section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term.

**Part 2. User Interface**

6. Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface.

7. Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful.

**Part 3. Documentation and User Guide**

8. Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited.

9. Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear.

# APPENDIX B

# INDIVIDUAL REVIEWER COMMENTS

**COMMENTS SUBMITTED BY**

**Alesia C. Ferguson, MPH, Ph.D.**

**Peer Review of EPA's Consumer Exposure Model and Draft User Guide**

**Post Comments:**

After discussion with other reviewers and EPA, I wish to keep my comments as is. I believe they are valid areas of concern and areas for improvements. Some comments are minor and some more major. I suggest in the future that EPA be allowed a time to review our responses and indicate where perhaps we had a misunderstanding and also indicate what might be easy changes versus more difficult changes. Or why perhaps certain functionalities or models were not considered at the time. It is easy for reviewers to come along and suggest everything, but we may not understand the original intention of the model or certain difficulties encountered. This should occur before the conference call. In general I felt that there was an overall concern that current models needed to be further validated and verified to ensure models were working as expected according to algorithms as presented and against data in the field. In addition, although some reviewers felt mass balance checks might be difficult, I think further effort can be made to create subroutines that indicate the exposure and dose for all receptors as a function of the original mass (this ensures at least some impossibility does not occur although exposure and dose may be magnitudes of order less).

I overall felt there was great variability in the complexity of models that needed to be explained to the user, and later improved (e.g., evaporation of products applied to a surface but no evaporation of product from a skin or diffusion through one layer of the skin but through multiple layers for the dermal models). There are areas for future enhancements, suggested by reviewers, that involve developing models for other exposure scenarios, but I suggest that EPA fully focus on improving current models in the current CEM and adding explanations on the functionality of these models where they reveal to the user what is and is not considered at this time.

I am looking forward to the release of the improved model over time.

**Part 1. Equations used in Models and Exposure Defaults**

1. **Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies.**

   Answer: There are a few areas where improvements can be made (also please note that some of these comments are related to understanding the modules better but also improving the content of the user guide which pertains to Question 9 below-ERG may choose to arrange parts of my response under that question):

   a) I see equation numbers in CEM for equations. The user guide needs equations numbers that match CEM equation numbers.

   b) In some areas, where an equation is repeated, remove this repetition and refer to the equation number. For example, the equation for mass of product used (g) is at least repeated 4 times, starting on page 23 of the user guide. The equation does not change, and so use the equation number (when assigned) to refer back to it.

c) The naming pattern for models and equations should be better explained. INHO1, INH02 for example are concentration determination models, but ING01 and all DER models are exposure and dose models. Consider a renaming format for those models that only determine an environmental concentration and those that determine an exposure and dose. Some inhalation and some dose exposure/dose models use the concentration determination models.

   Some additional point related this:

   - Page 29: Calculation of Inhalation Dose from Product Use really should be a separate numbered model and stand out to the reader. This model can utilize INO1, IN02, INH03, IN04, the emissions models, which I believe should be named differently from exposure and dose models.
   - In Section 2 (page 17): Insert an overall explanation of the various models in this summary section (you have some of that content at the beginning of Section 3). I would also suggest a schematic of models and equations and how they can feed into each other, after a renaming has occurred. The schematic would answer the questions, "what concentrations models can feed into what exposure and dose models by route and based on whether the chemical is found in an article or product?"
   - For a model when naming, it should be clear what this model will do? So as an example in your current naming format: INHO2: Product Applied to a Surface Indoors Double Exponential Model", would be better called: INH02: Air Concentration Determined from a Product Applied to a Surface Indoors Using a Double Exponential Model". Consider a renaming scheme for models.

d) The user guide often goes back and forth between the terms algorithm (e.g., page 15), equation and model. I suggest sticking to equation and models. Also when does an equation rise to the level of a model (when it is a series of equations)?

e) In the Introduction (Page 16), after describing the contents for the user guide, please list all secondary models utilized in CEM (e.g., PARAMS, E-FAST and so forth). Also describe their function in CEM. This would be very useful to the user and will demonstrate the utility and parameter estimation functions in CEM.

f) Section 3 (page 20): When the two Zone model is explained (Figure 1), Q12 and Q21 is confusing. Just use one Q for a bidirectional flow or interzonal flow, like the figure on page 22 (Figure 2). It may have been a typo.

g) At first I had a hard time understanding the parameter H in the IH01 model on page 24. The term H helps to determine which part of the model is being applied; When H is zero, this is the first use or application period. Maybe just a couple words on this parameter and the user will better envision the different aspects or phases of this equation.

h) E(t) on page 24 is the same as E(t2) on page 27, because in the model INH03 a product sprayed has INH01 emissions as one component. You can eliminate this equation being repeated by numbering and referring to it and then users can see the relationship between models, where there is an

extension of INHO3 over INHO1. Or at least point this out to the user, and use consistent terms and equation numbering.

i) Page 27: Product added to water: Evaporation might depend on whether it is added to a container that is then closed, such as a washing machine. The chemical's 90 percent evaporation time might not be relevant to dynamics in a washing machine. This is an empirical equation, please say the reference for this equation for "EvapTime" here and how it was determined by Chinn 1981. In other words provide some further explanation on "EvapTimes" used to reduce the emission rate for a chemical added to water and how it might vary based on a closed container versus an open container. Once the container is closed, should emissions be truncated? Right now it says truncation will occur when everything is washed down the drain.

j) Page 30, LADC is mentioned for the first time without a definition as "Because of this iterative process CADD cannot be calculated directly from the LADC presented in the model results." Please note, the definition for LADC "Potential Lifetime Average Daily Concentration (mg/kg-day)" is first defined on page 32. Therefore this section needs some re-organization to perhaps present the various air concentrations that are actually determined and presented to the user (i.e., LADC, Peak Concentration, time integrated concentration) before then presenting time integrated dose over 60 days used for ADR and time integrated dose over one year used for calculating CADD. Some smaller section label or titles are also needed for this very important inhalation exposure and dose section.

k) Page 41, "Inhalation Dose of from Article Exposure" uses InhalAfter as a parameter. The glossary defines these "Inhalafter" and "InhalBefore" as use during and use after a product. Please clarify in all these inhalation models when these parameters would be used and why we assume breathing rates would be different during the use of a product and after the use of a product. In addition, this parameter "Inhalafter" is first mentioned with inhalation for article exposure, page 41 and a "inhal" parameter was used for inhalation after product use on page 30. Glossary also needs to match these definitions."Inhalbefore" is not used in any of the equations. I see "InhalBefore" use as a selection in the CEM model but not in the equations of the model in the User Guide.

l) Page 43, D is used for Density of Formulation in the AR equation for DER01. Den is used for Density of formulation on the next page and D is used for Duration of use on page 50. Please check these equations for consistency and ensure actual CEM model is using the right parameters. Please also note earlier that Den is used for density of product. I suggest two separate terms for density of product and density of formulation where formulation is intended for a product applied directly skin like a cosmetic.

m) Page 51, DER03, the Factor says "weight fraction of chemical in product". DER03 model is for article where skin contact occurs. Change to "weight fraction of chemical in article" or explain the "product". This also occurs in the ADR equation on Page 52.

n) Although I think in most cases the dose will be far lower than the exposure or the chemical concentration in the environment, is there an underlying mass balance check on the chemical mass that is released from product and article uses. So if a product is assigned three routes of exposures, is the final dose amount (chemical mass) experienced by all receptors added to ensure that they

total does not exceed total product mass released from product use. Can the model also report total dose as a function original chemical mass?

o) Some clarity needed here. Dermal exposure from use of product outside on soil is actually considered. Currently ingestion exposure is considered in CEM (ING02) from product used on ground, but the product user is more likely experience dermal exposure during use or a child playing on grass outside is likely to experience dermal exposure for days after the product use. This was not well explained. I choose fertilizers and ING02 and DER01 are used for product used outside. This was not explained in the user guide. DER01 is suggested as product applied to skin, but was used for product accidently applied to skin (where the percent retained is key). Again, does the model keep track between the DER01 and ING02 for such a scenario. If I choose 90% retained on skin, what restrictions are placed in the mass available for the ING02 model.

p) Another note: I ran a test with fertilizers and it allowed me to change the use environment to Residence-Whole House from Yard, but on the input page CEM still asked for the Yard Area and soil properties, so although it appears the model flexible on use environments, it is not. This needs to be explained.

**2. Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios".**

Answer:

a) There is a wide range of scenarios available to the user. If the user guide is rearranged and ordered more clearly according to some of my earlier suggestions to Question 2, this may be more apparent to the user.

b) On page 4, can you give example of when to use near field for product. Meaning how stationary is near-field. Would painting a room and moving around slowly be considered near field? Would walking through two rooms and spraying to be rid of "stinky teenager boy" smells be near field? In other words you have the product in your hands, but you are leaving the immediate vicinity of some of the air concentration. Maybe suggest to the user examples of product usage in near field. This may be a more trivial point, but it might help the user.

c) The percent retained on skin (Ret) in DER01 (page 43) is an extremely important factor. After searching a while I see that Table B-2 has this for products. Please indicate the references for these values and refer to this table in Section 3. Do these values consider wash and wipe events within a certain time period or consider the maximum loading possible on a skin surface over the time period? The implications of this factor may need to be further explained to the user, because heavily weighted factor for determining exposure and dose estimates. For some cosmetics applied to the skin (which I believe this model could also be used-although no cosmetics are listed as products) estimates could made on the mass of the product and expected use period of the product. For example, is facial cream expected to last 30 to 60 days

and therefore daily exposure is just chemical mass divided by the number of days? So, ultimately however this model for CADD just means the person is exposed to all the chemical in certain fully used products, and the dilution factor is all that matters. This would be an assumption of no wash or removal event.

d) On page 24 for INH02, a study from Wilkes et al., 1996 is quoted as determining the 25% of mass is released typically. On page 26, f is described as the fraction of mass emitted from first exponential as 0.1. This f should be allowed to vary from 0.1 to 1.0 by the user, and should be dependent on volatility of chemical and product. However, why is it described as 25%, but 0.1 is used in description. Again 10% is mentioned in the write-up on page 25. I may be confused and 10% what is released at first but overall only 25% mass of the chemical mass is ever released. Also combine the explanation of 25% and 10% release into the same paragraph for clarity.

e) Page 49, for DER02, please clarify to the user that the Kp is a permeability coefficient through the stratum corneum only (actually derived from Potts and Guy 1992 and then used by EPA in their dermal document-I gave reference for the EPA document below). Kp also exist for permeability through the hydrophilic epidermis (other 4 layers beneath SC). Models that consider movement through the two layers might be better predictors (Bunge 1995). At least let the user know this as this might be confusing, especially since DER04 uses a more complex and more recent model from Weschler and Nazaroff, 2012 that does consider a Kp for SC/viable epidermis composite and even permeability all the way through to blood (i.e., dermal capillaries). Explain that one model may be more complex than the other (many assumptions made also for partition coefficients). DER04 considers more barriers to movement. Really CEM is pulling different models together with varying levels of complexity and the reader needs to know this. Again there is consideration for volatiles and semi-volatiles, but once and if they cross the air-skin or liquid-skin barrier it is their solubility and molecular weight in both layers that will determine movement through layers and uptake into the bloodstream. The lipophilic and hydrophilic properties of all chemicals will need to be considered consistently in all layers or one layer.

f) Related to my point above, the “transfer coefficient” in DER03 is no more than a permeability coefficient through the skin. Please explain if the user determines this transfer coefficient and if it is different than kp in DER 02. Please note that the “transfer coefficient” in DER01 has units of cm/hr (length-time). The “transfer coefficient” in the glossary is cm2/hr (area-time). Terminology for permeability coefficient and transfer coefficients need to be clarified. It gets further confusing when table –B13 has diffusion coefficients through a materials in units of m2/s (area-time). If differences in these models are dependent on the phase of the chemical (VOC versus SVOC) or media (air, versus liquid) that the chemical is housed in a better explanation is needed for the user for these dermal models and their considerations of movement of the chemical through the skin. Merging models from different sources can pose the additional challenge of establishing parameter terms consistently. In the exposure field transfer coefficients are also used to denote the mass of a chemical that transfer from a surface to the skin following one or multiple contacts (mg/cm2). In DER03, you use fraction of chemical

on surface that is dislodgeable as a proxy for mass transfer coefficients along with the mass of the chemical on the article in the contact layer.

g) Equations for INH05 and INH04 are identical on page 27 and page 28. So will a product placed in the environment will have the same emissions as the product placed in water? The only difference explained as I understand it, is that when the product goes down the drain or Csat is exceeded for INH04 the emissions is truncated then, while for INH05 emissions is truncated at the end of the product use or when Csat is exceeded. I do have a hard time seeing that "EvapTime" the chemical product poured into water is the same as the "Evaptime" of the chemical from only the product. What might be different is the weight fraction of the chemical in the product. For INH04, it may now be weight fraction of the chemical in the mixture of water and product (not while pouring the product into the water-but for some time of exposure after). There must be some variable difference between the models, aside from emissions truncation time. In fact one model could be presented for both scenarios and just the truncation difference explained then.

**3. Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered.**

Answer:

a) This model is <u>not</u> geared for probabilistic calculations, where a number of calculations could be run by varying multiple parameters to look at worst case (i.e., Monte Carlo simulations using distributions). The user could carefully select an input for each parameter to get to worst case, with an understanding of parameter's influence in the equation. But the range of values and exposure possibilities cannot be determined using this model. This statement is made in the user guide on page 6, and could be moved into an executive summary since this is very important to understand. The model allows the user to enter their own parameters for a particular scenario to offer flexibility in the model and in the case of the user to capture the variability using a unique set of parameters in a single run.

b) A product user could become a receptor during the duration of use of the product. I just experienced this. I painted for a while, allowed my partner to paint for a couple hours, but I stayed close to source. The CEM could allow the user to add exposure for the two scenarios to a total exposure. The first scenario entails "near field" exposures, and later a far field with the time frame of the acute or chronic dose calculations.

c) The user is required to enter air exchange rates and ventilation rates. These largely depend on type of building, layout of building (upstairs/downstairs), use of building and type/performance of HVAC system (room HVAC and central HVAC). The user can be referred to a few references to determine this. ASHRAE recommended ventilation rate is 50 cfm and changes for house size. ASHRAE has a formula for recommended ventilation rates dependent on the number of bedrooms in the building.
See: https://resaveguide.lbl.gov/step-3-whole-building-ventilation-rate

d) The "60-day modeling period is used to calculate the total exposure associated with a single use of a product". Can this be flexible, and more dependent on mass of product and ultimately environmental concentration of some significance over time?

e) Model can ask if other receptors in in the same room as product user or a different room during the use period. This would increase the exposures for some receptors and offer some flexibility in the model. Right now on page 14 of the user guide it is not clear to me where the receptors are located (zone 1 or zone 2 when at home)?

f) For Activity Patterns, currently only one type of activity pattern (i.e., full time or part) will be calculated all receptors in the user guide. This is an area of flexibility the model can consider changing later.

g) User has to choose between DER01 and DER02 (absorption fraction or permeability method) on the Scenario tab. Allow user to also select both for comparison.

**4. CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc.). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways.**

Answer:

a) The exposure/dose metric to consider might also be relevant to the toxicity of the chemical, the question the user might want to ask is….is it likely to cause an acute effect or a chronic effect to a particular user, and is it based on how the product or article is used. However in the home setting, odd use patterns can occur and all exposure metrics should be available for every product and article. However as a start, in the excel sheet of product and article functional use categories, you might consider adding columns for product and articles on likely use patterns in terms of weekly, month, and yearly. When additional dose metrics are added, it will guide the user on selecting what dose metrics are suitable. Naturally you would allow lifetime measures for those articles and products that are used quite commonly over very long periods (e.g., cleaners, cosmetics).

b) Many products cause a dermal/skin local effect equation (e.g., harsh cleaning agents like bleach). Allow the dermal dose equation to focus on determining what remains on the skin surface over the exposure period. In model DER01 for example this is more appropriate for the Acute Dose Rate equation, FRabs would not be needed. The model in CEM should ask if a skin exposure or a dose is needed. Likewise DER02, DER03, and DER04 can be adjusted also to accommodate this extra feature.

**5. There are several items listed in the "Areas for Future Enhancement" section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term.**

Answer:

**a)** **For exposure metrics for Short_Term, Chronic and Lifetime Exposures:** Yes, these additions would be important for certain classes of chemicals, and in part would depend on the toxicity of the chemical. Chronic and Lifetime exposures would be important where people use products on a very regular basis. Cosmetics, cleaning products, and air fresheners would fall into that category. The acute use rate would be used with a multiple to calculate some reasonable use patterns. Cosmetics are used daily and cleaning products can have a use rate of 52 (once a week), twice a week (104) or once a month. These could be set a low, medium and high use rates. I would think that short term exposure can be easily determined in the model to reflect just the time of product use. Instead of averaging over a day, just determine the exposure for dose for the use period and report as such.

Please reorganize this section for better flow. Move the second paragraph below the third.

**b)** **For Products intended to go down the drain**: I am not understanding how this concentration equation relates to a residential or public environmental exposure in CEM. What do you mean by the concentration in the river water? We need concentrations in media that the residential or office building receptor would contact. This scenario is either not explained well or irrelevant to what CEM is trying to do. Perhaps, concentration in river water needs to be related to concentration in a media in or around the home. If the approach or intent is how this concentration helps to account for mass loss of product in the home, this potential scenario needs to be explained as such.

**c)** **For Vector-facilitated Releases from Articles Not intended to go Down the Drain**: Here you describe movement of additives from articles to vectors, where in fact vectors are still articles (e.g., clothing and this is confusing to the reader). Again why are we concerned about the greywater being a source of exposure, or are we considering chemical are being lost from articles in this manner from the home environment. Is this a consideration of a mass balance equation accounting for all losses? Keeping track of all exposure to a chemical that is moving from one article to the next will be complicated without a type of detailed human activity pattern. So please clarify whether the vector is a source of exposure, an exposure pathway, or a consideration of mass balance for the chemical of concern. Please also clarify CEM as a residential or building exposure model for exposures. These are losses to the larger environment and then we also have to trace removal at a wastewater facility.

**d)** **Products that Spill or Leak over Time**: The description needs to clarify if this would affect exposure for the product user or other receptors. Or would this decrease or increase the exposure for the product user from one route vs. the other route and how would models would keep track of overall product and chemical mass balance between routes. Because I do not think that there are standards for product percent spills in the residential and office setting (a person clumsiness might help dictate that on any given day), the model can just have the user enter variable spill rates to see how it affects product mass, chemical mass and route exposures. Route exposure will depend on the volatility of the chemical and product formulation and likely use patterns.

**e)** **Elevated Temperatures During Application and After**: The user can be reminded in the user guide that emission rates (i.e., fate and transport) of the chemical are affected by temperature. Likewise ventilation rates are affected by temperature.

**f)** **Consideration of chemical or material specifics**: Currently, the ingestion model ING03 only uses a migration rate not a mouthing transfer efficiency (i.e., % or fraction removed during mouthing) found in Table B-5 of the appendix. These are not separate factors but are related, yet listed together in B-5, and might confuse the user about which is used. Mouthing activity (intensity) and acidity of saliva can indeed affect the migration rate of a chemical through and from the article. For models where articles are placed in the environment (e.g., INH06-one of the most detailed models), migration rates of the chemical is not a term used for the chemical as it moves from the bulk article to the air and then partitions to TSP and dust particles. Diffusion and mass transfer coefficients are utilized in those models (from Table B-12 and B-13). To some extent migration rates are related to diffusion or mass transfer coefficients (a chemical migrates because it diffuses and partitions). But to ensure the user does not get confused Table B-5 for "migration rates" needs to say "migration rate from saliva". Again when we are merging models from different sources, terms and concepts overlap or get confusing. Also please note the "product matrix" in Table B-13 and B-12 are articles by CEM definition not products (e.g., density board, vinyl flooring). For CEM "product matric may need to be changed to 'article matrix" for clarity. Vinyl floor for example is an article in Table B-1. If I am confused, someone else might be.

**g)** **Other scenarios:**

- Please consider a child in a bath. A dermal exposure model that considers water immersion is possible, where exposure can occur to soap products but also residual cleaning products in a bath. The EPA child specific exposure factors book has equations for exposure to chlorine products while swimming. This can be adapted for the CEM model.

- Consider adding exposures to chemicals in cosmetics. Some of my comments on considering local skin effects and percent retained on skin are relevant for exposures to cosmetics. But I notice under products that cosmetics are not included. Soaps and shampoos are considered, and for women exposures to harsh cosmetics that remain on the skin for many hours every day are of concern. When cosmetics are considered and if the chemicals are volatile or semi volatiles, then evaporation can be considered from the skin surface. This can already be done for DER01 and DER02 (product applied to skin). I suggest an article by Frasch et al., 2014 (found at http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3868874/ with some reluctance because I believe all the dermal models needs to be consistent in considering movement through layers or skin, evaporation from the skin surface and finite versus infinite skin loading conditions. But it is still a good read with some suggested model equations.

**Part 2. User Interface**

**6. Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface.**

Please note that some of these responses are very related to Part 3 (l) and refinement of the user guide, but it also affects the understanding and functionality of the graphical user interface.

Answer:

a) Helpful to tell the user to put the software program on "Full Screen", then the five tabs of CEM can always be seen. You advise the user on page 9 to use the scroll button to the right to move up and see these tabs.

b) It would be more useful to move "New Analysis" Button to the left of View Analysis. This button will be the most commonly used button and needs to be in immediate line of sight.

c) Please separate the product list from the article list in the CEM model on the scenario tab. If the user select a product then the rest of the interface only list "product". Therefore combination such like "product/article" goes away for the use environment and we know what we selected through the entire run and data screens. This might take a bit more programming and it would be like creating two clear paths in CEM, one for product and one for article. Right now when you select a product or article, the popup box always mentions "Do you want to use the defaults use environments for this product (RubberArticles:Toy). CEM and use guide need to remove any confusion between article and model for a better understanding of models applied and assumptions and defaults assigned.

d) The user should be given practice problem to run the CEM, if this was not in the plan. Reviewers had some training sets in the first Phone call with EPA and ERG.

e) I had problems trying to enter my own CAS or chemical string. It would not then find the chemical on the list. I have to select a chemical from the list. This may be code issue running on my computer. Can someone please check this?

f) Can any chemical be matched with any product or article? I tried fooling around and it appears so. Some combinations are highly unlikely. Let the user be aware that although every combination is possible in CEM, they need to check the ingredient lists (if available on the product or article label).

g) Consider some more direct statements in the introduction on the limitations of CEM per run, such as…. "Automated is the environment for a product or articles based on likely use environments and patterns. The product or article is then linked to the relevant exposure route and therefore relevant exposure models for in CEM. These likely scenarios, use patterns and exposure routes are shown in Table B-1. CEM determines one use environment at a time for a chemical in a product or article."

h) Page 10 of user guide, when product user and receptor are defined, description is misleading at first. It suggests the model can be run for more than one product user at a time, "CEM may be

run for multiple users and receptors". However, it can only be run for one product user at a time, and will automatically be run for 7 age groups of receptors (where one of those receptors is a product user). Of the 7 possible receptors, one of 3 can be a product user. I suggest refining the definition here for clarity.

i) For Activity Patterns please on page 10, also indicate clearly that only one type of activity pattern (i.e., full time or part) will be calculated all receptors in the user guide. This is an area of flexibility the model can consider changing later.

j) On the activity pattern tab of the CEM model, to the right is an explanation that activity patterns can be changed. It suggests you can go into the file and change the patterns by the hour. But this is not possible. You can only change from full time to part time, across all receptors. At least my version of the model does not allow these changes. However, if possible it would add great flexibility.

k) Page 10 for background Air and Dust concentrations, is it true that Products asks for background air concentrations and articles asks for background dust concentration? Can you include a better explanation of why here? This has to do with volatiles associated with products vaporizing to the air and articles associated with semi-volatiles attaching to dust and TSP particles? This would also help to explain how the models works.

l) Page 9: Modeling Options says that models that are not available are grayed out. I think in this version, they just do not show models that are not used.

m) Page 9 and page 10, I am not sure all the Help buttons are necessary if they did not add any more details than the label. So? button for "Product/Article Environment" adds no additional detail.

n) Page 12: for "2.a Chemical Properties" tab: Put all acronyms besides the parameters. I also found that this was not consistent in the glossary. Some parameters have the acronym as used in the model listed and some do not.

o) Page 12: Define QSAR when first used and explain what you mean by "training sets". These are the sets you used to develop and test the CEM model. This is confusing here.

p) Sections describing the input tabs are not balanced in the details they contain. 2.b. and 2.c. The 2.b tab describing the product/article properties tab on page 13 could further say: "Under this tab the user is required to enter use data for the product or article, and exposure factor information (e.g., mouth transfer, percent retained on skin). The model also has use inputs for acute and chronic assessment….." or something more to that effect.

q) Page 13 under the 2.d. If incidentally exposed humans are the 7 age groups defined as "receptors" please say "receptors" instead of incidentally exposed humans.

r) I think on page 13-14, under the 2.Receptor Exposure factors Tab, # 4 you mention surface areas. I think it is okay to say here that a table exists (what table?) for likely surface areas for each product type or article type. CEM uses that as the default, but the user can adjust. Is this correct?

s) Under the model selection tab, page 14, and throughout the document, I find that there are some key facts such as the "60-day modeling period is used to calculate the total exposure associated with a single use of a product" that is crucial in understanding how CEM operates and might need to be moved to a summary or overview.

t) In CEM, some inputs/parameters under the "model" tab are bolded and some are not.

**7. Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful.**

Answer:

a) Exposures to chemical having the same toxicological endpoint would be useful, as would the ability to estimate exposures to multiple chemicals from one product or article. Can you software initially ask if the client with be making any such calculation, and return to start each time, while retaining the information from the calculation from before. It is currently feasible for the user to download each report on one chemical at a time into access, but future versions of the this software could have an extra data entry screen to ask a series of relevant questions that would determine how many sets of calculations to perform and save into one report.

b) Multiple zone referred to in the "Future Enhancement" will facilitate the idea of distance from source in a room. This statement can be placed in this section to better explain when this would be used.

c) For the statement. "Consideration of Chemical and/or Age-Specific Transfer Efficiencies from Surface-to-Hand, Hand-to-Mouth, and Object-to-Mouth" The transfer efficiencies might depend more on article or product type, how it is used and pressure of contact, and whether skin is wet or dry. There are limitations however for maximum transfer.

d) Does the user have access to the excel files describing product category, article category and functional use categories from the CEM model interface?

e) Under the result tab, can the results remind you who you choose as the product user, even though you might be able to tell by the higher exposure results?

**Part 3. Documentation and User Guide**

**8. Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited.**

Answer:

a) I recommended referring to tables in the appendices when the parameters are presented in the user guide. I mentioned an example above for the parameter "percent retained on skin for product usage" refer to table B-2.

b) Recommended formula for ventilation rate dependent on number of bedrooms: See: https://resaveguide.lbl.gov/step-3-whole-building-ventilation-rate.

c) Readings on deposition of particles in Lungs (portion swallowed)

1) http://www.archbronconeumol.org/en/deposition-inhaled-particles-in-lungs/articulo/S1579212912000845/ … Ana Fernández Tena, Pere Casan Clara, 2012.

2) Also see http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.275.9282&rep=rep1&type=pdf,

3) Also see www.mass.gov/eea/docs/dep/cleanup/laws/inh0708.do for the following more precise information

i. 100% of respirable particulate mass is equal to or less than 30 microns in diameter (≤ PM-30) (ORS 1994, MassDEP 1997)

ii. 50% of total respiratory particulate mass is equal to or less than 10 microns in diameter (≤ PM-10) (ORS 1994; Weidner et al.; ORS 2006).

**iii. 100% of inhaled particulates greater than 10 microns but less than or equal to 30 microns are swallowed (ORS 1994).**

**iv. 50% of inhaled particulates equal to or less than 10 microns are swallowed, and the remaining 50% enter the lungs (MassDEP, 1997).**

d) Use EPA's own simple dermal exposure model to suggest consistency in the complexity of the dermal models, Kp values and other terms used: Refer to EPA/600/R-07/040F. Also use this document to look at skin loading from various media and specifically for my suggestion for dermal exposure for "treated surfaces" for dermal exposure to pesticides applied to grass (Eq. 6 of this document). One of the existing DER models in CEM can also be adjusted.

e) See http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3868874/ for evaporation from skin surface, especially when cosmetics that might have some more volatile compounds are considered (things like nail polish remover for example). Frasch et al. "Analysis of finite dose dermal absorption data: Implications for dermal exposure assessment", J Expo Sci. Environ Epidemiol. 2014, 24 (1): 65-73.

f) EPA child specific factors handbook for children in pools and exposures to chlorinated products (EPA/600/R-)8/135). Ingestion of water while swimming find in Chapter 3). A dermal model can be adapted for dermal exposure while swimming.

**9. Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear.**

Answer:

a) Be sure to include and executive summary with an overview of model for the user. This can be similar to "Note to Peer Reviewers" section but can omit the 9 list of changes made in last version. This can be incorporated into other model capabilities.

b) On page 8 of user guide it indicates a tab for Lookup Table, but not a tab for Reports.

c) Page 10: Indicate briefly how many different product and article categories, and chemicals are currently available in CEM.

d) In the Introduction to Reviewers the following statement occurs. “Product use categories define various kinds of products. Examples include aerosol spray paints, laundry detergent, foam-based furniture, hard-plastic toys, and motor oil.” I might be confused. Are certain types of furniture defined as products? Check all documents for consistency in definition of products and articles.

e) I consider this suggestion very optional. The glossary can be moved up under a description of the user interface. It helps the reader get familiar with terms and acronyms very quickly and they can understand Section 3 more effectively. Make sure to not include equations in the glossary and move all equation to descriptions of models and equations, in Section 2 and Section 3 (this last part of the suggestions should be done anyway).

f) Delete Button: Does not allow you to unselect a selection, once you select. It asks if you are sure about deleting. If you say no, it needs to go back to screen and un-highlight all choices automatically, please check. Or explain that “Done”, closes the screen without deleting anything. Just in case this makes someone nervous.

g) Can the user download or view the entire user guide from CEM. Currently CEM generates short descriptions from a search now.

h) Appendix A says “Output from INH06-ING05-DER04 and Conversion to Dose. The first part describes assumptions for SVOC concentrations then used to estimate inhalation and ingestion doses. Four doses are described, one for the ingestion route and three for the inhalation route. Please explain how DER04 is involved here. DER04 is “Article with Direct Transfer from Vapor Phase to Skin”. There is no SVOC parameter or ingestion or inhalation parameter used for this DER04 model, or the relationship is not clear for reference to this vapor phase model here.

i) For Table B-12, please put material-air partition coefficient in the table title.

j) For table B-11, please include a reference or state assumptions for these near-field assumptions.

**Specific Glossary suggestions:**

a. The zone one concentration can be called Cff or CR1 depending on whether a near field is selected or not? We need to check all equations and stick to one term that might not be confusing to the reader. This comment also applies to near and far field volumes versus Zone 1 and Zone 2 volumes and also for air exchange rates? Check glossary and equations.

b. What does the word “harmonized” when referring to the SHEDS-HT model in the definition of “Amount Retained on skin” is the SHEDS-HT model the reference for the ‘mount retained on skin” in table B-2. Then this reference needs to be added to this table for clarity.

c. For some definitions in the glossary or guide-parameters the reference is given to where the defaults for the parameter were taken, but for some not.

d. In the definitions for chronic average daily dose and from acute average daily dose please again mention the averaging time for exposure and for the product concentrations for clarity (daily and yearly, 60 days, etc.).

e. Cleaning frequency: Cleanings per hour applied to an acute dose rate calculation will likely underestimate exposure where particulate exposure is concerned. Check if the models allow this cleaning frequency can be set to zero for these short term exposures and an explanation be provided to user.

f. Degradation half-life in soil. Most of the product mentioned for outdoor ingestion exposures are applied to grass (e.g., fertilizers and pesticides-both herbicide and insecticides) are applied to grass. This exposure pathway needs to be reconsidered or better explained to users, or that a soil half-life is used as a proxy

g. Earlier on it should be explained that soil exist outside, dust refers to large particles that settles inside and TSP refers to finer particles in air inside as media of exposures.

h. Diffusion coefficient models used here refer to Fickian law of diffusion assuming steady state concentration. Fickian second law of diffusion would account for time changing variation of concentration on the surface. Page 39, a solid-phase diffusion coefficient is mentioned to determine mass transfer for the complex" IN06 model: Inhalation Article placed in Environment." Diffusion coefficients are not used for the dermal models (permeability and transfer coefficient related terms are used), should we just call this the solid-phase diffusion coefficient determined in the PRAMS model for IN06 here in the glossary. Again the user guide may need to take some care in defining transfer coefficients, permeability coefficients and diffusion coefficients for what and through what as used in various models.

i. Under the First Order Emissions Decline you have a couple of equations in the glossary. To be consistent move this to Section 3 where extended descriptions of models and parameters are found. Also a 25% mass release is mentioned but 10% is used in the model.

j. Fraction of Contact (unitless) is described as "fraction of touches of all surfaces that are in contact with the article of interest", took me a few times to understand. Would it be better to say "fraction of all contacts with surfaces in the environmental that are with the article of interest?"

k. Fraction Ingested. The default is 1. It would mean everything inhaled is ingested. The default should really be 0 unless you have other information. The primary route is inhalation originally. How are the inhalation and ingestion model matched here for mass balance. There are size recommendations for what portion of particles are ingested after inhalation. See my included references above.

l. HVAC penetration, mention the range of value used from Creech et al., 1996.

Additional note: I did not thoroughly review INH06, because this type of fate, transport is less my area of expertise but I hope one of the reviewers did review. It is a complex model and separate runs/beta testing hopefully were performed on the standalone with various chemicals to see if it makes sense based on chemical parameters and time.

**COMMENTS SUBMITTED BY**

**Gary L. Ginsberg, Ph.D.**

## Peer Review of EPA's Consumer Exposure Model and Draft User Guide

**General Comments**

It is excellent that USEPA is developing an integrated set of peer reviewed consumer exposure models suitable for understanding exposures from the use of products and from household articles for a range of human receptors and scenarios. There are 15 different models and each has a variety of elements (e.g., migration of chemical, estimation of chemical concentration in exposure medium, estimate of human contact rate, estimate of human intake dose). Further, there are a wide variety of potential chemicals that could be involved in these scenarios. Thus, there are many aspects to review. Given time constraints I have decided to focus on one article (vinyl flooring) and one product (pesticide indoor application) and have reviewed each of the 3 pathways considered in these models (inhalation, oral, dermal).

My overall finding is that model parameterization could be more thoughtful in certain places and that opportunities for calibration and validation of model output have not been fully utilized. A sensitivity analysis and reality check of the article (flooring) model suggests that the output does not match what is anticipated based upon the literature while the product (pesticide) model appears to provide reasonable inhalation estimates.

### Part 1. Equations Used in Models and Exposure Defaults

1. **Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies.**

Article Equation (Page 36):

This equation focuses on the release of SVOC from the article into the gas phase with partitioning into suspended particles and deposited house dust. Separate tracking of suspended particle and house dust concentrations, with their own mass transfer coefficients makes the modeling more complex and may be of questionable value depending upon whether TSP contribution to house dust (for oral exposure) and influence on inhalation exposures is sufficient to warrant this level of detail. The main portion of the equation shows a steady state mass balance partitioning of SVOC between the article and gas phase with an exponential term apparently used to represent the back pressure of built up gaseous SVOC to partition back into the article over time. While this appears to be a reasonable mathematical representation, one potential issue is that the equation predicts the change in air SVOC mass (dNair/dt) by subtracting out the existing air amount (-Q*Nair/V). However, the incremental change over time may be best modeled by adding not subtracting what is already in air, which could allow the inclusion of background sources of Nair from other indoor and outdoor sources of the SVOC. By subtracting the baseline of Nair that exists from the previous time step it is worth asking whether the model has the potential to underestimate indoor concentrations. Further, the set of model equations for this scenario (pp 36-39) do not show how the model gets from the differential (change in Nair per time) to what is needed in the next set of equations (the consumer dose equations) and that is a concentration of SVOC in gas for inhalation. I would assume that the mass balance equations which produce mass of SVOC in air are fed into an equation which divides this quantity by Q*V, but I didn't see this described. Further, the mass balance equations which partition SVOC into TSP and dust

on a mass basis must be fed into equations which dilute this mass into a total amount of house dust and TSP in the room or house. However, these equations are not shown and the way to estimate how dusty is the interior space is also not shown. Finally, there is no effort given to relate predicted TSP and house dust concentrations to actual data for these quantities in homes. Given the importance of dust loading levels on the release of SVOCs from flooring, it would be comforting if USEPA provided a comparison between predicted loading levels and measured loading in homes that showed that the CEM estimates are reasonable.

The Page 36 equation shows SVOC partitioning into dust and TSP. The definitions and abbreviations for dust and TSP parameters are somewhat confusing, for example $A_{TSP}$ is "Mass of TSP suspended in the floor" – it would make more sense if that were "suspended above the floor" to distinguish it from $F_{TSP}$, which is "Mass of TSP settled on the floor".

$L_{art}$ is part of the exponential term on Page 36 but is not defined. The exponential appears to remove chemical from gas phase by partitioning back into article over time based upon the partition coefficient and $L_{art}$? Is that length of article? If so, shouldn't it be surface area of article instead of length of article?

The description of chemical specific mass transfer coefficient on Page 37 suggests that there are 3 ways to calculate it but then decides to use one of the methods (thermal convection) based upon a 2007 EPA modeling document. This decision should be better documented, and if there are substantial differences between the 3 methods, this parameter uncertainty should be discussed given the importance of this parameter. Further Equation 11 shows H to be a simple function of chemical molecular weight. It is worth describing whether other physical and chemical properties of the SVOC might impact H.

$K_{TSP}$, Page 38, Equation 12: this partitioning is based solely on octanol/air partition coefficient and the percent organic matter in the TSP or dust. As stated in this section, it is also possible to parameterize this partitioning based upon SVOC vapor pressure but this is suggested to be more complicated. However, SVOC vapor pressure may be more easily obtained from the literature for a wide range of chemicals than Koa, and in fact Page 38 did not say how Koa is derived (I assume it's the oct/water divided by the water/air (Henry's Law coeff?)). Further complicating the chosen approach (Koa based) is that the organic carbon matter percent of TSP and dust may vary and is not known but assumed to be 0.4, without further reference. It would be helpful to have further explanation about the possible differences between these two approaches and further justification for selecting the Koa approach.

Kart, Page 38, Equation 13: this partition coefficient is said to be based upon SVOC vapor pressure. However, when I ran the article model for vinyl flooring using DINP as SVOC, I tried a wide range of vapor pressures and found the model completely insensitive to this chemical parameter. The fact that Equation 13 is a log-log function should not prevent the model being responsive to VP if in fact it is used to create Kart and Kint. Further, it is conceptually inconsistent to base one partition coefficient, $K_{TSP}$, on Koa while a similar partition coefficient, Kart, is based upon vapor pressure.

Overall impression of the Article/SVOC Model (pp 36-39)

Model equations and parameterization appear reasonable except as noted above. However, the modeling is complex with chemical released from the article and ending up in air, dust or TSP based upon a few chemical specific properties (concentration in article, Koa, VP, MW) and the eventual concentration in dust or TSP

based upon some undescribed estimate of the dustiness of the interior space, or in the gas phase based upon some undescribed estimate of the volume of air the SVOC mass is diluted within. Given the various extrapolations and uncertainties, it would be very helpful for model results to be cross-checked against actual data. I exercised the article model for flooring using DINP as SVOC since it was a chemical already in the modeling parameterization database and since there are interior air and dust measurements for DINP in the literature to cross-check against. This exercise yielded an indoor air concentration of DINP of 93 ug/m3 and a TSP concentration of 3.59 ppm, while the model output did not report the house dust concentration. In contrast, Cousins et al. 2014 modeled indoor air and dust concentrations of DINP from Swedish flooring based upon actual emission tests of the flooring, with their model output estimating DINP in indoor air at approximately 0.003 ug/m3 and in indoor dust at approximately 10 ppm. Actual measurements of DINP in interior dust from a range of studies reported in Cousins et al. 2014 are in the 50-100 ppm range. These studies did not report on DINP in indoor air. However, the implication is that because of the low volatility of DINP, whatever is released from flooring and other household products will tend to be in particles and dust, not in the gas phase. This is not what the CEM article model predicts for DINP. Compared to a predicted indoor air concentration of 93 ug/m3 for DINP by CEM, Cousins et al. predict much lower levels in indoor air as mentioned above. Another point of comparison is the California Prop 65 review of DINP in vinyl flooring in which they estimated a gas phase indoor air concentration of 0.207 ug/m3 and a house dust concentration of 3416 ppm ( Cal OEHHA, 2016, available at: http://oehha.ca.gov/media/downloads/crnr/ sud1supportingmaterials06212016.pdf). Again this is a much different air to dust ratio than what my trial run of the CEM flooring model yielded.

There are more data for DEHP, another large molecular weight phthalate with similar chemical properties as DINP. Modeling of DEHP emission from vinyl flooring and indoor measurements in homes from several studies involving hundreds of samples (summarized in Xu et al. 2012) show that DEHP in indoor air is uniformly well below 1 ug/m3 while in house dust its concentrations are routinely above 100 ppm. I suggest the CEM article model be revisited by EPA to explore how it can better simulate patterns for phthalates and perhaps over SVOCs that appear in the modeling literature as emanating from household articles and consumer products (e.g., flame retardants). Further, it was somewhat surprising that a commonly studied chemical such as DEHP was not included in the CEM database. Even if many uses of DEHP have been phased out, it is not banned in household articles and still appears to be at substantial levels in house dust. Given all the experimental data for DEHP, it would be helpful if the CEM contained DEHP to directly compare model results with empirical data and other modeling efforts.

A further indication of differences between CEM vinyl flooring results and that reported by others is with respect to the apportionment of doses to different routes. The DINP CEM run showed house dust ingestion for young children at 0.1x the inhalation dose to gas phase DINP. This is opposite to what was forecast by Little et al. 2012 for DEHP emanating from vinyl flooring and taken up by young children (ingestion of house dust = 700 times more dose than inhalation of gas phase DEHP). An interesting feature of the CEM results with DINP for vinyl flooring is that the childhood mouthing dose was 25 times the house dust ingestion dose. This would appear to be a highly uncertain estimate as it would appear to require a child's direct mouthing of the floor for sustained periods and appears to be based upon a mouthing methodology developed by CPSC (2014) for toys. The CEM documentation (Page 55) states the numerous uncertainties in the mouthing modeling.

I attempted to run a second CEM model, this one for an indoor crack and crevice treatment of a pesticide. Since there are several chlorpyrifos studies in test rooms and houses, my first goal was to simulate those experiments with the CEM. However, the CEM does not have chlorpyrifos as a chemical ingredient. Rather than import parameters for this pesticide, I scrolled through the list and found that diazinon is in the CEM database and so looked for studies which tested or modeled diazinon in indoor applications. A pesticide indoor modeling paper by Bennett and Furtaw (2004) provided fugacity model estimates for chlorpyrifos and diazinon air concentrations after a test application with actual data provided for chlorpyrifos. Their fugacity model was able to simulate the chlorpyrifos air concentrations in the test house. In trying to use their diazinon application parameters in the CEM I quickly found that there was no pesticide indoor scenario. The closest scenario I could find was "one component sealants and caulks", within which I ran Inh01: Product Applied to a Surface, Incremental Source. Applying the diazinon application information (amount applied, application area and house size) from the Bennett and Furtaw paper to this CEM scenario and running INH01 yielded a peak exposure concentration of 7.7 ug/m3 which was within 2 fold of the reported peak of the fugacity based model from a single application (4.5 ug/m3) (Bennett and Furtaw, 2004). Thus, based upon this one attempt at checking CEM product application results against the literature yielded a confidence-building good fit. However, this is a limited cross-check as the CEM report only provides peak and chronic air concentrations instead of the full temporal pattern as reported in the literature. Further, the CEM does not provide a pesticide indoor application scenario so the user has to improvise which creates uncertainties in whether this is really an appropriate use of the model. It would be helpful for CEM to describe how to adjust the existing scenarios for products and applications not contained within the default array of scenarios.

On Page 25 of the user's manual, Wilkes et al. 1996 is used to support an estimate of 25% in one place and 10% in another for the fraction of applied product that rapidly vaporizes in the double exponential model. This apparent inconsistency should be fixed.

Additional comments post review group teleconference: The comments made by Dr. Ferguson regarding renaming of type of equations as environmental concentration prediction vs dose prediction I think would help, together with a flow chart of how one goes from product or article to contamination of media contacted by humans and then to dose in those humans. I agree with Dr. Ryan especially when he talks about the need for better documentation of models and parameter values, and in fact it would be very helpful to include a bit of mechanistic text to introduce the equations for a given pathway so that the reader knows what's going on physically and knows what the key assumptions are (e.g., boundary layer conditions, diffusional flux in different media, sorption/partitioning based upon organic carbon content of particles and other properties, etc.)

2. **Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios".**

The scenarios represent an impressive array of product uses and household articles, with these scenarios appropriately tied to inhalation, oral and dermal exposure models. The scenario depictions of size of area treated, size of room and house, frequency of application, near and well mixed model, ventilation rates, etc.

appear to be what is necessary to simulate a real world consumer exposure. As described above, the range of scenarios could be expanded to include pesticide crack and crevice treatment given the variety of studies with empirical data to ground-truth the model, mouthing of fabric to become exposed to dyes and flame retardants, and emission of phthalates from additional plastics such as shower curtains and Christmas trees. However, there will always be additional scenarios and products one may encounter that merit consumer exposure modeling. Therefore, it would be helpful if there was a general discussion of how the existing modules could be adapted to unique scenarios and product uses or articles in the home.

Near field modeling is mentioned repeatedly as an option and yet no guidance is given as to when it should be used. I would think that if exposures to young children are being modeled one may want to use the well mixed room model assuming that most cleaning, painting, stripping, pesticidal, etc. products would be applied by an adult and the young child would be somewhere else in the room (or house) rather than in the near field. However, such an assumption is not health protective of children. Guidance on when near field modeling is appropriate would be helpful.

Product Sprayed (Page 17) – would the overspray that is available for direct inhalation differ between aerosol cans and pump bottles used for cleaning chemicals?

DOES THE MODEL COVER PRESSED WOOD OFFGASING? COOKING EXPOSURES? RELEASE OF PERFLUORINATEDS?

**3. Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered.**

The CEM modules are populated by many different equations and parameters. In most cases the uncertainty and variability associated with a model parameter is not described. The product usage modules do contain a low, medium and high range of default estimates for product content and use rate which is helpful to bound estimates. But for many other parameters such ranges are not provided. As described above under Charge Question #1, the uncertainty with using Koa instead of VP-based partition coefficients is not described and the uncertainty of matrix interference with release of SVOCs from articles is also not described, although some of the data presented in Appendix tables B12 and B13 show the potential effect of matrix on diffusivity and emission. Further, the uncertainty and possible alternative values for other parameter defaults (e.g., percent organic carbon in TSP of 0.4) is not described. Finally, the large range in human activity patterns, breathing rates, body weights, dust ingestion rates, dermal parameters, etc. is captured to some extent in the modeling options but a better description of intra-human variability related to age groups and activity patterns would be helpful.

It appears that the low/medium/high scenarios are not necessarily representative of low, medium or high exposure rate as is implied by the labels. For example, App Table B-12, top of Page 87, shows that the high scenario has greater TSP and house dust generation rates than the low scenario. These higher particle generation rates will likely dilute the emitted chemical into a greater mass and thus reduce the concentration in the particle. Further, the high scenario is associated with a higher frequency of cleaning and efficiency of cleaning which would tend to lower TSP and house dust levels. The net effect on chemical concentration mean for these inhalation models.

Seasonality is not considered in the modeling. This could affect temperature, humidity and building ventilation. Phthalate emissions from plastic surfaces and flooring is known to be affected by humidity and temperature. Discussion of such sources of variability would be a helpful addition.

The lack of model calibration and validation against actual data is a source of considerable uncertainty. Greater confidence could be obtained by cross-checking model output for TSP levels, house dust levels, and chemical concentrations in various media, against actual studies from test houses. Under charge question number 1 I provide two such modeling cross-checks, one which did not provide very comforting results (vinyl flooring) and another which did (pesticide application). Other such cross-checks are recommended in an iterative process to improve model reliability and confidence.

4. **CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways.**

It is helpful that the modules provide both an acute peak exposure profile as well as a chronic dose. However, the CADD doses on Page 30 are calculated based upon 1 year of exposure. How does this relate to the chronic averaging of dose needed in risk assessment to compare against an RfD or CPF? If basing exposure upon only 1 year, which year of life for children – the maximal year of exposure? It would also be advantageous for the model to provide dose estimates that are more in line with what is needed in risk assessment to calculate risk for chronic cancer and non-cancer endpoints.

5. **There are several items listed in the "Areas for Future Enhancement" section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term.**

In the above responses I have already made a variety of recommendations for enhancements to the models themselves (iterative calibrations against actual data, cross-comparison to other modeling efforts), to the CEM user's guide, to the computer interface and to variability and uncertainty descriptions. I agree with EPA that enhancements are also possible with respect to shorter term averaging times for products used sporadically and briefly (eg. paint stripping scenario), calculation of LADD to better match up with risk assessment needs, and a variety of other scenarios mentioned by EPA in this section. I also believe it imperative that models include leaching of chemicals from consumer products in relation to food and water uses (e.g., phthalate release into water from plastic tea pots). In terms of chemicals to add, flame retardants, perfluorinated compounds, pesticides, DEHP, dyes, and a variety of other ingredients (aside from phthalate) present in plastic would be helpful.

**Part 2. User Interface**

6. **Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface.**

The CEM is cumbersome to use because of the many scenario-specific and chemical-specific parameters needed to run models. In trying to execute a model it was common to get an error message that some

parameter not particularly germaine to what I was seeking to learn (e.g., film thickness on skin) was missing. It would be helpful if there were simplified ways to run the model, e.g., without all the exposure dose calculations, so that one might focus on the difference between chemicals or use rates on indoor air concentrations.

While the user's manual is helpful, it is not detailed enough for a casual user (e.g., an average risk assessor) to use the model in default mode or to make adjustments to the model with confidence. A bit more background on how the model works in terms of diffusion, boundary layer conditions, partitioning, and exponential decay would help with understanding of what is going on with chemical release, fate and availability for exposure.

The user's manual refers to USEPA's EPI-Suite Version 4.11 to obtain chemical-specific parameter values. However, it is not obvious what information must be known about a chemical (e.g., MW only?) to get the rest of the information needed to run the CEM scenarios. A table of chemical-specific information needed to extrapolate to other higher order information would be helpful. A direct interface with EPI-suite would be an advance so that it would be easy to bring additional chemicals into the modeling with confidence.

In terms of the user interface, I found it disappointing that some parameter values input for a scenario were not saved the next time that scenario was opened, but other parameters were saved. Further, it is unclear why some parameters are automatically provided with a default value and others require one to hit a button requesting an estimated value (essentially a default).

The report produced from a model run is limited, focusing mostly on dose estimates for different pathways and acute vs chronic scenario. Information such as house dust concentration or chemical loading on surfaces would be excellent to have to compare to literature values. Additionally, graphic representation of the time course of air concentrations after a product use would be useful to present.

**7. Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful.**

This is already covered in my response to other questions but I think the main points are reporting of additional data from model runs such as shorter term peak exposures (<24 hr), house dust concentrations of SVOCs and a time course for indoor air concentrations after a product use.

**Part 3. Documentation and User Guide**

**8. Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited.**

References that I cite above are:

Cousins et al. 2014, Sci Tot Env 470-471: 527-535.

Little et al. 2012 – already cited in CEM user manual.

Bennett and Furtaw (2004) Environ. Sci. Technol. 38, 2142-2152.

Xu et al. 2012, ES&T 46: 12534-12541.

**9. Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear.**

My previous responses go into some detail on how the user's manual could be more comprehensive and accessible to a risk assessor.

**COMMENTS SUBMITTED BY**

**P. Barry Ryan, Ph.D.**

## Peer Review of EPA's Consumer Exposure Model and Draft User Guide

### Part 1. Equations used in Models and Exposure Defaults

**1. Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies.**

Overview - Two-Zone Model

The Section entitled: 3. Detailed Description of Models and Equations used within CEM, as the title might suggest, lays out the models used in CEM. The two-zone model diagram and differential equations are clear and represent a standard two-compartment approach affording different concentrations for materials in the near-field and the far-field. At the bottom of Page 20, there are a pair of empirical expressions relating inter-zone exchange for two scenarios- Closed Rooms and Open Rooms. One must assume that the data used to develop these empirical models is sufficiently generalizable to account for most situation, at least at the level of a screening tool, but a reference to the work that developed this empirical expression would be of interest. The variables in the differential equations are defined sufficiently to enable the user to identify them clearly. By and large, the equations used appear sound and rely on fundamental physics. The coupled differential equations will be used extensively as they will determine the air concentration, and consequently the inhalation exposure and dose, in later models.

General Overview of Specific Models

As a general overview of the specific models, the equations, with some exceptions, rely primarily on typical combinations of variable, e.g., concentration, contact time, volumes, etc., that are manifestations of fundamental physics. These are not in question. However, many rely on specific data or specific manuscripts and reports. These need to be made available for users. One might envision a repository or compendium of documents that would be maintained by EPA for this project. As noted in the text, some of the key references are not generally available and it would be useful for the reader to have easy access.

INH01: Product Applied to a Surface Indoors Incremental Source Model Pages 22-24.

What is questionable is the reliance on certain empirical relationships that appear to be based on regression models of data not readily available. For example, in the Section entitled: INH02: Product Applied to a Surface Indoors Double Exponential Model, the emission rate is determined using an exponential decay of emissions with time. The total time for evaporation is given by an empirical relationship developed by Chinn in a DOD reference, i.e., Chinn 1981 reference given as: Chinn, KSK. (1981). A simple model for predicting chemical agent evaporation. Alexandria, VA: U.S. Department of Defense, Defense Technical Information Center, Cameron Station.
http://www.epa.gov/opptintr/exposure/presentations/efast/chinn_1981_a_simple_method_for_predicting.pdf

The link is dead and thus the expression cannot be evaluated. As this is an important reference, the link must be refreshed. I cannot understand the physics that leads to a product of molecular weight and vapor pressure without his work, which appears to be the results of a regression model relating the log of evaporation time with the log of this product. This evaporation times is then used to determine the time

over which 90% of the material has evaporated. This seems feasible from a physical point of view, but difficult to assess.

The next equation references Evans (1994), which will be discussed presently. However, this is a relatively straightforward look at the time dependent emission rate and does not require a reference.

The equation at the top of page 24 has a constant in it, namely $1.33 \times 10^5$. It would be useful to describe this constant, which I believe is a conversion among torr, g/mol, and perhaps other units in order to make the saturation concentration come out to the correct units.

### INH02: Product Applied to a Surface Indoors Double Exponential Model

I have no particular problems with the initial set of equations in this section, but have questions regarding the statements made and the references called. The equation at the bottom of Page 24, appears soundly based, however, the parameters that go into it, most notably, the fraction of material emitted and the exponential constants are less well developed.

The first paragraph contains the text:

> Only 25% of the applied chemical mass is released, because a substantial fraction of the mass becomes trapped in the painted substrate when it dries. Empirical studies reported by (Wilkes et al., 1996) support the assumption of 25% mass released and have estimated a relationship between the fast rate of decline ($k_1$) and vapor pressure ($VP$), and between the slow rate of decline ($k_2$) and molecular weight ($MW$), leading to the equation below for the time-varying emission rate (Evans, 1994).

The references are repeated here to illustrate a problem:

> Wilkes, C; Koontz, M; Ryan, C; Cinalli, C. (1996). Estimation of emission profiles for interior latex paints. Paper from proceedings of Indoor Air '96.
>
> Evans, WC. (1994). Development of continuous application source terms and analytical solutions for one- and two-compartment systems. In Characterizing Sources of Indoor Air Pollution and Related Sink Effects (pp. 279-293). ASTM STP 1287, American Society for Testing and Materials. http://www.astm.org/DIGITAL_LIBRARY/STP/PAGES/STP15627S.htm.

The Wilkes reference is to a Proceedings paper from 20 years ago. It cannot be found anywhere online. The Evans reference is behind a pay wall requiring a payment of $25 in order to get a copy of the paper and an additional $109 for the "Complete Source (pdf)." Yet these two references are essential to the understanding where the empirical emission constants came from in the equation on Page 24 as well as the assumption that 25% of the mass is released while the rest is bound up in the matrix of the surface. This is not satisfactory. These two papers should be distributed as an appendix or kept online with simple access for users of the model. The quality of the modeling equation cannot be determined without them.

While I agree that the concentration must be limited to the saturation vapor pressure of the compound under investigation, one must still ascertain the inflow and outflow concentrations, and the inter-zone flow rates in order to determine rates of evaporation well. We blow on soup to increase evaporation and thereby

cool the hot soup and such an analogy might be included here to explain the process. This is the basic physics of two-zone concentrations here.

### INH03: Product Sprayed

I have no specific comments on this model. I was able to find the Delmaar reference, but not able to find the appropriate version of the EPA 2007 reference. A reference to page and paragraph in this large document would help. The equations for emission rates are similar to INH01 equations.

### INH04: Product Added to Water

While not directly called, this model also makes use of the Chinn empirical equation for Evaporation Time, which cannot be assessed. This model also uses the method of fixing the maximum concentration in air at the saturation vapor pressure and reducing the emission rate so that, when coupled with the inter-zone and overall exchange rate, that the concentration does not exceed saturation. Under some conditions, evaporation would cease. I believe that this is accounted for in the model, but it is a bit unclear.

### INH05: Product Placed in Environment

I have no new comments in this section. This model also makes use of Chinn's empirical formulation of evaporation time and the same treatment of saturation concentration.

### Calculation of Inhalation Dose from Product Usage

The CADD calculation is a standard application used in screening risk assessment. I do have one comment regarding the adaptive time step: there is a big jump that occurs after 24 hours of exposure. In the first 24 hours, the time increment is 30 seconds. This is increased to one hour for the next 59 days. This is a two-order-of-magnitude increase in time step, which seems large. I believe the assumptions is that emission characteristics should be stabilized and flat after this after 24 hours. For a screening tools, this may be adequate, but I think caution is a watchword here as some substances or Articles may require a more adaptive time course. An adaptive time-step algorithm could be invoked here, but it is not my purview to tell the modelers how to do their work.

It is noteworthy that the authors have elected to determine the Potential Acute Dose using the maximum one-hour concentrations observed during the 60-day period. While this is a conservative estimate, I think it is appropriate for this screening tool. In our meeting discussions, this component was addressed. There is some concern about using this approach. I still think it is a valid conservative approach.

### INH06: Article Placed in Environment

Figure 3 on Page 33 gives is a good depiction of the components affecting concentration and dose under these conditions. One might ask for more discussion of the figure for clarifying purposes.

A small point- the use of TSP as nomenclature for particles <10 µm in diameter is not quite standard notation. TSP, when EPA regulated it, included larger particles, perhaps as large as 100 µm. The <10µm particles were referred to as "respirable" particles, or RSP.

The 50% figure for settled particle mass transfer area can be readily seen, but might require a reference or a figure depicting the action.

On page 35 is the first equation in this Section. It relates surface area to volume ratio of the zone. This is an empirical relationship, not a physical one. It requires a reference or a model indicating why the number 2.08, which has units of inverse length, assumed to be meters, is appropriate. At this point, it seems completely arbitrary.

On Pages 36 and 37, there is a series of differential equations giving emission rates, denoted as change in particle number, for various emission surfaces. These are difficult to understand and would be quite a bit more transparent if there were explanations of the terms. For example, the very first equation includes a term:

$$\frac{A_{TSP}}{\rho_{TSP}} \text{ X } \frac{3}{r_{TSP}}$$

I looked at this, and the equations that followed trying to figure out where the constants 3 and 1. 5 came from; is the physics appropriate? After some manipulation, I realized that the term is conversion of volume to area assuming a spherical particle. The equation would have been much clearer if the Area had been put in and a notation used that effected the conversion, e.g.

$$\frac{\text{Mass of TSP}}{\text{Density of TSP}} = \text{Volume of TSP}$$

$$\text{Surface Area of a Sphere} = \text{Volume of a Sphere X } \frac{3}{\text{Radius of a Sphere}}$$

The concept is simple, but not at all transparent when one skips the steps. The 1.5 constant indicates particles on a settled surface that then emits only in the upward direction. This is also appropriate, but there is no need to make the equations so opaque. The equation is appropriate, as are all of them others with "3" in them as the surface area is the appropriate variable for emission of SVOCs bound to the surface of particles. But why make is so difficult to understand, especially in light of the central nature of these equations to the model?

At the bottom of Page 38 is the equation:

$$D_s = \frac{0.00000000003}{(MW \div 292)^{0.65}}$$

Why do the authors choose to use the long decimal number instead of scientific notation, i.e., 3 x $10^{-11}$? I found myself counting zeroes, for no good reason, again obfuscating the use of the equation. I do note the use of scientific notation for the same number on Page 39 and the definition of the value as the diffusion coefficient of PCP-52, the reference compound, which has a MW of 292 g/mol. At least in this section, the EPA document references as USEPA 2005, is readily available for download. Note that this relationship probably came from a regression model as well. A simple Graham's Law of Diffusion approach would have the exponent on the denominator as 0.5. The last sentence on page 39 gives the default assumption for surface diffusion thickness as 0.005 m, and supports this with three references. It would be nice to get an assessment of the variability in this parameter and perhaps a sense of the sensitivity of results to this assumption. However, for a screening tool, this is likely accurate enough.

### Calculation of Inhalation Dose from Article Exposure

I have no comments in this section; the equations seem quite appropriate given the correct values for input.

### ING01: Product Applied to Ground Outdoors

The first reference in this section, USEPA 2012b, is readily accessible for download. In addition, the equations appear appropriate from a physical point of view. I have no additional comments.

### ING02: Product Ingested via Swallowing

The first reference in this section, ACI 2010, is readily accessible for download. In addition, the equations appear appropriate from a physical point of view. They are typical of screening equations used in risk assessment for other types of exposures. I have no additional comments.

### ING03: Article Ingested via Mouthing (Migration Rate Method)

The primary reference for this section USCPSC 2014, is readily downloadable. However, the reference focuses on phthalates for baby toys and similar items. One may question the validity of the application to other materials. Can the authors justify the leap from phthalate exposure to other exposures? Further, the so-called "migration method" may be operable on some materials, while a "bound-to-surface approach" maybe more valid on others. I would speculate that the user would select one or the other of these and evaluate the differences noted. Nonetheless, I believe the model to me adequate for the purposes of screening and offer no further comments. The dose equations are typical of screening equations used in risk assessment for other types of exposures.

### ING04: Incidental Dust Ingestion (Article Model)

This model presents no new modeling approaches. It is similar to the other ingestion models discussed just above. I believe the model to me adequate for the purposes of screening and offer no further comments. The dose equations are typical of screening equations used in risk assessment for other types of exposures.

### ING05: Ingestion after Inhalation (Article Model)

This model is modestly more complex in that it includes an inhalation component. However, it is relatively straightforward and similar to other models used in risk assessment for exposure and dose. I have no further comments.

### DER01: Product Applied to Skin (Fraction Absorbed Method)

Dr. Ferguson is the expert on the panel in dermal exposures. I defer my comments to her extensive review.

The primary reference for this section is, again USEPA 2007. I was unable to download the appropriate version of this reference and thus cannot fully evaluate the model. However, see below.

The equation at the bottom of Page 47, uses the term D, which is confusing given equations above that use D as a diffusion coefficient. In the legend for this equation "Dens" is used and it is defined as "density." Density is usually symbolized as ρ (Greek letter rho), in is, in fact, symbolized this way in other parts of the manual. Others commented on this problem as well, further suggesting editing the document for symbol consistency throughout. The rest of the equations used in this model are fairly straightforward and similar to those used in other exposure/dose screening models. I have no further comments.

### DER02: Product Applied to Skin (Permeability Method)

I was not able to find the expression for Kp in the first reference in this section, USEPA 1992, despite the reference being relatively easy to download. Hence I cannot fully evaluate the model. However, the expressions used are fairly straightforward and similar to those used in other exposure/dose screening models. I have no further comments.

### DER03: Article where Skin Contact Occurs

There are three references cited in the first sentence of this section. ECETOC 2012 requires membership. As I am not a member, I cannot evaluate it. USEPA 2012b is readily downloadable from EPA. Delmaar 2005 is readily available from RIVM. Regardless, the equations used are fairly straightforward and similar to those used in other exposure/dose screening models. I have no further comments.

### DER04: Article with Direct Transfer from Vapor Phase to Skin

The principal reference for this model is a paper by Weschler and Nazaroff obtainable from Environmental Science and Technology. Their equation for penetration the stratum corneum is a regression model they have developed. It is well described in their paper. This is the type of reference the modeling section needs, i.e., one that is readily available and can readily be evaluated. The remainder of the equations are standard flux equations based on relatively straightforward physics. I have no further comments.

**2. Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios".**

The scenarios available are extensive and range throughout typical activities encountered by individuals in their daily activities. I did not explore each and every scenario, activity, and default values, as that would have required modeling runs numbering in the thousands. However, the ones I did explore appeared to have default values that were, at least, reasonable, and quite adequate for the screening tool design of the CEM. Data sources appeared quite complete, given the caveat that not everyone could be explored in the allotted time.

As is the case with the models themselves, I am concerned that some of the data may be from sources not easily evaluated such as reports, proceedings presentations not later published in the peer-reviewed, etc. USEPA should strive to document these as well as can be done and develop a library of such data in readable format for downloading and evaluation.

The MSExcel spreadsheet includes an extensive list of Products, Articles, and Functional Use Categories, with 88, 79, and 123 items listed respectively. The worksheet labeled "Product cat_Scenario Overlap" offers a useful compendium of cross-referenced Product Categorist and usage that should aid the user in selecting appropriate scenario, activities, articles, etc.

The discussion in the meeting requested both more scenarios and fewer scenarios, which is obviously contradictory. Personally, I think a simpler approach- one with a limited number of scenarios- is the way to go, but some of my colleagues thought otherwise. I am just putting my vote in.

**3. Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered.**

The approaches presented in the CEM are deterministic in nature and thus contain no information on variability and uncertainty. I saw no way of implementing such beyond the brute-force method of varying input parameters by hand to assess the impact of such. I think the approach followed here is appropriate for a screening method. It could, perhaps, be modified to reflect calculations of uncertainty and variability, but the CEM is complicated enough as it is and would be complicated substantially by further modification to include this type of analysis. I think that most users of CEM would be interested in measures of central tendency or high/screening values that could be modeled directly. The CEM does have the ability modify the input parameters to simulate variability and uncertainty through direct changes in input parameters, but I do not think that this is essential to the utility of the system. The system is meant to be a screening tool and I think uncertainty and variability in a screening tool may be misplaced. More sophisticated models may be required as the uncertainty introduced by taking conservative parameter estimates and models is large and would likely dominate.

**4. CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc.). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways.**

All of these exposure metrics are important depending on the context. Specific activities of the various age groups influence which are considered most important. Since these are commercial products, most would be used by Adults. However, the Child and Youth categories are also important. I will express concern that the latter two categories may be too broad. Activity patterns for the Child category differ widely over the age range (1-10 years) with differential skin contact for many compounds varying substantially. In the Youth category, the older ages may actually experience activities similar to Adults in that they will be using some of the same Articles and Products, as Adults in the same way. Further, Adults, themselves, may experience use of Commercial Products differently as they age- particularly after age 65. All of these shortcomings may be overcome by using user-inputted data, but more flexibility on the scenarios, activity patterns, etc., including default values for other categories may be of utility, especially in screening scenarios. But see my updated comments on increasing the number of scenarios.

One may reasonably argue that the screening nature of CEM precludes the need for more detailed scenarios as outlined above. This argument has some merit as long as the default values selected represent, if not worst-case scenarios, at least high-end exposure scenarios for all classification of individuals. Under this umbrella, the screening tool can give results that, if shown protective, are sufficient. Potentially, however, they may give “false positive” results that require further exploration. Balance must be maintained and such balance is precarious.

**5. There are several items listed in the “Areas for Future Enhancement” section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term.**

Several Areas for Future Enhancements are presented in the User's Manual. Essentially all are feasible and their implementation is based on the needs and expectations of future utility by USEPA. I will comment on them individually and give my assessment of the need and utility of each. Data sources are varied for the enhancements. I have no special knowledge of specific sources for the data needed to develop the specific enhancement, however.

My personal preference, not discussed here, is the ability to perform variability assessments and uncertainty evaluations before implementing any of these modifications of CEM. However, this must be tempered by the increasing complexity of such a system. Even implementing the strategies suggested below in a deterministic fashion will complicate an already-complicated system to a significant degree. Such modifications should be evaluated cautiously. It would be easy for this system to become complicated enough to overwhelm the typical user and reduce its usefulness in the field.

### Exposure Metrics for Short-term, Chronic, and Lifetime Exposure

It would seem that this is the next logical step in the development of CEM. Estimates of shorter- and longer-term metrics would be a relatively straightforward modification and could be of interest to many users. Implementation would not result in substantial complication of the model as viewed by the user as it would simply be a few more boxes that could be checked in the Input section. This would be a useful addition. Further, I believe the implementation would not be overly difficult, which would clearly be a desirable trait. However, USEPA has "carved in stone" the acute, sub-chronic, and chronic temporal exposure regimes, and modification may not be possible at this time for USEPA use. But other Agencies and researchers may find other temporal regimes of interest.

### Articles in Routine Contact with Water

While certainly of interest, I believe this component would be of lower priority than some others as the number of Articles that fit under this rubric would likely be limited and not commonly implemented. Further, data may not be ready available to develop the modeling approaches. I would give this lower priority.

### Products Intended to go Down the Drain

Again, this could be an interesting addition to the CEM and is receiving interest in, for example, medical waste and endocrine disrupting chemicals. However, as pointed out in the text, while the model addition as shown in the text, is straightforward, the data to support some of the parameters is lacking. Given this, I would place this at lower priority as well.

### Vector-Facilitated Releases from Articles Not Intended to go Down the Drain

As reported in the text, data are emerging on this subject. Further this may be tied in with para-occupational exposures in the home and elsewhere. There was lively discussion of para-occupational exposures on our conference call. This may be an important additional scenario, at least it light of that discussion. Such an implementation is of intermediate priority, but it is my opinion that the data are not yet available to develop the modeling parameters. However, they are likely to become available in the next few years upon which time implementations could be done. I suggest developing the modeling components- equations, data reduction methods, etc., but wait for better data prior to implementation.

### Products that Spill or Leak Over Time

Implementation of this component should be of lower priority as it requires an unusual set of circumstances to be operational. I recommend waiting on this one. Data may become more available with time and, if it is deemed an appropriate measure, a set of modeling equations could be developed. I do not think such a system is currently available.

### Elevated Temperatures During Application and Use

I had not considered this aspect at all in evaluating the models used in CEM. Essentially all of the approaches may want to consider these temperature-related effects in some fashion. Such an implementation would be quite difficulty, however, as one would need to develop, for example, a temperature profile over seasons for the application of materials and subsequent volatilization. Changes in vapor pressure and Henry's law constants as a function of temperature are notoriously difficult to model. At least one reviewer expressed the need for Henry's law approaches as opposed to Raoult's law (vapor pressure) approaches. Regardless, both have temperature dependence that is not well characterized for most compounds of interest. Further, emissions associated with personal care products must take into account interaction with body-cooling mechanisms such as sweating. This is quite complicated and I am not at all sure on what data exist. I think this is a higher-priority item, but that implementations would be especially difficult and may require substantial work to ascertain their utility.

### Consideration of Multiple Zones in the SVOC Article Model

Multiple zone models are relatively easy to design but require substantially more data to implement than single-zone or two-zone models as one must ascertain the zones that are interacting. Implementation is straightforward, but the data to support such implementation is not readily available. I agree with the statement made in the text, that such a system should be implemented when data become available but the complexity goes up like the square of the number of zones. I do not see such data becoming general available for multiple locations in the near future and even if it does, the applicability goes down quickly as they models become more focused on a single scenario rather than generally applicable. This observation places the implementation of such a modeling system on a lower priority.

### Consideration of Chemical and/or Age-Specific Transfer Efficiencies from Surface-to-Hand, Hand-to Mouth, and Object-to-Mouth

Again, Dr. Ferguson is the expert and I defer to her judgement. I discussed this in a general sense early in my review. Generally, I think that there is substantial variability in age groups on any of the parameters in CEM. The Child age group is too wide, and the Youth age group needs further examination. Toddlers are very efficient in transferring materials from hand to mouth and the system CEM should make use of such knowledge. This may be the first priority of modification of CEM.

### Consideration of Chemical or Material-Specific Migration Rates

Implementation of this rubric may open an extremely large can of worms as I can see no place to stop. Materials, Articles, etc., may have to be considered almost on a unit by unit basis increasing the complexity of the model exponentially. I would punt on this one as CEM is a screening tool, not the be-all and end-all model. It may be possible to increase complexity in a manageable fashion by classifying Articles and Materials into general categories to keep the complexity manageable, but the categorization itself would be

problematic. I would put this at low priority not because of its perceived lack of importance, but rather because of the difficulty of implementation.

### Consideration of Total Ingestion Rates of Indoor Dust and Particles

There is consideration in the text of variability and uncertainty in implementing this component. I do not think data exist to look at variability and uncertainty in this parameter or many others. I would not consider implementing this at this time. Should more data become available, one could reconsider.

### Absorbed Dermal Dose

Again, Dr. Ferguson is the expert and I defer to her judgement. This approach could be readily implemented by offering a different check box in the input section. Data are available for many of the needed parameters and are already stored in the chemical compound section. Assuming that models of dermal dose are good, the implementation is relatively straightforward, then it becomes a higher priority. This is a simple, deterministic alternative to what is already available for implementation.

### Consideration of Additional Exposure Scenarios and Exposure Defaults

There is little to add to what has been said in the text. As more data are gathered, more scenarios can be implemented. Further, more Articles, compounds, and activities could be implemented as well. This should be an ongoing activity with modifications of CEM occurring on a regular basis. The priority is high and continuing for this modification. But caution due to increasing complexity is important. Maybe develop a simpler model with limited scenarios that account for much of the population exposure and reserving additional scenarios to a larger model is an appropriate strategy.

## Part 2. User Interface

**6. Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface.**

The user interface is complicated and, at times, proved difficult to use. I found myself often having to readjust the screen so I could see the top row. Admittedly, there are explicit instructions to do this, but it was annoying. There are a large number of input lines on multiple screens. It is quite easy to miss one (or more) of these. Fortunately, when the “Run CEM Models” button is hit, the system does a quick scan and tells you what you have left out. As I became more familiar with the interface, I was able to navigate more quickly to the correct location, but at the beginning this was cumbersome and frustrating. If one runs the model a few dozen times, it becomes more intuitive, but the “intuition” must be learned.

I have no real ideas on how to improve the interface. There is a lot going on, and a lot of things must be done to get useful information out. The menu of compounds, activities, articles, scenarios, etc., is extensive. Thus it is difficult to see how the process could be streamlined without eliminating the flexibility. The authors have made an excellent effort in dividing tabs up into related areas so that the user, if s/he is systematic in the approach to the CEM system, can streamline the process her/himself.

One thing that may be of use is, when the scan for missing data is done, categories that require additional input could be highlighted somehow. The system tells you which model is problematic, and which parameters are missing, but when you go to that model, you have to hunt around for the parameter of

interest, often re-running the model to get the error back up and follow it through. I would really like to see this implemented- and it should be pretty simple to do sao as the items missing have already been identified.

**7. Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful.**

Batch mode would be useful as the number of input values is large and one would like to evaluate the effect of certain changes. This can be accomplished by building upon an existing scenario, but the batch approach would be useful a well. I am not familiar with the capabilities of MSAccess in this regard, but if it would be relatively easy to implement. This could be a way of assessing uncertainty in the model a well by affording a method of quick entry of data varying an input parameter. Variability might also be assessed most easily with a batch mode method but one would have to know about distributions of parameters.

Operating in batch mode or even "inline," it could be useful to be able to direct the Save commands to a directory at the beginning of a session and have all the Report files show up there.

Although I am not sure what the format would look like, a graphical output system would be useful a well. A sheet containing appropriate input data and, perhaps, bar graphs of the output of various run scenarios in graphical form would be a nice package to have. This may not be implementable as I do not have any idea that a graphical input would be short of bar charts instead of numbers.

**Part 3. Documentation and User Guide**

**8. Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited.**

See discussion under Charge Question 1.

I have identified at least one broken link and a couple of instances of references being behind a (substantial) pay wall. I think that EPA should obtain a "fair use" license to distribute these references and others from a website at EPA. As an academic, I have access to most journal references. However, others not affiliated with a large University may have a much more difficult time getting references and evaluating the appropriateness of the various equations used. If USEPA is the sole target for this model, then it would be easy to have a private website for EPA staff only. But such a restriction would limit the use of the CEM and diminish its worth.

Other than the broken links, I did not identify any references that were inaccurately identified.

It would be useful in the models description section to identify where in the specific reference, e.g., page number, the given equation might be found. Some of the USEPA references are a couple of hundred page long and identifying the specific section and page number associated with a given equation was, at times, impossible. This is less critical when a particular published paper is referenced as such papers are typically 10 pages long rather than 200.

**9. Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear.**

I found no problems in this area. The User Guide presented all the equations for the models and these are repeated in the help screens that I encountered. As I did not open each and every possible help screen, there may be some that were not covered, but they were quite complete in what I saw.

As outlined in my response the Charge Question 1, certain of the model presentations were cryptic and could be improved markedly with a bit more explanation, and perhaps partitioning equations into parts then putting the parts together. This would add to the clarity of the presentation substantially and reduce frustration on the part of the novice user. However, I believe that many users would simply assume that USEPA had "done it right" and not dive into the equations at the level of a reviewer of the CEM might. This may be a dangerous assumption and many users would like the details before relying on the model for any specific purpose.

A suggestion for presentation of the User's Manual might include separating the section describing the details of the models into an appendix but including a brief description of each model where it is now but leaving out the detailed equations. That is, use a text description of the model and refer the User to the appendix for details. I am not clear on how this might best be done, however.

**COMMENTS SUBMITTED BY**

**Woodhall Stopford, M.D.**

## Peer Review of EPA's Consumer Exposure Model and Draft User Guide

### Part 1. Equations Used in Models and Exposure Defaults

**1. Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies.**

Outside my area of expertise

**2. Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios".**

A major oversight in the scenarios is for exposures to dusty materials or solid aerosols such as ceramic clays and glazes. Exposures to such products have been associated with lead exposures and/or poisoning in homes, schools, work places and nursing homes as well as exposures to crystalline silica and fibrous talc in studios and schools. Data on exposures can be found as follows:

Roth WR, Stopford W. Classroom Contamination from Lead Bearing Ceramic Art Glaze. 2007.
http://duketox.mc.duke.edu/EIA_Rev_4.doc

Stopford W, Turner J, Cappellini D. Determination of the Magnitude of Ceramic Glaze to Skin and Skin to Mouth Transfer. August, 2007
http://duketox.mc.duke.edu//ceramicglazetransfer.doc

Stopford W. Aerosol Production During the Use of Art & Craft Materials. Submitted to Consumer Product Safety Commission. 2003.

http://www.duketox.mc.duke.edu/recenttoxiissues.htm

Stopford W, Stanion C. Potential for Lead Dust Exposure During the Operation of Contemporary Ceramic Studios. Research Report Submitted to the American Society for Testing and Materials in Support of Test Method C1023, Labeling of Ceramic Materials for Chronic Health Hazards, 1998.
http://duketox.mc.duke.edu/CERAMICSlead.rtf

An alternate model for assessing peak exposure and average exposure over time is the general dilutional ventilation equation:

$C_t = C_i e^{-Qt/V}$

Where: $C_t$ = concentration (mg/m$^3$) at time t
$C_i$ = initial concentration
Q = Ventilation rate (m$^3$/min)
V = room volume (m$^3$)

This model has been used to determine peak exposure and average exposures to a number of aerosols and solvent vapors as summarized in the following article:

Stopford W. Aerosol Production During the Use of Art & Craft Materials. Submitted to Consumer Product Safety Commission. 2003.
http://www.duketox.mc.duke.edu/recenttoxiissues.htm.

This model was confirmed for exposure to marker solvents in the following paper:
Stopford W. Solvent Exposure from use of Whiteboard Markers. Submitted to CPSC.
http://www.duketox.mc.duke.edu/recenttoxiissues.htm. 2003

3. **Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered.**

Outside my area of expertise

4. **CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways.**

We are currently looking at skin exposure from the use of pastels, spray paints and airbrush paints. To assess risk of dermal effects (allergy and irritation), we are specifically looking at skin exposure in terms of micrograms of toxicant per $cm^2$ of skin. This approach is documented in the following article:

Stopford W. Protocol for the assessing dermal exposures while using pressurized aerosol sprays, airbrushing and drawing with pastels. 2014.
http://duketox.mc.duke.edu/dermal%20exposure%20to%20aerosols%20protocol9.doc

We have used both surveys of populations representative of the US both geographically and economically as well as user questionnaires to determine use patterns for various types of art materials. For spray aerosols use by artists, see:

Stopford W, Miller JS, Smith KN, Bosserman W. Solvent Exposure to Graphic Artists. Submitted to CPSC.
http://www.duketox.mc.duke.edu/recenttoxiissues.htm. 2002

For pastel use by artists, see:

Brock T, Stopford W. Bioaccessibility of metals in human health risk assessment: Evaluating risk from exposure to cobalt compounds. J Environ Management. 2003; 3(5):71N-76N.

5. **There are several items listed in the "Areas for Future Enhancement" section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term.**

*Exposure metrics*

For consumer exposures it is very important to know the peak inhalation exposure. Peak exposures to some sensitizers, such as diisocyanates, are the expected inducer of a sensitization reaction. Once sensitized,

however, determination of acute, daily exposure will provide data on the likelihood of a reaction to the environment.

For assessing cancer risk, determination of both a working lifetime (usually 40 or 45 years) and lifetime exposure would be needed.

*Vector-facilitated releases*

Skin or clothing contamination with materials that vaporize, such as solvents or mercury, can be the primary source of exposure both in the workplace and home. For one example of this type of exposure, see:

Stopford W, Bundy SD, Goldwater LJ, Bittikofer JA. Microenvironmental exposure to mercury vapor. Am. Industr. Hygiene Assoc. J. 1978; 39:378-384.

*Hand-to-mouth and object-to-mouth transfers*

We have collected data of the efficiency of hand to mouth transfer of the following:

Solid film (phthalates)

Pastes (polymer clays), see:

Stopford W, Turner J, Cappellini D. Determination of the Magnitude of Clay to Skin and Skin to Mouth Transfer of Phthalates Associated with the Use of Polymer Clays. 2003. Submitted to CPSC. http://duketox.mc.duke.edu/polymerclayresults2.pdf

Liquids (glazes), see:

Stopford W, Turner J, Cappellini D. Determination of the Magnitude of Ceramic Glaze to Skin and Skin to Mouth Transfer. August, 2007
http://duketox.mc.duke.edu//ceramicglazetransfer.doc

We have also looked at metal exposures from mouthing in the following paper:

Stopford W, Cappellini D. Bioaccessibility of Lead in Metal Pen Tips. Submitted to CPSC, 2009.
http://duketox.mc.duke.edu/recenttoxissues.htm

**Part 2. User Interface**

**6. Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface.**

The user interface is excellent. I particularly like the following:

- notices of what was overlooked during entry
- quick explanations for input parameters
- estimate tool

**7. Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful.**

One change that needs to be considered is defining the following in the report on exposure factors:

BW

Past_ing

Inhal_after

SABW_body

TC

**Part 3. Documentation and User Guide**

**8. Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited.**

Although USEPA (2007) E-Fast documentation manual is no longer available on line, the current manual (2014) is available at https://www.epa.gov/tsca-screening-tools/e-fast-exposure-and-fate-assessment-screening-tool-2014-documentation-manual

I am unable to find ECETOC's targeted risk assessment user's guide, though their model is readily available.

**9. Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear.**

On page 15 of the Draft User Guide, the authors note that:

"Primary sources of data methods or assumptions: Please see the "Product Properties Sources" look up table on the lookup tables and VBA Code tab for further information on parameter source information specific to each product."

The version we are reviewing has no such VBA Code tab or lookup tables. The appendices, however, are excellent giving the documentation for sources of mass data, duration data, frequency data and aerosol fraction data used in the models.

It would be nice to see similar documentation for environmental inputs, particularly for:

Building volume

Use environmental volume

Default air exchange rates (by zone and near field boundary)

**Additional Comments**

Background

*Markers*

I have completed an in depth study of exposures to solvents from the use of solvent-based whiteboard markers to address a concern raised by CPSC of the potential for excessive exposures with use of this type of consumer product either at home or in the classroom Stopford, 2003). Studies were done with up to 5 users in an unventilated room (0.4 air changes per hour) and with up to 4 users in a school room with a recirculating ventilation system (0.5 air changes per hour). The solvent system in these markers was a mixture of methyl isobutyl ketone (MIBK) and n-butyl acetate (NBA). Solvent consumption was determined by measuring marker weight loss. Exposures were measured in the breathing zone and at a background site with 3M Model 3500 samplers. Users drew for 30 minutes and then the sampler was moved to the background site for an additional 3.5 hours.

Measured personal exposures to MIBK for one user (30 minutes use plus 3.5 hours background) were 1.8 mg/m3 for classroom exposures and 3.8 mg/m3 for exposures in an unventilated room. For NBA, personal MIBK exposures were 0.67 mg/m3 for classroom exposures and 1.1 mg/m3 for exposures in an unventilated room. Modeling using the general dilutional ventilation equation was done to determine peak and average exposures. The highest average individual solvent consumption rate per user (424 mg for MIBK and 193 mg NBA per user) was used to determine exposures. For MIBK peak exposures using this model were found to be 1.69 mg/m3 in the ventilated classroom and 1.58 mg/m3 in the unventilated room. 4 hour average exposures were found to be as follows:

| | MIBK (mg/m3, measured) | MIBK (mg/m3, model) | NBA (mg/m3, measured) | NBA (mg/m3, model) |
|---|---|---|---|---|
| Classroom | 0.45 | 0.75 | 0.33 | 0.34 |
| Unventilated room | 1.52 | 0.94 | 0.28 | 0.43 |

Assuming a workplace inhalation exposure rate of 1.25 m3/hour for 40 hours a week and a body weight of 80 kg, the above would result in exposures of:

| | MIBK (mg/kg/d, measured) | MIBK (mg/kg/d, model) | NBA (mg/kg/d, measured) | NBA (mg/kg/d, model) |
|---|---|---|---|---|
| Classroom | 0.040 | 0.067 | 0.029 | 0.030 |
| Unventilated room | 0.136 | 0.084 | 0.025 | 0.038 |

*Spray Paints*

I have looked at exposure to spray paints using the following parameters: 47 m3 room with 1.1 air change/hour; measurement of exposures after filling out 6-12 sheets of artist paper per session with a total of 6 sessions; measurement of skin exposure using Ti as a marker with testing of Tyvek suits and nitrile gloves; measurement of air exposures using 10 micron personal exposure monitor, a PMA 10 in room monitor and a total particulate monitor in the room exhaust. Skin exposures to hands averaged 326 micrograms/cm2 and to total body (minus hands) 45.5 microgrms/cm2. No inhalation exposure was measured with the personal samplers or the PM10 monitor. The average total paint particulate levels

released to the room were 37.3 mg/session. Each session lasted 30 minutes. Each session consumed 26 gm of paint of which 5.7 gm was solvent.

Consumer exposure models

Markers

The above maximum highest average solvent consumption figures were used to test each consumer exposure model. The input parameters do not include markers or writing instruments. I used SOLVENT-BASED WALL PAINT as a default. Additional parameters used were as follows:

Environment of use: school/office

Users: adult

Background 0 mg/m3

User defined emission rate: 53 mg/hr (424 mg/8 hr)

Duration of use per event: 30 min

Mass of product used per event: 0.424 g

General comment: the chemical look up is very difficult to use by chemical name. It would be quite useful to allow look up by CAS# as well.

Spray Paints

For the solvent exposure, I used the Aerosol Spray Paints product type. I assumed an adult was using the product in a utility for a 30 minute interval and then stayed in utility room for 8 hours. 5700 mg of solvent was emitted in 30 minutes.

Results

INH02 (markers)

No near field area in zone 1: adult acute inhalation: 4.33-5.05 mg/kg/d.

Comment: these results are a factor of 100 fold greater than would be expected from exposure to solvent-based markers. It would appear that it would be prudent to develop a consumer product category for markers and writing instruments.

INH03 (spray paints)

There is no option to run this model for just for paint aerosols (no chemical identified). I added titanium dioxide (the marker in our studies) as a chemical for testing this model. All inhalation and dermal exposure parameters were 0.00E+00.

For solvent exposure, using the general dilutional ventilation equation (Brock and Stopford, 2003), the peak exposure was found to be 94 mcg/m3, the 8 hour average exposure was found to be 13.8 mcg/m3. Using the INHO3 model, and a garage with typed in values for duration of use (30 min) and mass of product used, the acute and chronic inhalation results were 0.00E+00., When using drop down values (45 min and 200 g/use with a dilution fraction of 0.22 inhalation exposures were calculated to be as follows:

Peak exposure: 595 mg/m3 (program defined emission rate)

2790 mg/m3 (user defined emission rate)

Comment: The peak exposure is a factor of 6000-30000 greater than expected

DER-01 (markers)

Acute dermal: 132-184 mg/kg/d, limited to hands

SA-BW ratio limited to both hands in youth (11-20 yo) in cm2/kg. youth 16-20 yo 71.6 kg, 11-15 yo 56.8 kg.

Comment: using a two hand skin area of 820 cm2 (Stopford, 2014), the above exposure would result in a dermal exposure to hands of 2.8-3.1 mcg/cm2.

DER-02 (spray paints)

There is no option to run this model for just for paint aerosols (no chemical identified). I added titanium dioxide (the marker in our studies) as a chemical for testing this model. All inhalation and dermal exposure parameters were 0.00E+00.

For solvent exposure, acute dermal exposure was 0.16 mcg/kg/d. For an adult, the SA/BW ratio was 12.4 cm2/kg for both hands. For an 80 kg adult, skin exposure to the hands would be expected to be 59 mcg/cm2.

Overall Assessment

The CEM models I evaluated were deficient in the following areas:

1. Lacking exposure scenario for markers writing instruments, pastels and chalks and ceramic clays and glazes.

2. Inability to enter non-volatile chemicals under chemical of interest. There is the ability to enter dust parameters for models INH06-ING04. I suspect this input could be modified to include dusts/aerosols where there is indoor exposures.

   An alternate would be to develop the general dilutional ventilation equation as a CEM model. This model could be used for determining peak exposures as well as exposures over time to both volatile chemicals as well as respirable particles.

References

Brock T, Stopford W. Bioaccessibility of metals in human health risk assessment: Evaluating risk from exposure to cobalt compounds. J Environ Management. 2003; 3(5):71N-76N.

Stopford W. Solvent Exposure during use of Solvent-Based Whiteboard Markers. 2003. http://duketox.mc.duke.edu/mibkmarkerstudy.pdf

Stopford W. Protocol for the assessing dermal exposures while using pressurized aerosol sprays, airbrushing and drawing with pastels. 2014. http://duketox.mc.duke.edu/dermal%20exposure%20to%20aerosols%20protocol9.doc

**COMMENTS SUBMITTED BY**

**Stephen T. Washburn, M.S.**

## Peer Review of EPA's Consumer Exposure Model and Draft User Guide

### Part 1. Equations Used in Models and Exposure Defaults

**1. Are the mathematical equations used in the modules of CEM adequately explained? Are they appropriate and accurately executed? Specifically, note any areas where errors were found, areas for improvement, or alternate calculation methodologies.**

In general, the equations used in the CEM are well explained, appropriate for the purposes of this model, and accurately executed. Note that I have not had the time to check to make sure that each equation in the CEM user guide is correct or agrees with the cited reference.

For modules that estimate volatilization of organic chemicals from water (e.g., INH03), I recommend that EPA consider models based on Henry's Law (using Henry's Law Constants) instead of Raoult's Law (using Vapor Pressure) when evaluating relatively low contaminant concentrations. While both Henry's Law and Raoult's Law are ideal vapor-liquid equilibrium relationships that are relevant to dilute component mixtures, Henry's Law tends to better approximate volatilization of the solute (i.e., lower concentration component) and Raoult's Law tends to better approximate volatilization of the solvent (i.e., higher concentration component). Raoult's Law assumes an ideal mixture and can result in much less accurate results than Henry's Law for dilute solutions of a contaminant (e.g., aqueous solutions of a chemical susceptible to hydrogen bonding).

Additional comments regarding inputs to the models are provided below.

**2. Comment on the breadth and depth of scenarios contained within CEM. For consumer product and article scenarios, comment on defaults and associated data sources used in the model. Specifically, are the default assumptions reasonable and adequately supported by relevant scientific data? If appropriate, provide suggestions and references for alternate default assumptions and associated references. Please refer to the excel file "Use Categories and Descriptions for CEM Scenarios".**

The breadth of scenarios contained within the CEM is impressive and actually a bit overwhelming, particularly given the large number of products and articles that are also included. While I have not tested all combinations of chemicals, products, articles and scenarios, some clearly represent relatively lower potential for exposure, are less common, and/or are based on less established modeling approaches. I recommend that EPA strongly focus the initial version of the CEM on a smaller number of scenarios, articles and products that under most exposure conditions are likely to be the most significant or most common, and put effort into refining those scenarios rather than attempting to be as exhaustive as the version release for peer review.

Although the current list of products is relatively exhaustive, cosmetics is conspicuously absent. Unless cosmetics are being addressed separately by EPA, I recommend that they be included in the current CEM or, at a minimum, be a top priority future enhancement.

Regarding the scenarios that are included in the CEM:

- Products appear to be limited to "consumable liquids, aerosols or semi-solids". What about powders, such as dishwashing powder or abrasive cleaners?

- Explain why SVOC emissions, but not VOC emissions, are evaluated for articles while presumably both VOCs and SVOCs are evaluated for products.
- Why are metals and other essentially non-volatile chemicals not included for any products or articles? They could be particularly important when evaluating exposure to particulates.

In most instances, references are provided for default values or approaches. Some exceptions appear to include the following:

- p.19, Section 3. Reference or basis for 60-day emission period needed.
- p. 33. Reference or basis needed for assuming that 100% of the area is available for suspended particulates and 50% is available for settled particulates
- Table B-2. Reference or basis needed for film thickness values.
- Appendix B should provide all default physical-chemical property data with references. While some physical-chemical data are provided (e.g., diffusion coefficient), others are not (e.g., vapor pressure).

How frequently will the database of physical-chemical data for individual compounds be reviewed and, as necessary, updated? Who will be responsible for making sure that the physical-chemical database is maintained and reflects the current scientific literature?

**3. Does CEM consider variability and uncertainty for both defaults and calculation methodologies adequately? Specifically, note any areas where variability and uncertainty could be further considered.**

Overall, the CEM does an acceptable job of considering variability and uncertainty – especially and primarily because it allows the user to readily conduct his or her own sensitivity and uncertainty analyses by entering alternatives to the defaults. I believe this is one of the chief values of the CEM. I do not believe that we have sufficient data to conduct reliable probabilistic (Monte Carlo) simulations for most components of the model and thus do not recommend that additional level of complexity. However, I think the User Guide should include a separate sections that emphasizes the variability and uncertainty in the models and their inputs, and the results summaries should also distinguish between default, model-calculated and user-supplied inputs.

**4. CEM contains several exposure metrics (acute dose rate, time-averaged air concentration, chronic average daily dose). Other exposure metrics could be reported as well (Lifetime Average Daily Dose, loading present on skin, intake per day, etc.). Please comment on which exposure metrics are most appropriate for use in considering different age groups, exposure scenarios, and exposure pathways.**

As discussed below, the CEM should include Lifetime Average Daily Dose (LADD), rather than leave it for a "future enhancement", given the importance of cancer as an endpoint. Calculation of the LADD should be a fairly simple matter for the CEM given that I believe that the model already includes all of the information needed for such a calculation. I note that, in the "Calculation of Inhalation Dose from Product Usage" (p. 32), CEM already calculated Lifetime Average Daily Concentration (LADC).

I believe that the calculation of chronic average daily dose is misleading (and probably not scientifically defensible) in those instances where exposures are relatively infrequent. For an exposure to be considered

chronic, it usually should be continuous (or at least relatively continuous) over time. In a number of the exposure scenarios in the CEM, the exposures occur only a few days a year, and then a default averaging period of 1 year is used to calculate the chronic exposure. (For example, for "whole appliance cleaners", "anti-freeze liquids", and "interior car care cleaning and maintenance products", the default "medium" exposure frequency is 3 days per year and the default "low" exposure frequency is 1 day per year. The default exposure frequencies for "fertilizers" are even lower – 4 days for "high" exposure, 2 days for "medium" exposure and 1 day for "low" exposure. I believe that such exposures, when averaged over a year, do not really represent chronic exposure and are generally best characterized as either separate acute exposures or subchronic exposures depending on the chemical and scenario, and should be handled as such.

The appropriate averaging time for chronic exposures will depend on the chemical. The 1 year default for averaging time is likely quite conservative in many instances. In any case, the CEM should prohibit the user from specifying an exposure duration (ED) that is longer than the chronic averaging time or automatically adjust the chronic averaging time to be equal to the ED if an ED of greater than 1 year is specified – otherwise the calculation will be incorrect (see related comment below).

5. **There are several items listed in the "Areas for Future Enhancement" section of the User Guide. These describe other calculation methodologies or data sources that were considered during the development of CEM and could be considered in the future. Please comment on feasibility of current incorporation of one or more of these into CEM. Provide specific suggestions and data sources that could assist with integration in the near term.**

As discussed above, the current version of the CEM should include Lifetime Average Daily Dose (LADD), rather than leave it for a "future enhancement". Calculation of the LADD should be a fairly simple matter for the CEM given that I believe that the model already includes all of the information needed for such a calculation. I note that, in the "Calculation of Inhalation Dose from Product Usage" (p. 32), CEM already calculated Lifetime Average Daily Concentration (LADC).

Of the other identified "Areas for Further Enhancement", I recommend that the focus be on the following as being the most significant:

- Products that Spill or Leak Over Time", particularly in occupational settings.
- Elevated Temperatures During Application and Use".

As previously discussed, if exposure to cosmetics is not incorporated into the current version of the CEM, I recommend that they be included as a top priority future enhancement.

**Part 2. User Interface**

6. **Are the exposure models easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the graphical user interface.**

Overall, I found the user interface relatively easy to use although I did run into a number of problems. However, I obviously did not have time to run all combinations of scenarios/products/articles, so there may be other issues/problems in combinations I did not attempt. To illustrate the types of problems that I did encounter, I refer to an example I ran for bubble solution product for two chemicals with very different

properties (formaldehyde and a zinc formulation, CAS #4259158), for a number of different combinations of inputs and different sensitivity analyses:

- No controls on impossible/incorrect inputs
  - Entered an exposure duration (ED) of 30 years, without changing default averaging time (AT) of 1 year. This mistake could easily be made by a non-expert. Model accepted input of a 30 year ED and calculated the CADD result with an ED of 30 years and an AT of 1 year, which is clearly incorrect (ED must be =< AT).
  - Entered a film thickness on skin (FT) of 100cm (1m) which is clearly impossible. Model accepted 100cm FT when using the "estimate" button to calculate the amount retained on skin (AR).
  - I also noted that once an FT valued was entered, it was impossible to recalculate the AR value by correcting/changing the FT value. In other words, once I had entered a 100cm value for FT and used the "estimate" feature to calculate AR, the model would not change the AR value after I changed the FT value to 0.1cm.
  - In addition, I was able to enter both an AR value and an FT value, which should not be allowed, since the FT value is used only to estimate the AR value. In other words, if I specify the AR value, then I should not be able to also enter a film thickness value since they may be inconsistent. In fact, if I enter an AR value, I am actually still required to enter an FT value in order to run the model even though the FT value is not used.
- Report Format
  - The "Full Analysis" report does not appear to include all inputs. For example, for the bubble solution test described above, I was not able to find the ED value on any page of the report.
  - The "Full Analysis" report does not appear to properly present all inputs entered. For example, for the bubble solution test described above, the film thickness on skin was always presented as "0" no matter what value I entered into the input screen.
  - For some sensitivity tests on the bubble solution test described above, the report did not show the scenario name or chemical, although other inputs were shown. I was not able to determine what caused the scenario name or chemical to be shown in the report – the problem was difficult to duplicate.
- I found the "View/Save Report" process after producing a report to be confusing. Also, I found it very unclear what the "Access" and "PDF" buttons are for, or how they are related to "View/Save Report". I think this should be made much clearer when working within the CEM (without having to refer back to the User Guide).
- I had a difficult time trying to save report files outside the CEM model (e.g., to another file folder). This is something I think all users would want to do so that, for example, they could send a Full Analysis report to a colleague. Eventually, I tried printing a Full Analysis report to a PDF but after waiting 10 minutes while the Adobe program said it was "creating" the PDF file, I gave up. There should be an obvious and easy way to save report files outside CEM (unless I missed it).

- Notification that required inputs are missing
  - When leaving the "Scenarios" page, I am immediately notified which required inputs are missing. However, this feature doesn't seem to be incorporated for the other pages.
  - For example, if required inputs for the "Inputs" page are missing, I do not find out until I try to run the CEM model itself. I suggest that the user be notified upon leaving each page if any required inputs are missing.

**7. Are there additional features that you would like to see such as batch mode, additional help screens, or alternate options to save reports? Describe any additional features that you would find useful.**

The "Full Analysis" report should highlight when default or model-calculated input values have been used, and when user-specified values are used.

The user should be required to provide reference or source for user-specified values, or denote that they are based on professional judgement and this information should be included in the "Full Analysis" report.

**Part 3. Documentation and User Guide**

**8. Are the references accurately identified? Would any additional references be helpful? If so, please provide additional references that should be cited.**

p. 19, Section 3. Why are indoor sinks not considered for SVOC emissions from products?

p. 35. Reference for highlighted equation for interior area.

p. 41. Must user specify half-life in soil? If unknown, how does CEM address?

p. 43. How in migration rate from article to saliva (MR) estimated? This factor is identified as an "Area for Future Enhancement" but it is not clear to me what is being done in the current version of CEM.

**9. Does the model user guide and help screens present the equations, defaults, and results, in a clear, complete and useful manner? If not, specifically note areas that are unclear.**

The User Guide properly characterizes the models within CEM as appropriate for screening level assessments. However, I believe that the CEM should more clearly discuss the intended purpose of the CEM and target user profile, and emphasize its limitations in estimated actual exposures, particularly in site-specific and individual-specific analyses. While the CEM represents a noteworthy accomplishment in compiling models and information that allow for a characterization of potential exposures, there are generally very significant uncertainties in the results. This does not mean that the CEM does not have true value, but it does mean that EPA should be very careful to emphasize that the results cannot be assumed to represent reality. When EPA issues a model like the CEM, there is often a tendency for users (and those who receive the user's reports based on the models) to accept the output as "gospel" when in this case, in particular, there are very limited data for confirming the accuracy of models in predicting potential human exposures. It is my opinion that the CEM is most useful as a range-finding tool, in evaluating the likely sensitivity of exposure estimates to changes in exposure conditions or assumptions, in assessing the relative importance of different exposure pathways and scenarios, and in identifying what data would be most valuable to collect so that we can improve our understanding of potential exposures – in other words, as a risk management tool rather than in evaluating absolute magnitude of dose.