ERG
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Consumer and Occupational Model Draft Peer Review Summary

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1.0 INTRODUCTION

The United States Environmental Protection Agency (EPA) evaluates inhalation and dermal exposures to chemicals in consumer/commercial products and pesticide products. EPA uses these exposures along with hazard and dose-response information to estimate risks to chemicals contained in these products. In many cases, suitable monitoring data to estimate exposures are not available and EPA must use models to estimate exposure. EPA has developed two computerized models to assist in the determination of inhalation and dermal exposures to chemicals in consumer/commercial products and pesticide products: the Consumer and Occupational Model (COM) and the Multi-Chamber Concentration and Exposure Model (MCCEM). This report summarizes comments solicited on COM.

COM estimates consumer inhalation and dermal (skin) exposures (acute and chronic) to chemicals in consumer products. The model allows users to select predefined consumer product scenarios to estimate consumer inhalation and dermal exposure levels.

Six experts attempted to complete the peer review for COM. One expert was unable to complete all items in the charge due to time constraints, but did submit general comments. All peer review comments submitted by the experts are summarized in the following report. The comments are summarized by type in the following sections:

- Section 2.0 - Inhalation Exposure;
- Section 3.0 - Dermal Exposure;
- Section 4.0 - COM Input and Output Summary Reports;
- Section 5.0 - Individual COM Help Screens Provided; and
- Section 6.0 - General Comments and Suggestions for Improving COM.

The appendices present the comments as submitted by the COM peer reviewers.

2.0 INHALATION EXPOSURE

COM estimates inhalation exposures to consumer products using the following predefined scenarios:

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Sprayed on Surface - Fabric Protection, Aerosol Paint
- Product Added to Water - Laundry Detergent
- Product Placed in Environment - Solid Air Freshener

COM also allows users to develop custom inhalation exposure scenarios under a user-defined scenario option. Peer reviewer comments on these inhalation scenarios are discussed in this section.

2.1 Default Inhalation Scenarios

One reviewer comments that the default inhalation scenarios seem appropriate, and easy to understand and use. One reviewer believes that the data from the most recent edition of the U.S. EPA's Exposure Factors Handbook should be used for the default values.

Another reviewer indicates that the duration and frequency of use for the general purpose cleaner seem excessive and that 0.67 to 1.47 hours of use per day for 300 uses per year are not typical.

A different reviewer notes that the frequency of use for aerosol paint seems high for the average consumer. Based on the median usage rate default, the reviewer calculates that the one gallon used per event should cover approximately 400 ft^2. If the default frequency of six events per year is usual, the reviewer calculates that this default corresponds to painting three-fourths of a 321 m^3 house every year for 11 years (see Appendix E for the detailed calculations provided by the reviewer). He feels that this amount is excessive, and suggests revising the defaults to two or three events per year. Another reviewer states that the aerosolized fraction

0.01 may be reasonable for the product sprayed on surface scenario, but seems too small for use in an upper bound estimating process.

One reviewer stated that the input tabs for the "default scenarios" generally lacked default values (except body weight), and suggests that it would be helpful if each scenario would automatically enter the default values given in the documentation. The reviewer goes on to comment that requiring the user to enter values manually defeats the purpose of having default exposure scenarios. He notes that suggested default values and the sources cited appear appropriate.

2.2 Emissions Rate Assumptions

Most reviewers found it difficult to determine how the indoor air emissions rates are calculated for each default scenario since no equations or calculations are given. None of the input screens, the reports, or help files describe the emission rate assumptions or calculations in detail.

One reviewer could not determine from the material provided and the time available which, if any, exposure scenarios use the Chinn algorithm. This algorithm seems to apply primarily to calculating evaporation from an aerosol or droplet, but is not valid for all COM uses. The reviewer agrees that an exponential model is appropriate for general purpose cleaners, latex paint, and applied aerosol paint that form a surface film. The reviewer feels that laundry detergent calculations should use Henry's Law, but the documentation did not provide the calculation's equations. Solid air fresheners are unlikely to emit at a constant rate throughout their life unless they are actually removed by the user according to the schedule based on the manufacturer's test data showing when it will deviate from a constant "permeation" rate. The reviewer indicates that a full analysis of the evaporation model used in each scenario and their possible differences in outcome would take more time (and perhaps more information) than was available.

One reviewer comments that the default aerosolized fraction of 0.01 seems to small for an upper bound estimating process.

2.3 User-Defined Inhalation Scenario

Reviewers commented that the User-Defined Scenario is easy to use; however, it does not seem functional. It provides the same choices as the Standard Scenarios, which seems contrary to the purpose of a User-Defined Scenario. One reviewer suggests allowing users to fill in the blanks on this screen.

Another reviewer notes that it takes some time and effort to understand the organization of the Inhalation Input, Day of Use, and Days After Use input screens.

2.4 Exposed Population Assumptions

Reviewers noted that the default values for body weight and incorporation of exposed population considerations seem appropriate and well documented. Again, one reviewer suggests that the recommended default values should agree with the latest edition of the Exposure Factors Handbook.

One reviewer finds the assumptions of exposed populations rigid. For example, infants and children, particularly older children, will have some inhalation exposure to general purpose cleaner air concentrations and latex paint air concentrations, while the model's population consists only of adults for these scenarios. The reviewer feels that the user should be given the opportunity to define relevant populations for all scenarios.

2.5 Inhalation Inputs

One reviewer feels that the inhalation rate defaults during and after use are not appropriate for all situations, but are otherwise reasonable values.

Another reviewer feels that the default values seem appropriate; however, the documentation should specify a default value or input for the interzone air flow. The reviewer also notes that it is confusing to enter the volume of the house on one tab and the volume of the source room on another. This reviewer also comments that the value for the portion of aerosol in air seems low.

Several of the inhalation input default values are based on "best professional judgement." One reviewer notes that the model should provide documentation on the group or committee that was involved in determining these values.

One reviewer's personal exposure assessment files suggest that the Westat 1987 report contains frequency of use and other information for general purpose cleaners (listed in the Westat report as liquid cleansers and powdered hard surface cleaners). The Westat report apparently states that these products are used once per day, and a total of twice per week. He also notes that COM default values do not agree with the values provided in the most recent exposure factors handbook.

2.6 Day of Use and Day After Use Activity Patterns

The room volumes seem reasonable to most reviewers; however, one reviewer feels that this parameter is not a sensitive parameter in the model calculations. One reviewer notes that the "whole house volume" default value of 321 m^3 in COM does not correspond with the recommended value in the most recent edition of the Exposure Factors Handbook of 369 m^3.

One reviewer is unsure of the source of the default activity pattern information. The reviewer suggests that information in the EPA-sponsored National Human Activity Pattern Study (NHAPS) that was done in 1992-94 could be used to supplement COM. The reviewer also feels that users should be allowed to define activity patterns in one-minute increments versus one-hour increments, if needed.

Another reviewer feels that these tabs are very easy to use, especially in comparison to the equivalent tabs in MCCEM. The COM feature that links the duration of use to the activity location is very helpful. However, COM requires the product user to be in the source room for the upper bound duration of use, rather than the average duration; therefore, a scenario where the user leaves the source room immediately after completing a task cannot be modeled. For example, the model could not accomodate a scenario in which a consumer might use aerosol paint or fabric protector in a utility room and then immediately exit to another room.

2.7 Physical/Chemical Property Information

Without better documentation of COM's calculation procedures, one reviewer is unable to determine if the weight fraction is used properly. In addition, he requests that a reference for the weight fraction data be included.

One reviewer notes that the units for "milliequivalent weight" in the Physical/Chemical Property tab as well as in the input page of the report are incorrect. The reviewer states that the proper units for the milliequivalent weight are milligrams per mole equivalent. In the Input tab, the reviewer feels that COM should request either the equivalent weight in grams per mole equivalent or else request the number of equivalents per mole (valency). Another reviewer suggests that, rather than having the user divide the molecular weight by the valance number to determine millequivalents, the user should only input the valence number [default = 1] and COM should complete the calculation.

Another reviewer notes that it seems more logical to enter the K_{ow} in this tab rather than in the Scenario tab.

A different reviewer assumes that the input vapor pressure value is for the pure chemical compound and that COM will calculate a reduced vapor pressure using Raoult's Law for ideal mixtures and non-aqueous mixtures, and Henry's Law for aqueous mixtures. If this assumption is correct, the reviewer suggests clarifying the documentation as well as the text on the screen.

This reviewer also suggests that COM list "mmHg" along with torr as the units for vapor pressure since they are equivalent. The reviewer notes that a weight fraction estimate of 0.013 for enzymes in laundry detergent seems exceedingly high and would expect a value more in the range of 10^{-4} to 10^{-6}.

2.8 Estimated Indoor Air Concentrations

Most reviewers agree that the calculations used to estimate indoor air concentrations were adequate, especially considering the stated goals of COM's usage. One reviewer feels that earlier versions of MCCEM and/or WINSCIES may have gone through more validation and verification of results than COM. The reviewer feels that validation of COM should be a priority, and is something beyond what peer review should provide.

Another reviewer feels that for many products it may be more accurate to model evaporation of volatile chemicals into a "breathing zone." Two reviewers indicate that additional documentation describing source calculations should be included in COM.

2.9 Inhalation Exposure Calculation QA/QC

One reviewer feels that the COM QA/QC files do not explain the exposure calculations and states the COM documentation provided does not clearly and adequately describe these calculations. The reviewer is unable to offer improved or alternate calculations methods without better documentation. A suggested alternate QA/QC procedure is to compare model predictions against actual exposure data for a particular scenario.

Another reviewer feels that the inhalation exposure equations are appropriate, except for the presence of the weight fraction term. The reviewer comments that it may be more appropriate to include the weight fraction in the calculation of the emission rate. The reviewer also notes that COM documentation states that the LADD is based on the median weight fraction, but does not explain whether the median or 90th percentile values of the other parameters are used.

The reviewer feels that the overall approach used in the COM QA/QC documentation, validating the indoor air concentrations against MCCEM, is reasonable. An alternative approach would be to duplicate the calculations on a spreadsheet, as was done for the dermal exposures.

2.10 Inhalation Exposure Descriptors

Two reviewers concur that the inhalation exposure descriptors are adequate and correspond with assumptions and calculations that they have seen in other models. One reviewer is unclear about the meaning of Descriptors and is unable to provide comment on this topic.

One reviewer feels that the High-End/Bounding descriptor applied to all the inhalation exposures is not described in enough detail. The documentation states that the lifetime average daily dose (LADD) is based on the median weight fraction and that the acute potential dose rate (APDR) is based on the upper bound weight fraction. However, the reviewer notes that the documentation does not state whether the inhalation exposures are based on the 90th percentile exposure duration, frequency, and amount used. COM would be more useful for other purposes if both best estimates and upper bounds are reported.

The reviewer notes that a "reasonable worst case" exposure is generally defined by setting one or a few of the parameters in an exposure equation to the upper bounds, while the remaining parameters are average or typical values. For example, if the frequency and duration of use are 90th percentile values, the resulting dose could be described as a "reasonable worst case." In the reviewer's past experience, using this approach gives exposure estimates that are within the distribution predicted by Monte Carlo methods, perhaps between the 75th and 95th percentile exposures.

The reviewer suggests that the only alternative method to estimating reasonable upper bounds would be to use Monte Carlo methods. However, Monte Carlo methods require detailed information or assumptions on the distributions of the input values, and the resulting exposure estimates are only as accurate as the input data. For screening purposes, the reviewer

indicates that the approach used in COM is probably just as accurate as Monte Carlo methods, and requires fewer input data.

Another reviewer states that COM does not calculate bounding estimates. The reviewer notes that statistically speaking, using 90th percentile values for input variables does not result in calculation of a 90th percentile values for inhalation estimate outputs. The reviewer suggests a distribution or Monte Carlo simulation be done to estimate 90th percentile values for the outputs based on the median and 90th percentile value inputs.

2.11 References

The inhalation estimation references seem adequate to the reviewers. Reviewers suggest citing sources for input variables and calculations, such as the U.S. EPA Exposure Factors Handbook and the Chinn report. Another reviewer suggests using and referencing activity pattern information from the EPA-sponsored NHAPS.

3.0 DERMAL EXPOSURE

COM estimates dermal exposures to consumer products using the following predefined scenarios:

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Added to Water - Laundry Detergent
- Product Directly Contacting Skin - Bar Soap, Used Motor Oil

COM also allows users to develop custom dermal exposure scenarios under a user-defined scenario option. Peer reviewer comments on these dermal scenarios are discussed in this section.

3.1 Default Dermal Scenarios

Most reviewers agree that the Default Dermal Scenarios are appropriate and adequate. One reviewer comments that the scenarios are easy to use. Another reviewer suggests that the scenarios are a good starting point for COM, but that COM should be expanded to include additional scenarios.

Another reviewer believes that the dermal surface area for the latex paint scenario is unclear. From the descriptions of the default surface area to body weight ratios, the reviewer assumes the scenario models only one hand coverage. He feels that this default may be an underestimate of typical situations.

A different reviewer commented that the Default Scenarios seem appropriate, based on professional judgment. Because the Input tabs for the Default Scenarios generally lacked default values (except body weight), he suggests that each scenario should automatically enter the default values given in the documentation. The reviewer states that entering the values manually defeats the purpose of default exposure scenarios. He also suggests including an option, such as the one in the user-defined scenario, to enter or to estimate a dermal flux, and to estimate absorbed dose.

One reviewer is unclear about the source of the number of liquid laundry detergent events per year. Assuming that each event is a washing cycle, he believes that 52 dermal events per year seem low compared to the inhalation default value of 312 inhalation events per year. The reviewer is unclear whether the model assumes that spillage, dispenser leakage, or water immersion occurs. He notes that spillage may occur in one out of six washes, but contact with a contaminated dispenser or water immersion is likely to be much more frequent, perhaps approaching 312 events. The reviewer also questions whether a consumer would contact detergent with both hands from spillage (assuming two hand contact based on the dermal surface area of 1,120 cm^2); or immersion (assuming COM is referring to automatic washers and not ringers). He comments that COM may account for some of this variation in the calculation of the Amount Retained on the Skin, but that the documentation does not provide enough detail.

Another reviewer is uncertain about the derivations of the surface area to body weight ratio and amount retained on skin values. The reviewer suggests incorporating additional text, examples, or footnotes to help users. He does not believe that simply stating "These values are equal to the product of the Film Thickness, Density, and Dilution (values not shown)" is sufficient. The reviewer suggests including information from the Westat 1987 report to supplement the default dermal scenarios, specifically the film-thickness data.

3.2 User-Defined Dermal Scenario

The reviewers found the User-Defined Dermal Scenario fairly easy to use. However, one reviewer feels that the User-Defined Scenarios provide little to no value. The reviewer feels that it is not really a "user-defined scenario" but rather a user-defined input to set scenarios.

One reviewer suggests that COM automatically carry over parameters common to both the inhalation and dermal scenarios, such as events per year and averaging time, as is done for the Default Scenarios. Doing so would ensure internal consistency in the assessment for scenarios that have concomitant inhalation and dermal exposures.

He also notes that in the User-Defined Scenario tab, the list of fluxes is blank. The tab itself and help file do not provide the proper units for entering a known flux. The units are given in the documentation, but they are not associated with the Scenario tab. The reviewer feels that the dermal flux should be entered in a tab other than the Scenario tab. The reviewer is unsure whether the K_{ow} should be entered as the partition coefficient itself or as the log K_{ow}.

3.3 Dermal Inputs

According to one reviewer, the values of the general purpose cleaner frequency of use (300 times per year) and exposure duration (0.47 median, 1.47 90th %) seem excessive, based on personal knowledge. For bar soap, COM indicates that the amount retained on skin is approximately 10^{-3} less than for general purpose cleaner, interior latex paint, and used motor oil. The reviewer notes that it is difficult to determine the validity of the difference since the citation for this value is "best professional judgement." Another reviewer strongly recommends exploring the "Applicator Scenarios" considered by EPA's Office of Pesticide Programs (OPP).

One reviewer would prefer to input the exposed surface area rather than the surface area-to-body weight ratio. The reviewer comments that since the body weight has already been entered in a previous tab, calculating the ratio before entering the data increases the likelihood of entering the wrong value. The reviewer has a sense for what a valid surface area value is, but not for the surface area-to-body weight ratio.

One reviewer finds the surface area to body weight ratio needlessly obscure and suggests inputting the exposed skin area for the average person. These values can be obtained by multiplying the current defaults by the nominal 71.8 kg or from values in the Exposure Factors Handbook. The reviewer feels that it would be easy to add a drop-down list of the areas of body parts or some series of subjectively selected default body areas that would yield the current default Ratio values. Similarly, one could much more easily interpret the assumed exposure scenario from the default body areas, and any variation in these areas could be calculated in proportion to other than default body weights input on the Inhalation screen.

The reviewer also notes that the single asterisk footnote is incorrect. For instance, the Ratio values have nothing to do with Frequency of Use but do appear to correspond to the exposed part of the body, which is only the whole body for the Bar Soap users. The reviewer suggests the following alternate footnote: "These values equate to exposed skin surface area divided by the body weight." If the input is changed to exposed area rather than the surface area to weight ratio, a footnote is probably not necessary.

The reviewer finds amount retained on skin more confusing that the surface area to body weight ratio. COM documentation indicates that density is supposedly used but the user does not enter this information via any scenario (default or otherwise). Dilution is also supposedly used and seems to be input via the weight fraction on the physical/chemical parameters screen. As near as the reviewer can tell, changing the weight fraction does affect the output but does not affect the amount retained on the skin. Thus, it appears that amount retained on skin is really driven by film thickness (as it should be). The reviewer suggests that requesting the user to input film thickness or to select a value from a list would be simpler and more understandable than requesting the user to input the amount retained on skin. At the very least, the reviewer comments that a more detailed explanation of the amount retained on skin is needed. The reviewer also notes that COM has an unexplained, significantly large difference in the g/cm²/event for Laundry Detergent and Bar Soap versus the other dermal scenarios.

Another reviewer comments that surface area to body weight ratio and amount retained on skin require additional guidance and documentation. One reviewer recommends exploring the "Applicator Scenarios" considered by EPA's OPP.

3.4 Exposed Population Assumptions

Most reviewers agreed that the default values for the exposed population assumptions are appropriate as they are based on values from the Exposure Factors Handbook.

One reviewers feels that for general purpose cleaner, older children may perform household cleaning chores and should not be excluded from the scenario. The reviewer also

feels that for used motor oil, older adolescents may have the opportunity for contact and should not be excluded from the scenario.

3.5 Physical/Chemical Property Information

One reviewer notes that the source for the weight fraction data should be cited. As previously mentioned in Section 2.5, this tab requires the molecular weight in grams per mole, and the milliequivalent weight in equivalents per mole. One reviewer states that equivalents per mole is not the same as milliequivalent weight and finds this tab confusing. The reviewer suggests either changing the label to mole equivalents per mole (or valency), or changing the units to grams per mole equivalent.

3.6 Dermal Potential Dose Rate

One reviewer feels that the surface area/body weight ratio is an awkward input parameter. It is unclear to the reviewer how COM applies the dermal exposure formula described in the documentation, since the equation does not seem to include mass of product or the dermal area covered. Although the calculation process addresses these parameters somewhere, the reviewer found it difficult to identify where and how.

Another reviewer notes that the use of the potential dermal dose is reasonable if the dermal flux is not known or cannot be estimated. However, the reviewer suggests that the output report should specify whether an absorbed dose or exposure is estimated. As mentioned in Section 3.3, one reviewer strongly recommends exploring the "Applicator Scenarios" considered by EPA's OPP.

3.7 Dermal Flux Rate Equation

One reviewer comments that the equation for estimating the flux is well-documented and validated. Another reviewer feels that the source for the flux rate equation

should cite the original source instead of an EPA Interim Report. At a minimum, the EPA Interim Report citation should include the section and page number.

One reviewer suggests reviewing the descriptions and units in the dermal flux rate equation. Flux has the units of (mass)/[(length)^2(time)]. The reviewer notes that the absorbed dermal exposure equation (in the case of User-Defined Scenario) is not appropriate, since it does not contain a variable that represents the amount dermally exposed.

3.8 Dermal Exposure Calculation QA/QC

One reviewer notes that the QA/QC files seem to show that COM calculations are accurate; however, these files do not demonstrate that the equations deliver reasonable estimates. The reviewer suggests validating the results by comparing COM estimates to measured data for selected scenarios.

Another reviewer feels that the equations for calculating dermal exposure are appropriate, based on professional judgment and experience. The reviewer regards the QA/QC approach that was employed, calculating the exposures using a spreadsheet, as a reasonable approach.

3.9 Dermal Exposure Descriptors

One reviewer comments that the dermal exposure descriptors are appropriate. Two reviewers agree that the documentation does not adequately define the term "What if." One reviewer finds the default values, equations, and calculation process unclear and feels that COM lacks peer reviewed references for the defaults and other parameters.

COM states that the median weight fraction is used to calculate the LADD and average daily dose (ADD), while the upper bound weight fraction is used to calculate the APDR. However, one reviewer is unclear whether the median or upper bound values for exposure duration and frequency are used. COM would be more useful for other purposes if both the best

estimate and upper bound were reported. The upper bound estimates of the frequency and duration of use can be used to estimate a reasonable upper bound. The reviewer feels that the report should indicate whether the dermal exposure is a potential dose (exposure) or absorbed dose.

One reviewer feels that dermal doses should have an equivalent high-end/ bounding estimate. According to the reviewer, based on experimental field survey data, dermal doses are even more variable than inhalation doses.

One reviewer questions why the descriptor "What if" is applied to dermal exposures when an actual flux rate was entered.

3.10 References

One reviewer notes that many additional references are used in COM but not cited in the documentation. Although Reference 4 (U.S. EPA 1992b, Dermal Exposure Assessment) may serve the purpose, citing the original sources is preferable. The reviewer feels that the developer (not peer reviewers) should make the correction.

Another reviewer suggests that the user should know how to obtain and view latest edition of Exposure Factors Handbook. If general references are added, the reviewer feels the following would be useful: G. K. Whitmyre, J. H. Driver, and P. J. Hakkinen, "Assessment of Residential Exposures to Chemicals," Chapter II.1, Pages 125-141 in "Fundamentals of Risk Analysis and Risk Management," edited by V. Molak. CRC Press, Inc., Boca Raton, Florida, 1997. This reference discusses EPA's SCIES, MCCEM, Exposure Factors Handbook, Dermal Exposure Assessment: Principles and Applications, etc.

One reviewer recommends use of EPA's OPP information, and notes that OPP has conducted numerous dermal exposure assessments that could be useful guidance for COM.

4.0 REPORTS

According to most reviewers, the input and output summary reports are not adequate. Two reviewers suggest incorporating a printout of the equations, emissions assumptions, and values in the equations. Another reviewer suggests adding a graph depicting the concentration profiles in the two zones.

One reviewer notes that the ability to save reports in a WordPerfect format is very useful, and comments that the reports are well designed. Two reviewers were unclear about the meaning of the Descriptor column. One reviewer feels that neither the documentation nor the help files for inhalation exposure provided a detailed definition of the descriptor High-End/Bounding. The documentation states that the LADD is based on the median weight fraction. The reviewer is unclear whether or not the inhalation exposures are all based on the 90th percentile duration and mass used. The reviewer feels it would be helpful if the report provided both best estimates and upper bounds.

Another reviewer does not feel that the documentation or help files for dermal exposure provided an adequate definition of the descriptor "What if." It is unclear to the reviewer why dermal exposures should be characterized differently from the inhalation exposures. The report should indicate whether the dermal exposure is a potential exposure or an absorbed dose.

He also notes that the input page reported values (0 or 1) for parameters, such as K_{ow} and Henry's Law constant, even when these values were not input by the reviewer. In addition, the averaging time was reported as 2.555×10^4 days, when 70 years would be more appropriate.

The reviewer recommends adding a box to the report form that allows the user to enter a brief description of the simulation. This information could be entered in the Introduction tab.

5.0 HELP SCREENS

Overall, the reviewers find the help screens adequate and clearly written, especially if the user has an understanding of modeling techniques. However, one reviewer searched for a number of terms, such as "flux" and "dermal" that were not in the index. It would be helpful to expand the search capability to include additional search terms.

One reviewer suggests adding an explanation in the help screens describing how the different sources releases are handled. Calculations similar to the ones provided for mass balances of a chemical in two zones could be provided to explain the source models (incremental, etc.).

6.0 GENERAL COMMENTS

Several reviewers commented that overall, COM is easy to use and navigate. Most reviewers noted that COM documentation could be expanded to more explicitly define the equations used to calculated emissions and exposures, data sources for default parameters, and references. Reviewers also noted that best professional judgement should not be cited as a reference, but should be replaced with more descriptive information. In addition, one reviewer noted in several places that COM should incorporate data from the most recent EPA Exposure Factors Handbook (August 1997), and mention that this document is available either via phone or on the Internet.

6.1 Suggestions for Improvement

One reviewer states that the peer review charge seems premature because the program's sparse documentation makes COM difficult to thoroughly review. The reviewer believes that the assumptions (and limitations) should be stated in the documentation for the COM. Relying on best professional judgements, as is frequently cited for default values for both the inhalation and dermal components, calls to question the value of the model.

The reviewer feels that the number of significant digits presented by COM may mislead users on the accuracy and precision of the results, since many of the input factors are accurate only to the "order of magnitude" level. The reviewer also feels that funding would have better been spent demonstrating validity of COM calculations by comparing COM exposure estimates to measured exposure data from set scenarios rather than funding peer review. Expanded and more detailed documentation would also have been a better use of resources.

According to the reviewer, sensitivity analyses are not easily performed. Because parameter sensitivity analyses are important in demonstrating the certainty of the results, the process for performing them should be incorporated so it is easily completed.

The reviewer believes that the predictive power of COM is limited. Although COM is intended for use as a screening tool, the reviewers comment that more suitable screening approaches may be available. For example, the EASE model in EU EUSES system uses actual data from surveys in an expert system approach to screening. A similar approach based on actual consumer exposure data may be more useful. The reviewer suggests that COM could incorporate a search for the most similar scenario for a material with similar physical/chemical properties. Then, calculations to adjust for composition and physical/chemical property differences could be completed.

Two reviewers feel that overall, COM is easy to use; the methods and default assumptions are appropriate; and the prompt, status, input, and help screens are commendable. One reviewer suggests the following minor changes to improve COM:

- Provide additional details on the methods used to calculate emission rates and upper bound exposures;
- Expand the search capability of the help files to include additional search terms;
- Include a "breathing zone" for active inhalation exposure scenarios; and
- Revise the units for mole equivalents.

Another reviewer suggests that care should be taken to consider and use all relevant exposure factor values from the most recent edition of U.S. EPA's Exposure Factors Handbook. He also suggests making the approaches used in COM more transparent, especially the derivation of the surface area to body weight ratio and the amount retained on skin value.

Another reviewer notes that the COM software should reference the latest edition of the U.S. EPA's Exposure Factors Handbook (August 1997), and mention that it can be obtained from EPA by calling 513-569-7562 or from the Internet at http://www.epa.gov/ORD/WebPubs/exposure. He mentions that of special importance for COM users are the two new chapters added to this edition, "Consumer Products" (Chapter 16) and "Residential Building Characteristics" (Chapter 17).

Two reviewers suggest addition of a "back" key that would allow the user to easily move between screens to revise input parameters while working on a scenario.

Three reviewers mentioned that the COM software "crashed" while running sample scenarios; one reviewer is unable to remember the exact data entry steps leading to the crashes. The second reviewer recommends that the program be tested more thoroughly. The third reviewer experienced crashes while attempting to enter a flux rate and while attempting to overwrite a report file that was in use by WordPerfect. In addition, COM accepted invalid values yet gave no warning until the user submitted the data for calculation. The reviewer notes that the inputs cannot be saved before the calculations are completed, which means that the inputs are lost.

One reviewer feels that the assumption that teens (or at least some children under 17) would not use hard surface cleaning products, detergents, or latex paints and encounter dermal exposures is contrary to what would be expected to occur in the real world. The reviewer suggests adding a "teen" category for these scenarios, or that COM could recommend that users evaluate teen under the adult category.

While the majority of the exposure factor values seem reasonable for use in screening-type exposure assessments to one reviewer, some exposure factor values seem either too high or too low (e.g., the 312 laundry detergent events per year seem high while the air freshener events seem low compared to the typical consumer). The reviewer recommends requesting data from industry associations, like the Soap & Detergent Association, to refine current judgements. The reviewer also suggests including a complete listing of the sources of all COM parameters to help the user understand the reasoning behind the use of a particular value.

One reviewer notes that to obtain high-end estimates, a procedure to conduct Monte Carlo simulations must be considered. The reviewer also suggests improving the dermal scenario using information available from EPA's OPP.

6.2 Ease of Use

Most reviewers find COM easy to use. However, one reviewer notes that COM is also easy to misuse and suggests that reasonable ranges be provided on all input variables. The reviewer mentions that COM accepted an input value of 70,000 kg for a person and completed all calculations.

The purpose of the ADAPI program was unclear to one reviewer. During installation, the program asked for permission to overwrite an existing file, but did not specify the file name. The reviewer does not understand why COM installation would overwrite any existing files, unless it is to modify the config.sys or win.ini files. The reviewer also suggests including some example exposure assessments (*.cmi files) to aid in learning to use the program.

When entering inputs into any tab, the reviewer finds it annoying that he was unable to move to another tab unless all the required inputs were entered. The reviewer suggests incorporating a warning that indicates "data entry is not complete," but still permit the user to move to another tab.

The File drop-down menu does not allow the user to open an existing file from the tabs. The user must essentially exit the simulation and return to the Introductory Image. According to the reviewer, he could not find a way to view a previously saved report directly; he either had to print the report or recalculate.

One reviewer encountered many difficulties during installation of the COM. The inhalation calculations would not function properly when installed in other than the root directory. Repeated attempts resulted in either execution errors or a complete lockup. He had a problem trying to output to a printer (an HP6L) that eventually resulted in him having to reinstall the printer drivers. It would also be useful if users could install IDAPI without having to exit the installation sequence and reboot.

The reviewer also provides a detailed list of format and grammar suggestions for the COM. These suggestions are included in Appendix E, page E-2.

One reviewer mentioned that the use of two different type of menus, drop down (File, etc.) and tabbed (Scenario, etc.), could be confusing. The reviewer suggests the following enhancement of the COM interface:

- At COM startup, grey all the tabs except Scenario. When a scenario is chosen, grey Scenario and ungrey the next relevant tab; and so on.
- It would be visually more appealing if all the titles were in one color, all the input variable names in another color, and all the input values in yet another color. Another reviewer suggests color coding require data input boxes.
- Rearrange input tabs as follows: Introduction, Scenario, Inhalation Input, Day of Use, Days After Use, Dermal Input, PChem Properties.
- Rename the "PChem" tab.
- Move the Submit Data for Calculation button outside the input regions rather than including it as part of PChem Properties.

6.3 Exposure Estimates

The inhalation exposures estimated using COM correspond to EPA's high end or bounding exposure descriptors. High end estimates focus on estimates of exposure in the exposed populations. Bounding estimates, on the other hand, are constructed to be greater than the highest actual exposure in the population. The dermal exposures estimated using COM correspond to a "What if" scenario. A "What-if" scenario only states that if this model and these assumptions are used, this result will be obtained. OPPT has not attempted to classify the dermal exposure estimates further and currently evaluates them on a case-by-case basis. Reviewer comments on the appropriateness of these descriptors and COM outputs are detailed in the following subsections.

6.3.1 High-End/Bounding Screening Level Inhalation Estimates

Comments on the appropriateness of High-End/Bounding descriptors for the inhalation exposure estimates range widely among the reviewers. One reviewer has low confidence in the results. The reviewer comments that no data were provided that validate this model with measured data from similar use scenarios. If earlier versions of COM component calculations were validated, it is not obvious to the reviewers. He also notes that High-End/ Bounding estimates from one day do not rationally extrapolate to lifetime average exposure.

One reviewer indicates that the method used to calculate High-End/Bounding estimates is unclear. If the estimates are calculated using the 90th percentile values for the exposure duration and frequency of use, then they may be considered reasonable upper bound estimates. The reviewer states that it is generally accepted that a reasonable upper bound exposure estimate may be obtained by setting one or a few of the parameters in an exposure equation to the upper bounds, with the remainder being average or typical values. In his experience, this procedure gives exposure estimates within the distribution of exposures predicted by a Monte Carlo approach, perhaps between the 75th and 95th percentile exposures.

The reviewer also notes that for many inhalation scenarios, it is likely that the product user is exposed to two- to three-fold higher pollutant concentrations than the average room concentration. COM does not account for this phenomenon, however, the personal exposure estimates could be improved by including a "breathing zone" in the model.

Another reviewer feels that a more detailed explanation of the High-End/ Bounding descriptor is required. The reviewer assumes that all the 90th percentile values are used in the high-end/bounding calculation; however, this assumption could not be confirmed. Normally a 90th percentile outcome would be based on the distribution of results from a random combination of input values. Thus, the high end calculated as above is more extreme than a 90th percentile outcome. As a quick guess, the reviewer would predict that the probability of the high-end outcome would be about the inverse of the product of the number of 90th percentile values that went into it. Thus, the probability for n = 3 (two 90ths from the Inhalation screen and

one from the PChem screen) is about 1 - (1 -. 90)^3 = 99.9th percentile. The reviewer feels that using the high end calculation is appropriate as long as it is clearly documented. One alternative is to calculate the cumulative 90th percentile variance using Propagation of Error theory which would not be too difficult within the program.

One reviewer has a fairly high level of confidence in the high-end/bounding estimates from review of the scenarios and data used.

One reviewer feels that based on the descriptions of high-end/bounding screening level inhalation estimates, COM does not calculate bounding estimates. Statistically speaking, in the case of high-end screening level inhalation estimates, using the 90th percentile values for the input variables does not give the 90th percentile values for the outputs. Based on the median and the 90th percentile values that are used as inputs, a distribution should be specified and a Monte Carlo simulation (or something similar) done to estimate the 90th percentile values for the outputs. Also, not all the input variables are correctly represented for their median and 90th percentile values. In light of the above two issues, the reviewer has a low level of confidence in COM's high end screening level inhalation estimate.

6.3.2 What If Screening Level Dermal Exposure Estimates

Comments on the appropriateness of the "What if" description for dermal exposure estimates provided by COM range widely among the reviewers. One reviewer has a fairly high level of confidence in the "What If" estimates from review of the scenarios and data used. Another reviewer has a low confidence in the results. He comments that no data were provided that validate this model with measured data from similar use scenarios. If earlier versions of COM component calculations were validated it is not obvious to the reviewer.

One reviewer feels that the model does not provide opportunity to choose in a straight forward manner the area of skin to which the product is applied. When COM's underlying models were developed, limited data were available on skin surface area by body part;

however, this database has evolved and should be incorporated into COM. Also, the reviewer states that the default gram/cm^2 values should be clearly documented and referenced.

A different reviewer was not certain of the meaning of the "What If" descriptor, while another reviewer was unclear how the "What If" exposure estimates are calculated. If the estimates are calculated using the 90th percentile values for the exposure duration and frequency of use, then they may be considered reasonable upper bound estimates and should be characterized as such. The reviewer feels that the dermal exposures should be further characterized as either exposures (i.e., potential doses) or absorbed doses, depending on the option selected.

One reviewer states that estimating amount retained on skin (g/cm^2) is a very complex process. The manner in which this input variable is represented in COM is very uncertain to the reviewer. Therefore, the reviewer has a low level of confidence in COM's "What If" screening level dermal exposure estimate.

Appendix A

PEER REVIEW COMMENTS
SUBMITTED BY THOMAS ARMSTRONG

COM Peer Reviewer COMMENTS

GENERAL COMMENTS

1. Summarize your comments in order of importance. In addition, please summarize any suggestions for improvement or alternate estimation methodologies.

The model as produced and as documented is a "black box" and not easy to thoroughly review. The peer review charge seems premature based on program's sparse documentation.

The documentation "Introduction to COM - Draft" states COM "uses the same approach and calculations as the Multi-Chamber Concentration and Exposure Model (MCCEM) ..." This does not seem to be the case; MCCEM considers decay in air due to sinks/degradation, but COM does not.

Mathematical models are simulations that depend on simplifying assumptions. The assumptions then impart limitations on the model's predictive power. I believe that the assumptions (and limitations) should be stated in the documentation for the program.

The most frequently cited reference for default values for both the inhalation and dermal components is "Best Professional Judgement." These values may well drive many assessment results, and should be based on data from peer reviewed publications. Relying on these judgements so extensively call to question the value of the model.

The number of digits carried probably generate a misimpression about the accuracy/precision of the results; many of the input factors have accuracy only to the "order of magnitude" level.

At this stage of the model's evolution, funding would have better been spent on demonstrating validity via comparison to measured exposure data from set scenarios than funding spent on peer review. Better documentation would also have been a better use of resources.

The model has little in the way of controls for reasonable value selection for input fields.

Sensitivity analyses are not easily performed. Parameter sensitivity analyses are important in demonstrating the certainty of the results, and the process for doing this should be incorporated so it is easily completed.

I believe the predictive power of the model is limited. Although it is intended as a screening tool, there may be more suitable screening approaches. For example, the EASE model in EU EUSES system uses actual data from surveys in an expert system approach to screening. A similar approach, drawing on actual consumer exposure data, may be more useful. It could incorporate a search for the most similar scenario for the material with the most similar

COM Peer Reviewer COMMENTS

physical/chemical properties. Then, some calculations for composition and physical/chemical property differences could be completed.

2. What is your overall level of confidence in COM's "high end/bounding" screening level inhalation estimates? Please provide your rationale for assessing level of confidence.

I have low confidence in the results. No data were provided to show validation of this model against measured data from similar use scenarios. Possibly, earlier versions of component calculations were validated, but this is not obvious in COM.

The documentation describes equations used in a general way. (Granted, the references provide further details.) However, the input variables transfer to a "black box" for calculations that are opaque to the user. This does not engender confidence in the calculation process and results.

"High end/bounding" estimates from one day do not rationally extrapolate to lifetime average exposure.

3. What is your overall level of confidence in COM's "what-if" screening level dermal exposure estimates? Please provide your rationale for assessing level of confidence.

I have low confidence in the results. No data were provided to show validation of this model against measured data from similar use scenarios. Possibly, earlier versions of component calculations were validated, but this is not obvious in COM.

The model does not provide opportunity to choose (in a straight forward manner) the area of skin to which the product is applied. When the underlying models were developed, there were limited data on skin surface area by body part. This database has evolved and should be incorporated into COM.

The default gram/cm^2 values should be clearly documented and referenced.

4. COM Ease of Use

Is the model easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the user-friendliness of COM.

The model is easy to use. However, it is also easy to misuse; reasonable ranges should be provided on all input variables. Currently, the model is content to accept such items as a 70,000 kg person and complete the calculations.

COM Peer Reviewer COMMENTS

5. COM Help Screens

Are the Help screens adequate? Describe any additional help screens that you would find useful.

The help screens are adequate, as long as the user has an understanding of the modeling techniques to begin with.

6. COM Reports

Are the report input summary and output reports adequate? Please note any additions to the reports that you would find helpful?

The reports are not entirely adequate. A print of the equations, emission assumptions, and values in the equations would be helpful.

INHALATION EXPOSURE

7. Default Inhalation Scenarios

Are the default inhalation scenarios appropriate and adequate? Note, the default scenarios currently included in COM represent those most often encountered by OPPT. Are these scenarios easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario. Specifically note any areas or assumption that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint

  The dermal surface area for the latex paint scenario is not described in simple terms. From the descriptions of the default surface area to body weight ratios, it appears to assume one hand coverage; this may be an underestimate of typical situations.

  The duration and frequency of use for general purpose cleaner seem excessive; 0.67 to 1.47 hour of use per day for 300 uses/year seems far more than typical.

- Product Sprayed on Surface - Fabric Protection, Aerosol Paint.

  The aerosolized fraction 0.01 may be reasonable, but seems too small for use in an "upper bound" estimate process.

COM Peer Reviewer COMMENTS

- Product Added to Water - Laundry Detergent

  I do not have an opinion on this scenario.

- Product Placed in Environment - Solid Air Freshener

  I do not have an opinion on this scenario.

8. Emissions Rate Assumptions

Are the indoor air concentration emissions rate assumptions (i.e. incremental, constant, aerosolized) appropriate for each default scenario?

Unfortunately, it is difficult to figure out what emission rate assumptions are applied in a given scenario from the COM program. Neither the input screens nor the reports indicate the emission rate assumption. These are commented on to some degree in the "Introduction to COM - Draft" document. However, the draft does not demonstrate the assumption's use in equations for predicting concentrations.

The default aerosolized fraction (0.01) seems too small if to be used in a "upper bound" estimating process.

9. User-Defined Inhalation Scenario

Is the user-defined inhalation scenario easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

The user defined scenario is easy to use, but does not seem to be useful. All COM provides for is redefining the parameters of the pre-defined scenarios. This is rather far from a user defined scenario.

10. Exposed Population Assumptions

Are the default body weight and incorporation of exposed population considerations appropriate? Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

As far as they go, the defaults seem reasonable as point values. However, the assumptions of exposed populations are not entirely appropriate. For example, infants and children will have some inhalation exposure to general purpose cleaner air concentrations, and latex paint air

COM Peer Reviewer COMMENTS

concentrations. Particularly for older children, they may use these products and have direct contact. This aspect of COM is needlessly rigid; the user should be given the opportunity to define the relevant populations.

11. Inhalation Inputs

Are default frequency of use, years of use, mass of product used, duration of use, inhalation rate during and after use, portion of aerosol in air, and air exchange rate values appropriate for each scenario? Please provide your rationale for determining the appropriateness of the default values. Note any inputs or defaults that you feel are inappropriate and suggest alternate values.

The inhalation rate defaults during and after use are not appropriate for all situations, but are in other regards reasonable values.

12. Day of Use and Day After Use Activity Patterns

Please comment on the default activity patterns and default room volumes. Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

The room volumes seem reasonable, but this is not likely a very sensitive parameter in the model calculations.

13. Physical/Chemical Property Information

Information on physical chemical properties (such as weight fraction) are used along with the Chinn algorithm to estimate the emission rate. Comment on the default weight fraction estimates provided. Specifically note any areas of concern or areas for improvement in the estimation of emissions.

Without better documentation of COM's calculation procedures, I cannot discern easily that the weight fraction is used properly. Additionally, the source of the weight fraction data is not cited.

14. Estimated Indoor Air Concentration

Does the inhalation exposure mass balance equation calculate indoor air concentrations appropriately and adequately? Specifically note any areas of concern, areas for improvement, or alternate calculation methodologies.

COM Peer Reviewer COMMENTS

Earlier versions of MCCEM and/or WINSCIES may have gone through a degree of validation, and verification of results. However, COM seems to be a modification (to an uncertain degree.) and the MCCEM/WINSCIES verifications may not extend to COM.

Validation should be a priority, and is a project beyond what peer review should provide. The question of calculation correctness hinges on comparison to actual data. The calculations undoubtedly execute properly and accurately, but may produce flawed estimates.

15. Inhalation Exposure Calculations

Please review the enclosed COM QA/QC files. Are the inhalation exposure estimation equations adequately explained within COM and are they appropriate? Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

The "QA/QC" files do not explain the exposure estimate calculations. The COM documentation "Introduction to COM - Draft" covers the equations in an unacceptably meager manner. Without better documentation, I'm not sure how to offer improved or alternate calculation methods. An alternate QA/QC is to compare model predictions against actual exposure data for a particular scenario.

16. Inhalation Exposure Descriptors

Are the inhalation exposure descriptors of high end/bounding appropriate given the default assumptions and the models used? Please provide your rationale for determining the appropriateness of the descriptors. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

The descriptors are adequate.

17. References

Are inhalation estimation references identified appropriately? Would any additional reference citations be helpful? Please note any additional references that should be cited.

The references are adequate, but do not seem to be complete. The model may benefit by citing sources for input variables, such as the US EPA Exposure Factors Handbook.

18. Scenario-specific or Other Comments

COM Peer Reviewer COMMENTS

DERMAL EXPOSURE REVIEW COMMENTS

19. Default Dermal Scenarios

Are the default dermal scenarios appropriate and adequate? Note that the default scenarios represent those most often encountered by OPPT. Specifically note any areas or assumptions that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Added to Water - Laundry Detergent
- Product Directly Contacting Skin - Bar Soap, Used Motor Oil.

These scenarios seem appropriate as a starting point for COM evolution. Further scenarios should be added.

20. User-Defined Dermal Scenario

Is the user-defined dermal scenario easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

The scenario was easy to use, but provides little to no value. It is not really a "user defined scenario." Rather, it is user defined input to set scenarios.

21. Dermal Inputs

Are the default amount retained on skin, frequency of use, surface area to body weight ratio, years of use, and exposure duration values appropriate for each scenario? Please provide your rationale for determining the appropriateness of the default values. Note any areas of concern and suggest alternate values.

The general purpose cleaner frequency of use (300 per year) and exposure duration (0.47 median, 1.47 90th %) cite "Best Professional Judgement" as the reference. These values seem excessive, based on personal knowledge about typical patterns of use of general purpose cleaners in a household.

For bar soap, the amount retained on skin is approximately 10^{-3} less than for general purpose cleaner, interior latex paint, and used motor oil. Since the citation is "Best Professional Judgement," it is difficult to decide the validity of the difference.

COM Peer Reviewer COMMENTS

22. Exposed population assumptions

Are the default body weight and incorporation of exposed population considerations appropriate (active vs. passive exposure assumptions)? Please provide your rationale for determining the appropriateness of the default values. Note any assumptions that you feel are inappropriate and suggest alternate values.

For general purpose cleaner, older children may do household cleaning chores, and should not be excluded from the scenario. For used motor oil, older adolescents may have opportunity for contact and should not be excluded from the scenario.

23. Physical/Chemical Property Information

Comment on the default weight fraction values and the use of weight fraction in the dermal dose calculations. Note any areas of concern and suggest alternate values.

The source for the weight fraction data should be cited.

24. Dermal Potential Dose Rate

Please comment on the use of potential dose rates to calculate dermal exposures in the default scenarios. Note any areas of concern, areas for improvement, or alternate calculation methodologies.

The surface area/body weight ratio is an awkward input parameter. It is not clear how COM applies the dermal exposure formula (Eq. 3 on page 23 of the "Introduction to COM- Draft" document); the equation seems not to include mass of product or the dermal area covered. Although this is addresses somewhere in the calculation process, it is difficult to see where and how.

25. Dermal Flux Rate Equation

Is the flux rate equation for calculating absorbed dermal exposure in the User-Defined Scenario adequate and appropriate? Note any areas of concern, areas for improvement, or alternate calculation methodologies.

The source for the flux rate equation should be cited back to the original source. Citing the EPA Interim Report is a less than ideal approach. Even citing the section and page from the EPA Interim Report would be a substantial improvement in documentation.

COM Peer Reviewer COMMENTS

26. Dermal Exposure Calculations

Please review the enclosed COM QA/QC files. Are the dermal exposure estimation equations adequately explained within COM and are they appropriate? Does the dermal exposure equation calculate exposure appropriately and adequately. Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

The QA/QC files seem to show that COM calculates its equations correctly. However, this does not demonstrate that the equations deliver reasonable estimates. Validation should be completed by comparison of estimates to measured data for selected scenarios.

27. Dermal Exposure Descriptors

Is the dermal exposure descriptors of "what-if" appropriate given the default assumptions? For example, do you think that it may be appropriate to classify the dermal estimates as being high end or bounding? Please provide your rationale for determining the appropriateness of the descriptor. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

"What-if" is a vague term, not defined in the documentation. I find the default values, equations and calculation process so obtuse I do not know what to call the results. The lack of peer reviewed references for the defaults, etc. makes this impractical to resolve.

28. References

Are references identified appropriately? Would any additional reference citations be helpful? Please note any additional references that should be cited.

There seem to be many additional references that were used but not cited in the document. Although these may be cited reference 4 (U.S. EPA 1992b, Dermal Exposure Assessment), citing the original sources is preferable. This should be referred to the developer (not peer reviewers) for correction.

29. Scenario-specific or Other Comments

Appendix B

PEER REVIEW COMMENTS
SUBMITTED BY DR. MICHAEL BABICH

Comments by
Michael A. Babich

COM Peer Reviewer COMMENTS

Comments on COM
July 31, 1998

GENERAL COMMENTS

1. **Summarize your comments in order of importance. In addition, please summarize any suggestions for improvement or alternate estimation methodologies.**

Overall COM is easy to use. The methods and default assumptions are appropriate. Some minor changes would improve the program's utility, such as: (I) Provide additional details on how the emission rates and upper bound exposures are calculated. (ii) Expand the search capability of the help files to include additional search words. (iii) Include a "breathing zone" for active inhalation exposure scenarios. (iv) Change the units for mole equivalents.

2. **What is your overall level of confidence in COM's "high end/bounding" screening level inhalation estimates? Please provide your rationale for assessing level of confidence.**

It is not clear how the "high end/bounding" estimates are calculated. If they are calculated using the 90th percentile values for the exposure duration and frequency of use, then they may be considered reasonable upper bound estimates. It is generally accepted that a reasonable upper bound exposure estimate may be obtained by setting one or a few of the parameters in an exposure equation to the upper bounds, with the remainder being average or typical values. In my experience, this procedure gives exposure estimates within the distribution of exposures predicted by a Monte Carlo approach, perhaps between the 75th and 95th percentile exposures.

For many inhalation scenarios, it is likely that the product user is exposed to 2- to 3-fold higher pollutant concentrations than the average room concentration. COM does not account for this phenomenon. The personal exposure estimates could be improved by including a "breathing zone" in the model.

3. **What is your overall level of confidence in COM's "what-if" screening level dermal exposure estimates? Please provide your rationale for assessing level of confidence.**

It is not clear how the "what if" exposure estimates are calculated. If they were calculated using the 90th percentile values for the exposure duration and frequency of use, then they may be considered reasonable upper bound estimates, and should be characterized as such. The dermal exposures should be further characterized as either exposures, that is, potential doses, or absorbed doses, depending on the option selected.

COM Peer Reviewer COMMENTS

4. COM Ease of Use

Is the model easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the user-friendliness of COM..

Overall, COM was very easy to use. It was easy to install, except that the purpose of the ADAPI program was not clear. During installation, the program asked for permission to overwrite an existing file, but did not specify the file name. I did not understand why it would be necessary to overwrite any existing files, unless it was to modify the config.sys or win.ini files. It would be helpful to include some example exposure assessments (*.cmi files) to aid in learning to use the program.

While learning to use COM, I experienced several program crashes: due to floating point errors; while attempting to enter a flux rate; and while attempting to overwrite a report file that was in use by WordPerfect. I think that the floating point errors were due to entering an invalid house volume (equal to or less than the zone 1 volume). However, COM accepted the invalid value; there was no warning until submitting the data for calculation. There is no way to save the inputs before the calculations are completed, which means that the inputs are lost.

When entering inputs into any tab, I was unable to move to another tab unless all the required inputs were entered. I found this annoying. It would be better to have a warning that "data entry is not complete," but still permit the user to move to another tab.

The File drop-down menu does not allow the user to open an existing file from the tabs. The user must essentially exit the simulation and return to the "introductory image." There apparently is no way to view a previously saved report directly; the only way to accomplish this is either to print the report or else recalculate.

5. COM Help Screens

Are the Help screens adequate? Describe any additional help screens that you would find useful.

The Help screens were very clearly written. However, a number of terms that I searched for, such as "flux" and "dermal," were not in the index. COM was unable to find the help file when I was trying to enter a flux rate and needed to know the proper units. The most helpful change to the help files would be to expand the search capability to include additional search terms.

COM Peer Reviewer COMMENTS

6. COM Reports

Are the report input summary and output reports adequate? Please note any additions to the reports that you would find helpful?

The ability to save reports in WordPerfect format is very helpful, and the reports are well designed. Regarding the inhalation exposure, the descriptor High-End/Bounding (applied to all the inhalation exposures) was not defined in detail in the documentation or help files. The documentation states that the LADD is based on the median weight fraction. Are the inhalation exposures all based on the 90th percentile duration and mass used? It would be helpful if the report provided both best estimates and upper bounds.

Regarding dermal exposures, the descriptor What If is not defined in the documentation or help files. This descriptor was applied to all the dermal exposures, even when an actual flux was entered. It is not clear why dermal exposures should be characterized differently from the inhalation exposures. The report should indicate whether the dermal exposure is a potential exposure or an absorbed dose.

The input page reported values (0 or 1) for parameters, such as K_{ow} and Henry's Law constant, even when I did not input these values. The averaging time was reported as 2.555×10^4 days, when 70 years would have been more appropriate.

It would be helpful to have a box in the report form to enter a brief description of the simulation. This information could be entered in the Introduction tab.

INHALATION EXPOSURE

7. Default Inhalation Scenarios

Are the default inhalation scenarios appropriate and adequate? Note, the default scenarios currently included in COM represent those most often encountered by OPPT. Are these scenarios easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario. Specifically note any areas or assumption that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Sprayed on Surface - Fabric Protection, Aerosol Paint
- Product Added to Water - Laundry Detergent
- Product Placed in Environment - Solid Air Freshener

COM Peer Reviewer COMMENTS

The input tabs for the "default scenarios" generally lacked default values (except body weight). It would be helpful if the default values given in the documentation were automatically entered into each default scenario. Having to enter them manually defeats the purpose of having default exposure scenarios. The default values and the sources cited appear appropriate.

8. Emissions Rate Assumptions

Are the indoor air concentration emissions rate assumptions (i.e. incremental, constant, aerosolized) appropriate for each default scenario?

The general approach for modeling emissions for the various scenarios is appropriate. However, the documentation and help files do not describe in detail how the emission rates are calculated. No equations are given. The weight fraction appears in all of the inhalation dose equations. This would not be necessary if the weight fraction were used in calculating the emission rates.

9. User-Defined Inhalation Scenario

Is the user-defined inhalation scenario easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

The secondary screen for User-Defined Scenario simply provides the same choices as the standard scenarios. This seems to defeat the purpose of having a user-defined scenario. One of the choices on this screen should be to fill-in-the-blanks.

10. Exposed Population Assumptions

Are the default body weight and incorporation of exposed population considerations appropriate? Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

The default values appear to be appropriate, based on professional judgment, and are well-documented.

11. Inhalation Inputs

Are default frequency of use, years of use, mass of product used, duration of use, inhalation rate during and after use, portion of aerosol in air, and air exchange rate values appropriate for each scenario? Please provide your rationale for determining the appropriateness of the default values. Note any inputs or defaults that you feel are inappropriate and suggest alternate values.

COM Peer Reviewer COMMENTS

The default values seem appropriate. The value for the portion of aerosol in the air (0.01) seems low, based on professional judgment and personal experience, although it is documented by a memorandum. It was confusing to enter the volume of the house on one tab and the volume of the source room on another. I did not see a default value or input for the interzone air flow. This parameter should be specified in the documentation.

12. Day of Use and Day After Use Activity Patterns

Please comment on the default activity patterns and default room volumes. Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

These tabs are very easy to use, especially in comparison to the equivalent tabs in the MCCEM program. The default activity patterns seem appropriate, based on personal experience, although they are arbitrary. The program feature that connects the duration of use to the activity location is very helpful. However, the product user is required to be in the source room for the upper bound duration of use, rather than the average duration; therefore, one cannot model a scenario where the user leaves the source room immediately after completing a task. For example, one might use aerosol paint or fabric protector in a utility room and then exit to another room.

13. Physical/Chemical Property Information

Information on physical chemical properties (such as weight fraction) are used along with the Chinn algorithm to estimate the emission rate. Comment on the default weight fraction estimates provided. Specifically note any areas of concern or areas for improvement in the estimation of emissions.

The Physical/Chemical Property tab requests input for Molecular Weight in grams per mole, and Milliequivalent Weight incorrectly in milliequivalents per mole. The proper units for the milliequivalent weight are milligrams per mole equivalent. The input page of the COM Report incorrectly gives the Milliequivalent Weight as milliequivalents per milligram. These units are confusing and should be more consistent. In the input tab, request either the equivalent weight in grams per mole equivalent or else request the number of equivalents per mole (valency).

It seems more logical to enter the K_{ow} in this tab, rather than in the Scenario tab.

14. Estimated Indoor Air Concentration

Does the inhalation exposure mass balance equation calculate indoor air concentrations appropriately and adequately? Specifically note any areas of concern, areas for improvement, or alternate calculation methodologies.

COM Peer Reviewer COMMENTS

For many products it may be more accurate to model evaporation of volatile chemicals into a "breathing zone." The mass balance equations for calculating indoor air concentrations are appropriate. However, I found no equations for calculating source strengths. It was confusing to enter the volume of the house on one tab and the volume of the source room on another. I did not see a default value or input for the interzone air flow. The parameter should be specified in the documentation.

15. Inhalation Exposure Calculations

Please review the enclosed COM QA/QC files. Are the inhalation exposure estimation equations adequately explained within COM and are they appropriate? Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

The inhalation exposure equations are appropriate, except for the presence of the weight fraction term. It might be more appropriate to include the weight fraction in the calculation of the emission rate. The documentation states that the LADD is based on the median weight fraction, but does not explain whether the median or 90th percentile values of the other parameters are used?

The overall QA/QC approach that was used, validating the indoor air concentrations against MCCEM, is a reasonable approach. An alternative approach would be to duplicate the calculations on a spreadsheet, as was done for the dermal exposures.

16. Inhalation Exposure Descriptors

Are the inhalation exposure descriptors of high end/bounding appropriate given the default assumptions and the models used? Please provide your rationale for determining the appropriateness of the descriptors. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

The descriptor High-End/Bounding (applied to all the inhalation exposures) is not defined in detail. The documentation states that the LADD is based on the median weight fraction and that the APDR is based on the upper bound weight fraction. However, the documentation does not state whether the inhalation exposures are based on the 90th percentile exposure duration and frequency and the amount used. While OPPT requires upper bound estimates, COM would be more useful for other purposes if both best estimates and upper bounds are reported.

A "reasonable worst case" exposure is generally defined by setting one or a few of the parameters in an exposure equation to the upper bounds, while the remaining parameters are average or typical values. For example, if the frequency and duration of use are 90th percentile values, the resulting dose could be described as a "reasonable worst case." In my experience,

COM Peer Reviewer COMMENTS

using this approach gives exposure estimates that are within the distribution predicted by Monte Carlo methods, perhaps between the 75th and 95th percentile exposures.

The only alternative method to estimating reasonable upper bounds would be to use Monte Carlo methods. However, Monte Carlo methods require detailed information (or assumptions) on the distributions of the input values. The resulting exposure estimates are only as accurate as the input data. For screening purposes, the approach used in COM is probably just as accurate as Monte Carlo methods, and requires fewer input data.

17. References

Are inhalation estimation references identified appropriately? Would any additional reference citations be helpful? Please note any additional references that should be cited.

The report by Chinn should be cited.

18. Scenario-specific or Other Comments

No additional comments.

DERMAL EXPOSURE REVIEW COMMENTS

19. Default Dermal Scenarios

Are the default dermal scenarios appropriate and adequate? Note that the default scenarios represent those most often encountered by OPPT. Specifically note any areas or assumptions that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Added to Water - Laundry Detergent
- Product Directly Contacting Skin - Bar Soap, Used Motor Oil

The default scenarios seem appropriate, based on professional judgment. However, the input tabs for the "default scenarios" generally lacked default values (except body weight). It would be helpful if the default values given in the documentation were automatically entered into each default scenario. Having to enter them manually defeats the purpose of having default exposure scenarios. There should be an option to enter or estimate a dermal flux and estimate an absorbed dose, as there is for the user-defined scenario.

COM Peer Reviewer COMMENTS

20. User-Defined Dermal Scenario

Is the user-defined dermal scenario easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

It would be helpful if parameters common to both the inhalation and dermal scenarios, such as events per year and averaging time, would automatically carry over from the Inhalation tab, as they did for the default scenarios. This would ensure internal consistency in the assessment for scenarios that have concomitant inhalation and dermal exposures.

In the User-Defined Scenario tab, the list of fluxes was blank. The tab itself and help file did not provide the proper units for entering a known flux. The units are given in the documentation, but they are not associated with the scenario tab. The dermal flux should be entered in a separate tab. It does not seem logical to enter this parameter in the Scenario tab. It was not clear whether the K_{ow} should be entered as the partition coefficient itself or as the log K_{ow}.

21. Dermal Inputs

Are the default amount retained on skin, frequency of use, surface area to body weight ratio, years of use, and exposure duration values appropriate for each scenario? Please provide your rationale for determining the appropriateness of the default values. Note any areas of concern and suggest alternate values.

It would be preferable to input the exposed surface area rather than the surface area-to-body weight ratio. The body weight has already been entered in a previous tab. Having to calculate the ratio before entering increases the likelihood of entering the wrong value. I have a sense for what a valid surface area value is, but not for the surface area-to-body weight ratio.

22. Exposed population assumptions

Are the default body weight and incorporation of exposed population considerations appropriate (active vs. passive exposure assumptions)? Please provide your rationale for determining the appropriateness of the default values. Note any assumptions that you feel are inappropriate and suggest alternate values.

The default assumptions appear to be reasonable, based on professional judgment. At CPSC, we generally assume 10 kg as the body weight for an infant. The other assumptions are documented in the Exposure Factors Handbook, which is a source that we frequently use.

COM Peer Reviewer COMMENTS

23. Physical/Chemical Property Information

Comment on the default weight fraction values and the use of weight fraction in the dermal dose calculations. Note any areas of concern and suggest alternate values.

This tab requires the molecular weight in grams per mole, and the milliequivalent weight in equivalents per mole. Equivalents per mole is not the same as milliequivalent weight. This is confusing. Either change the label to mole equivalents per mole (or valency), or else change the units to grams per mole equivalent.

24. Dermal Potential Dose Rate

Please comment on the use of potential dose rates to calculate dermal exposures in the default scenarios. Note any areas of concern, areas for improvement, or alternate calculation methodologies.

The use of the potential dermal dose, that is, exposure, is reasonable if the dermal flux is not known or cannot be estimated. However, the report should specify whether an absorbed dose or exposure is estimated.

25. Dermal Flux Rate Equation

Is the flux rate equation for calculating absorbed dermal exposure in the User-Defined Scenario adequate and appropriate? Note any areas of concern, areas for improvement, or alternate calculation methodologies.

The equation for estimating the flux is well-documented and validated.

26. Dermal Exposure Calculations

Please review the enclosed COM QA/QC files. Are the dermal exposure estimation equations adequately explained within COM and are they appropriate? Does the dermal exposure equation calculate exposure appropriately and adequately. Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

The equations for calculating dermal exposure are appropriate, based on professional judgment and experience. The QA/QC approach that was employed, calculating the exposures on a spreadsheet, is a reasonable approach.

COM Peer Reviewer COMMENTS

27. Dermal Exposure Descriptors

Is the dermal exposure descriptors of "what-if" appropriate given the default assumptions? For example, do you think that it may be appropriate to classify the dermal estimates as being high end or bounding? Please provide your rationale for determining the appropriateness of the descriptor. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

The documentation does not adequately explain the meaning of "what if." It states that the median weight fraction is used to calculate the LADD and ADD, while the upper bound weight fraction is used to calculate the APDR. However, it is not clear whether the median or upper bound values for exposure duration and frequency are used. While OPPT requires upper bound estimates, COM would be more useful for other purposes if both the best estimate and upper bound were reported. The upper bound estimates of the frequency and duration of use can be used to estimate a reasonable upper bound. The report should indicate whether the dermal exposure is a potential dose (exposure) or absorbed dose.

28. References

Are references identified appropriately? Would any additional reference citations be helpful? Please note any additional references that should be cited.

The references cited are appropriate.

29. Scenario-specific or Other Comments

No additional comments.

Appendix C

PEER REVIEW COMMENTS
SUBMITTED BY DR. P.J. (BERT) HAKKINEN

Comments by
P.J. (Bert) Hakkinen

COM Peer Reviewer COMMENTS

August, 1998 Review of U.S. EPA's COM Software

Attn: Ms. Grace Kitzmiller
Eastern Research Group, Inc. (ERG)
14555 Avion Parkway, Suite 200
Chantilly, VA 20151

GENERAL COMMENTS

1. Summarize your comments in order of importance.

The COM software is easy to use, e.g., it is easy to navigate through, and has good prompt, status, input, and help screens. Overall, the software provides a very useful tool for EPA and others to use in developing residential dermal and inhalation exposure assessments; however, care should be taken to consider/use all possibly useful exposure factor values from the most recent edition of U.S. EPA's Exposure Factors Handbook (see below → examples include body weights, inhalation rates, and product usage data), and to make some of the approaches used in COM more transparent (see below → examples include the derivations of the "surface area to body weight ratio" and "amount retained on skin" values).

One possible improvement would be a "back" key, allowing the user to easily go back to the previous screen while working on a scenario if he/she wants to go back and make a change while inputting information. I realize that one can already go back on some screens; however, a "back" key option would be of further help on other screens.

I did have the software "crash" twice as I was running sample scenarios; however, I am unable to remember the exact data entry steps leading to the crashes.

In addition, please summarize any suggestions for improvement or alternate estimation methodologies.

The COM software should note the latest edition of the U.S. EPA's Exposure Factors Handbook (= August, 1997), and could mention that it can be obtained from EPA by calling 513-569-7562. It could also note that EPA has this document on the Internet's World Wide Web (http://www.epa.gov/ORD/WebPubs/exposure), and may offer it as a CD-ROM. Key to note for COM users are the two new chapters added to this edition, "Consumer Products" (Chapter 16) and "Residential Building Characteristics" (Chapter 17).

EPA's assumption that teens (or at least some children under 17) won't use hard surface cleaning products, detergents, or latex paints and encounter dermal exposures is contrary to what I would expect to sometimes occur in the real world [COM's screens do not allow one to select "child"

COM Peer Reviewer COMMENTS

(ages 2-17) as users of these types of products → perhaps a "teen" category could be added for these categories, or the teen usage could be noted as falling under the adult category].

While the majority of the exposure factor values seem OK for use in screening-type exposure assessments, some exposure factor values seem either high or low from what I'd expect, e.g., the 312 laundry detergent events/year seem high while the air freshener events seem low compared to the typical or likely consumer (the EPA values I'm talking about are based on best professional judgment → perhaps requests to industry associations like the Soap & Detergent Association would be helpful in refining the current judgments).

A thorough listing of the sources of the values would help guide the reader towards understanding the reasoning behind the use of a particular value and might lead to occasional use of other values, e.g., from the Exposure Factors Handbook or from other sources like industry associations.

2. What is your overall level of confidence in COM's "high end/bounding" screening level inhalation estimates?

I have a fairly high level of confidence in the "high end/bounding" estimates.

Please provide your rationale for assessing level of confidence.

From review of the scenarios and data used.

3. What is your overall level of confidence in COM's "what-if" screening level dermal exposure estimates?

I have a fairly high level of confidence in the "what-if" estimates.

Please provide your rationale for assessing level of confidence.

From review of the scenarios and data used.

4. COM Ease of Use

Is the model easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the user-friendliness of COM.

Please see above comments about ease of use.

COM Peer Reviewer COMMENTS

5. COM Help Screens

Are the Help screens adequate? Describe any additional help screens that you would find useful.

Please see above comments.

6. COM Reports

Are the report input summary and output reports adequate? Please note any additions to the reports that you would find helpful?

Please see above comments about possibly adding a more thorough listing of the sources of the values.

INHALATION EXPOSURE

7. Default Inhalation Scenarios

Are the default inhalation scenarios appropriate and adequate? Note, the default scenarios currently included in COM represent those most often encountered by OPPT. Are these scenarios easy to understand and use?

The default inhalation scenarios seem appropriate and adequate, and are easy to understand and use.

Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario. Specifically note any areas or assumption that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Sprayed on Surface - Fabric Protection, Aerosol Paint
- Product Added to Water - Laundry Detergent
- Product Placed in Environment - Solid Air Freshener

See other comments about making sure data from most recent edition of the Exposure Factors Handbooks are used (another example is Table 16-23's data for "Number of Minutes Spent in Activities Working with or Near Household Agents Such as Scouring Powders or Ammonia").

COM Peer Reviewer COMMENTS

8. Emissions Rate Assumptions

Are the indoor air concentration emissions rate assumptions (i.e. incremental, constant, aerosolized) appropriate for each default scenario?

No comments except the assumptions seem reasonably appropriate.

9. User-Defined Inhalation Scenario

Is the user-defined inhalation scenario easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

Yes (see above comments about user-friendliness).

10. Exposed Population Assumptions

Are the default body weight and incorporation of exposed population considerations appropriate?

Care should be taken to consider/use the recommended default values in the latest edition of the Exposure Factors Handbook, e.g., Table 7-3 of the Exposure Handbook has 13.3 kg as the body weight of a 2 year old and 36.3 kg for a 10 year old (the 71.8 kg for an adult does agree with the Exposure Factors Handbook). Other examples include consideration of the various recommended infant, child, and adult inhalation rates shown in Table 5-23.

Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

See above comments.

11. Inhalation Inputs

Are default frequency of use, years of use, mass of product used, duration of use, inhalation rate during and after use, portion of aerosol in air, and air exchange rate values appropriate for each scenario?

See above comments about need to consider/use/note values from the most recent edition of the Exposure Factors Handbook, e.g., Tables 16-2 and 16-3 have frequency of use and exposure time of use values for fabric protectors ("water repellents/protectors"), latex paint, and aerosol spray paint → the current COM default values do not necessarily agree with either the mean, 90th, or

COM Peer Reviewer COMMENTS

other percentile values in the Exposure Factors Handbook even though both COM and the Exposure Factors Handbook are both said to use "Westat, 1987" data.

Another example is COM's "Whole House Volume" of 321 m3 → the recommended value in the most recent edition of the Exposure Factors Handbook is 369 m3 (Table 17-1 and Page 17-24). (I will note that the 0.45 "Air Exchange Rate" is the recommended value in the current Exposure Factors Handbook.)

Also, my personal exposure assessment files suggest that the Westat, 1987 report contains frequency of use and other information for general purpose cleaners (listed in the Westat report as liquid cleansers and powdered hard surface cleaners according to my notes). Westat, 1987 apparently states that these products are used once per day, and a total of twice per week

Please provide your rationale for determining the appropriateness of the default values. Note any inputs or defaults that you feel are inappropriate and suggest alternate values.

See above comments about the Exposure Factors Handbook.

12. Day of Use and Day After Use Activity Patterns

Please comment on the default activity patterns and default room volumes. Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

See above comments about the Exposure Factors Handbook's information.

13. Physical/Chemical Property Information

Information on physical chemical properties (such as weight fraction) are used along with the Chinn algorithm to estimate the emission rate. Comment on the default weight fraction estimates provided. Specifically note any areas of concern or areas for improvement in the estimation of emissions.

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COM Peer Reviewer COMMENTS

14. Estimated Indoor Air Concentration

Does the inhalation exposure mass balance equation calculate indoor air concentrations appropriately and adequately? Specifically note any areas of concern, areas for improvement, or alternate calculation methodologies.

Yes, for the stated goals of COM's usage.

15. Inhalation Exposure Calculations.

Review of the COM QA/QC files: Are the inhalation exposure estimation equations adequately explained within COM and are they appropriate? Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

Yes.

16. Inhalation Exposure Descriptors

Are the inhalation exposure descriptors of high end/bounding appropriate given the default assumptions and the models used?

Yes.

Please provide your rationale for determining the appropriateness of the descriptors. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

My rationale included general agreement with other assumptions and calculations I have seen.

17. References

Are inhalation estimation references identified appropriately?

See above comments.

Would any additional reference citations be helpful? Please note any additional references that should be cited.

COM Peer Reviewer COMMENTS

18. Scenario-specific or Other Comments

DERMAL EXPOSURE REVIEW COMMENTS

19. Default Dermal Scenarios

Are the default dermal scenarios appropriate and adequate? Note that the default scenarios represent those most often encountered by OPPT.

The default dermal scenarios seem appropriate and adequate, and are easy to understand and use *except* for easy comprehension of the derivations of the "surface area to body weight ratio" and "amount retained on skin" values. Having additional text/examples (via footnotes?) describing these values would likely help many users [I do not think COM's simply stating "These values are equal to the product of the Film Thickness, Density, and Dilution (values not shown)" is enough].

Specifically note any areas or assumptions that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Added to Water - Laundry Detergent
- Product Directly Contacting Skin - Bar Soap, Used Motor Oil

The "General Purpose Cleaner" frequency of use of 300 is noted as "(e);" however, as noted above, my file notes suggest that the Westat, 1987 report has useful data. My files also note that the Westat, 1987 report's Appendix D contains U.S. EPA-developed film thickness data that might be considered for COM's "General Purpose Cleaner" and perhaps other products.

20. User-Defined Dermal Scenario

Is the user-defined dermal scenario easy to understand and use?

Yes. Also see above comments.

Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

See above comments.

COM Peer Reviewer COMMENTS

21. Dermal Inputs

Are the default amount retained on skin, frequency of use, surface area to body weight ratio, years of use, and exposure duration values appropriate for each scenario?

See above comments.

Please provide your rationale for determining the appropriateness of the default values. Note any areas of concern and suggest alternate values.

See above comments. My rationale included general agreement with the Exposure Assessment Handbook's and other sources of values I have seen.

22. Exposed population assumptions

Are the default body weight and incorporation of exposed population considerations appropriate (active vs. passive exposure assumptions)?

See above comments.

Please provide your rationale for determining the appropriateness of the default values. Note any assumptions that you feel are inappropriate and suggest alternate values.

See above comments. My rationale included general agreement with the Exposure Assessment Handbook's and other sources of values I have seen.

23. Physical/Chemical Property Information

Comment on the default weight fraction values and the use of weight fraction in the dermal dose calculations. Note any areas of concern and suggest alternate values.

No comments.

24. Dermal Potential Dose Rate

Please comment on the use of potential dose rates to calculate dermal exposures in the default scenarios. Note any areas of concern, areas for improvement, or alternate calculation methodologies.

COM Peer Reviewer COMMENTS

25. Dermal Flux Rate Equation

Is the flux rate equation for calculating absorbed dermal exposure in the User-Defined Scenario adequate and appropriate? Note any areas of concern, areas for improvement, or alternate calculation methodologies.

Yes.

26. Dermal Exposure Calculations

Review of the COM QA/QC files. Are the dermal exposure estimation equations adequately explained within COM and are they appropriate?

See above comments.

Does the dermal exposure equation calculate exposure appropriately and adequately?

Yes.

Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

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27. Dermal Exposure Descriptors

Is the dermal exposure descriptors of "what-if" appropriate given the default assumptions? For example, do you think that it may be appropriate to classify the dermal estimates as being high end or bounding?

Yes.

Please provide your rationale for determining the appropriateness of the descriptor. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

My rationale included general agreement with other assumptions and calculations I have seen.

COM Peer Reviewer COMMENTS

28. References

Are references identified appropriately?

No, see above comments.

Would any additional reference citations be helpful?

Should note how to obtain/view latest edition of Exposure Factors Handbook.

Please note any additional references that should be cited.

If general references are added, might be useful to include:

G. K. Whitmyre, J. H. Driver, and P. J. Hakkinen, "Assessment of Residential Exposures to Chemicals," Chapter II.1, Pages 125-141 in "Fundamentals of Risk Analysis and Risk Management," edited by V. Molak. CRC Press, Inc., Boca Raton, Florida, 1997.
(Discusses EPA's SCIES, MCCEM, Exposure Factors Handbook, Dermal Exposure Assessment: Principles and Applications, etc.)

29. Scenario-specific or Other Comments

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Appendix D

PEER REVIEW COMMENTS
SUBMITTED BY DR. MUHILAN PANDIAN

Comments by
Muhilan Pandian

COM Peer Reviewer COMMENTS

Charge

You are required to enter your comments on items 1 through 29 listed below in the enclosed electronic file, COM.WPD, using WordPerfect or Microsoft Word software. Return your comments no later than August 12, 1998 via U.S. mail or electronic mail. If you submit your comments via electronic mail, address the message to gkitzmil@erg.com. Feel free to comment on items not specified below.

GENERAL COMMENTS

1. Summarize your comments in order of importance. In addition, please summarize any suggestions for improvement or alternate estimation methodologies.

- To obtain high-end estimates, a procedure to conduct Monte Carlo simulations must be considered.
- Dermal exposure assessment can be improved by consulting with OPP (Office of Pesticide Programs).
- The program should be tested thoroughly. It crashed and hung up Windows quite a few times.
- Cosmetic changes mentioned below could be implemented.

2. What is your overall level of confidence in COM's "high end/bounding" screening level inhalation estimates? Please provide your rationale for assessing level of confidence.

Based on the descriptions of "high-end/bounding" screening level inhalation estimates, COM does not calculate bounding estimates. Statistically speaking, in the case of "high-end" screening level inhalation estimates, using the 90th percentile values for the input variables does not give you the 90the percentile values for the outputs. Based on the median and the 90th percentile values that are used as inputs, a distribution should be specified and a Monte Carlo simulation (or something similar) done to estimate the 90th percentile values for the outputs.

Also, not all the input variables are correctly represented for their median and 90th percentile values.

In light of the above two issues, my level of confidence in COM's high-end screening level inhalation estimate is low.

3. What is your overall level of confidence in COM's "what-if" screening level dermal exposure estimates? Please provide your rationale for assessing level of confidence.

COM Peer Reviewer COMMENTS

Estimating "Amount retained on skin (g/cm^2)" is a very complex process. The manner in which this input variable is represented in COM is very uncertain. Therefore, my level of confidence in COM's "what-if" screening level dermal exposure estimate is low.

Conceptually, "Amount retained on skin" is dermal exposure. Anything beyond that is dermal dose.

4. COM Ease of Use

Is the model easy to use? Specifically note any data entry screens you found confusing or unclear. Provide suggestions to improve the user-friendliness of COM.

COM is relatively easy to use.

An implementation that could be confusing: Two different type of menus - 1) drop down (File, etc.) and 2) tabbed (Scenario, etc.)

Specific comments:
- When COM is started, grey all the tabs except "Scenario". When a scenario is picked, grey "Scenario" and ungrey the next relevant tab; and so on .....
- It would be visually more appealing if all the titles were in one color, all the input variable names in another color, and all the input values in yet another color.
- Rearrange input tabs accordingly: Introduction, Scenario, Inhalation Input, Day of Use, Days after use, Dermal Input, PChem Properties.
- "PChem" dose not seem appealing.
- Why is the "Submit Data for Calculation" button part of "PChem Properties"? Could it be outside the input regions?

5. COM Help Screens

Are the Help screens adequate? Describe any additional help screens that you would find useful.

It is not clear how the different source releases are handled. Similar to the differential equations provided for mass balances of a chemical in the two zones, calculations should be provided to explain the source models (incremental, etc.).

What is PMN Number?

COM Peer Reviewer COMMENTS

6. COM Reports

Are the report input summary and output reports adequate? Please note any additions to the reports that you would find helpful?

A graph depicting the concentration profiles in the two zones will be useful.

INHALATION EXPOSURE

7. Default Inhalation Scenarios

Are the default inhalation scenarios appropriate and adequate? Note, the default scenarios currently included in COM represent those most often encountered by OPPT. Are these scenarios easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario. Specifically note any areas or assumption that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Sprayed on Surface - Fabric Protection, Aerosol Paint
- Product Added to Water - Laundry Detergent
- Product Placed in Environment - Solid Air Freshener

The default scenarios seem sufficient.

8. Emissions Rate Assumptions

Are the indoor air concentration emissions rate assumptions (i.e. incremental, constant, aerosolized) appropriate for each default scenario?

Cannot provide comments until the actual calculations behind the source models are transparent.

9. User-Defined Inhalation Scenario

Is the user-defined inhalation scenario easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

It takes quite a while to understand the organization of the following tabbed input sheets: "Inhalation Input", "Day of Use", and "Days After Use".

COM Peer Reviewer COMMENTS

10. Exposed Population Assumptions

Are the default body weight and incorporation of exposed population considerations appropriate? Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

Values provided are appropriate as they are based on values from the Exposure Factors Handbook.

11. Inhalation Inputs

Are default frequency of use, years of use, mass of product used, duration of use, inhalation rate during and after use, portion of aerosol in air, and air exchange rate values appropriate for each scenario? Please provide your rationale for determining the appropriateness of the default values. Note any inputs or defaults that you feel are inappropriate and suggest alternate values.

Quite a few of the values are based on "Best Professional Judgement". It should be mentioned somewhere who, what group, or what committee, was involved here.

12. Day of Use and Day After Use Activity Patterns

Please comment on the default activity patterns and default room volumes. Please provide your rationale for determining the appropriateness of the default values. Note any assumptions or defaults that you feel are inappropriate and suggest alternate values.

Values provided for room volumes are appropriate as they are based on values from the Exposure Factors Handbook.

There is no mention of where the default activity pattern information came from. There is a lot of useful information in the EPA-sponsored National Human Activity Pattern Study (NHAPS) that was done in 1992-94. Why is the user restricted to 1-hour chunks. Provision should be made to include activity pattern information in a one minute resolution, if needed.

13. Physical/Chemical Property Information

Information on physical chemical properties (such as weight fraction) are used along with the Chinn algorithm to estimate the emission rate. Comment on the default weight fraction estimates provided. Specifically note any areas of concern or areas for improvement in the estimation of emissions.

Defaults seem okay.

COM Peer Reviewer COMMENTS

14. Estimated Indoor Air Concentration

Does the inhalation exposure mass balance equation calculate indoor air concentrations appropriately and adequately? Specifically note any areas of concern, areas for improvement, or alternate calculation methodologies.

The methodology to calculate indoor air concentrations is okay. However, as stated above, it is unclear how the sources are treated mathematically.

15. Inhalation Exposure Calculations

Please review the enclosed COM QA/QC files. Are the inhalation exposure estimation equations adequately explained within COM and are they appropriate? Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

Inhalation exposure calculations and QA/QC methodologies are okay.

16. Inhalation Exposure Descriptors

Are the inhalation exposure descriptors of high end/bounding appropriate given the default assumptions and the models used? Please provide your rationale for determining the appropriateness of the descriptors. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

See comment for Question 2.

17. References

Are inhalation estimation references identified appropriately? Would any additional reference citations be helpful? Please note any additional references that should be cited.

Use activity pattern information from the EPA-sponsored National Human Activity Pattern Study (NHAPS) and reference it.

18. Scenario-specific or Other Comments

None.

COM Peer Reviewer COMMENTS

DERMAL EXPOSURE REVIEW COMMENTS

19. Default Dermal Scenarios

Are the default dermal scenarios appropriate and adequate? Note that the default scenarios represent those most often encountered by OPPT. Specifically note any areas or assumptions that you feel are inappropriate. Provide suggestions and references for alternate default assumptions.

- Product Applied to Surface - General Purpose Cleaner, Latex Paint
- Product Added to Water - Laundry Detergent
- Product Directly Contacting Skin - Bar Soap, Used Motor Oil

The default scenarios seem sufficient.

20. User-Defined Dermal Scenario

Is the user-defined dermal scenario easy to understand and use? Specifically note any areas that you found confusing or unclear. Provide suggestions to improve the user-friendliness of this scenario.

Considering the simplicity of the representation for the dermal scenario, it is easy to understand.

21. Dermal Inputs

Are the default amount retained on skin, frequency of use, surface area to body weight ratio, years of use, and exposure duration values appropriate for each scenario? Please provide your rationale for determining the appropriateness of the default values. Note any areas of concern and suggest alternate values.

Except for "Surface area to body weight ratio", all the other inputs are based on "Best Professional Judgement". I strongly recommend exploring the "Applicator Scenarios" considered by EPA's OPP (Office of Pesticide Programs).

22. Exposed population assumptions

Are the default body weight and incorporation of exposed population considerations appropriate (active vs. passive exposure assumptions)? Please provide your rationale for determining the appropriateness of the default values. Note any assumptions that you feel are inappropriate and suggest alternate values.

COM Peer Reviewer COMMENTS

Values provided are appropriate as they are based on values from the Exposure Factors Handbook.

23. Physical/Chemical Property Information

Comment on the default weight fraction values and the use of weight fraction in the dermal dose calculations. Note any areas of concern and suggest alternate values.

Defaults seem okay.

24. Dermal Potential Dose Rate

Please comment on the use of potential dose rates to calculate dermal exposures in the default scenarios. Note any areas of concern, areas for improvement, or alternate calculation methodologies.

Dermal exposure is used to calculate potential dose rate and not the other way around. I strongly recommend exploring the "Applicator Scenarios" considered by EPA's OPP (Office of Pesticide Programs).

25. Dermal Flux Rate Equation

Is the flux rate equation for calculating absorbed dermal exposure in the User-Defined Scenario adequate and appropriate? Note any areas of concern, areas for improvement, or alternate calculation methodologies.

Check descriptions and units. Flux has the units of (mass)/[(length)^2(time)]. The equation provided to estimate absorbed dermal exposure (in the case of User Defined Scenario) is not appropriate. There is no variable that represents amount dermally exposed.

26. Dermal Exposure Calculations

Please review the enclosed COM QA/QC files. Are the dermal exposure estimation equations adequately explained within COM and are they appropriate? Does the dermal exposure equation calculate exposure appropriately and adequately. Specifically note any areas for improvement, alternate calculation methodologies, or alternate QA/QC methodologies.

Dermal exposure calculations and QA/QC methodologies are okay.

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27. Dermal Exposure Descriptors

Is the dermal exposure descriptors of "what-if" appropriate given the default assumptions? For example, do you think that it may be appropriate to classify the dermal estimates as being high end or bounding? Please provide your rationale for determining the appropriateness of the descriptor. Note any assumptions or calculations that you feel are inappropriate and suggest alternate values.

"What-if" has no relationship with "high-end/bounding" estimates.

28. References

Are references identified appropriately? Would any additional reference citations be helpful? Please note any additional references that should be cited.

EPA's OPP (Office of Pesticide Programs) has conducted numerous dermal exposure assessments that will be useful guidance for this office.

29. Scenario-specific or Other Comments

None.

Appendix E

PEER REVIEW COMMENTS
SUBMITTED BY WILLIAM POPENDORF

Comments by
W. Popendorf

COM Peer Reviewer COMMENTS

GENERAL COMMENTS

1. **Summarize your comments in order of importance. In addition, please summarize any suggestions for improvement or alternate estimation methodologies.**

2. **What is your overall level of confidence in COM's "high end/bounding" screening level inhalation estimates? Please provide your rationale for assessing level of confidence.**

A better description of High End Bounding is definitely needed. I assume that all the 90th percentile values are used in the H-E/B calculation. Normally a 90th percentile outcome would be based on the distribution of results from a random combination of input values. Thus, the High End calculated as above is more extreme than a 90th percentile outcome. As a quick guess, I'd predict that the probability of the High End outcome would be about the inverse of the product of the number of 90th percentile values that went into it. Thus, the probability for n = 3 (two 90ths from the Inhalation screen and one from the PChem screen) is about $1 - (1 - .90)^3 =$ 99.9th percentile. That is OK if it is clearly stated somewhere. An alternative is to calculate the cumulative 90th% variance using Propagation of Error theory; that wouldn't be too hard within the program.

Furthermore, there is no equivalent High End Bounding for Dermal doses. Based on my experimental field survey data, Dermal doses are even more variable than are Inhalation doses. This high variability is also consistent with the mechanisms involved, if you think about how people get dermally dosed.

3. **What is your overall level of confidence in COM's "what-if" screening level dermal exposure estimates? Please provide your rationale for assessing level of confidence.**

(See question #6.)

4. **COM Ease of Use**

I had an egregious problem installing the software. The inhalation calculations would not function properly when installed in other than the root directory (I try to keep that directory to a minimum). Repeated attempts resulted in either execution errors or a complete lockup. There also seemed to be a major problem trying to output to my printer (HP 6L) that eventually resulted in having to reinstall the printer drivers. It would also be useful if one could install IDAPI before having to exit the installation sequence and reboot.

Page notations that follow (e.g. p. #) refer to the text in Attachment 2.

Comments by
W. Popendorf

COM Peer Reviewer COMMENTS

p. 1: Change It's (a contraction) to Its (a possessive). Similarly, on the very first screen, "site" should be changed to "cite."

p. 2: The double arrows on the Option screen can be misleading either by looking like a "do not" type kind of X or by appearing to cross-reference diagonal options, for instance "Begin New Consumer" with "Open Existing Occupational File", or the other two corners. Vertical arrows would still show color but at least appear to link something in common.

p. 4: Reference to COM in line 4 of the discussion of the Help button is confusing. When first reading this text, it appears that both references to COM should be "HELP." Only when seeing COM on the bottom of the screen does the text make sense; COM is apparently the title of the Help screen. However, it would help to change its title to HELP (it would avoid the problem of having to remember that the COM title means HELP). On the other hand, at least on my screen this point was moot in that the Help screen starts out smaller than the input screen.

The way back to the basic Option screen was not obvious. It seemed that once I got to the "Welcome" or "Introduction" screen, the only way back to select a new option (e.g. either a Beginning or Existing File) was to either submit a problem for calculation or to exit and re-enter. Eventually I found the inner X box would do the trick, but a note somewhere or a "previous screen" button would help.

p. 5: It is unclear which boxes are required data and which are optional. That is true beginning right at the opening Welcome screen (although the text does say these boxes are optional). If there is any chance of using something other than default values, the only way one finds out that a variable is required is by the message on trying to exit to the next screen. Color coding required data (or default data) would be nice. And upon trying to exit and getting a missing data message, it would be handy if the cursor went back to the missing data box.

In the same vein, the documentary descriptions supporting the model led me to believe that specifying the PMN and Product would allow the model to access a physical chemistry data file. I assume by experience that the input of PMN and Product are used only to label the output. Clarifying their more limited purpose could be aided by the above color coding or/and further changing the documentation. If there is a way to access imbedded data (e.g., the dermal flux data), it would be easier and help to avoid errors from synonyms to define these chemicals by their CAS number.

At the same time, it would seem that PMN and Product are **inadequate** to document the pertinent output of an individual chemical within a product especially if a mixture is being modeled. Several input parameters in the PChem screen such as Weight Fraction, Molecular Weight, and Vapor Pressure could differ within the same product and use scenario and cause

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changes in the dose. The Chemical Name is input but isn't used or output. The Chemical Name identified on the PChem screen should be carried through to all output files.

p. 8 and 11: It would help in both cases to tell the reader near the top of the page to "See the following table for default values." Finding them unexpectedly two pages later was frustrating.

p. 9: Cross-reference to the use zone volume (Zone 1 Volume in the "Day of Use" screen) should be made in the context of the Whole House Volume. These two volumes show up on separate screens and need some clearer linking. The marginal explanations of the use zone volume (Zone 1 Volume) on p. 14 could be improved.

p. 9 and p. 12: A small thing, but I would write the units for Acute Averaging Time like the other two averaging times (I first thought the units as written referred to Acute Potential Dose Rate).

p. 11: The Amount Retained on the Skin is probably both misleading or/and incorrect. Dilution does not seem to play a part in the amount retained (see further discussion in question #21).

p. 20: Despite the note at the top of the page, I am so used to seeing equations listed sequentially by number that I immediately started to renumber the references in parentheses after each equation into sequential equation numbers. One suggestion for incorrigibles like me is to add "ref. " into each parenthesis. Another is to list both equation number and reference, e.g. "(Eqn. 1 from ref. 1)".

The third equation has a subscripting error. $\sum$Sources + $\sum$CiQji should be $\sum$Sources + $\sum$CjQji etc. Some text defining those subscripts would help, such as inserting " subscripted as flows from and to" right after "Q refers to a flow rate."

p. 21: see question #8 about emission rates.

p. 21 - 23: It would help if a qualifier were added to each of these equations. E.g. the equation at the bottom of p. 21 is "Inhaled Dose...", that near middle of p. 22 is "Air Concentration...", that near the bottom of p. 22 is "Potential Dermal Dose...", and that in the middle of p. 23 is "Absorbed Dermal Dose..."

p. 23: Something is missing in the second sentence of third paragraph: "Potential dose is the amount a chemical contained..." doesn't quite make sense.

5. COM Help Screens

OK.

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6. COM Reports

The meaning of the "Descriptor" column was unclear. Similarly the AT data seemed to be the same as the input data. The H-E/B versus "what-if" did not seem to affect the AT column; I got both labels on the same run (H-E/B for dermal and what-if for inhalation). I presume the Descriptor might affect the Result, but somewhere I missed its significance, and still don't understand it.

INHALATION EXPOSURE

7. Default Inhalation Scenarios

Aerosol Paint Frequency of Use (6 times per year from Westat, 1987) seems high for the median consumer. Doing some calculations on 3635 grams median used seems to be about 1 gallon which should cover about 400 ft^2 on the label. Assuming an 8 foot ceiling for the default 40 m^3 room yields a floor area of 177 ft^2 which in a square room means 425 ft^2 of wall. Thus, each event is about right to paint about one 13 foot square room. There are about 8 such rooms in a 321 m^3 house. How many people paint 6 such rooms (about 3/4 of their house) each year for eleven years? That is a lot of painting. Two or three events per year seem high for me and most of my acquaintances but more plausible.

8. Emissions Rate Assumptions

It is not clear from the material provided (mostly on p. 21) and the time available which if any exposure scenarios used the Chinn method. That method seems to be suited specifically to evaporation from an aerosol or droplet. As outlined on p. 21, not all uses fall into that category. I agree that an exponential model is appropriate to general purpose cleaners, latex paint, and I'd even add applied aerosol paint that all form a surface film of one sort or another. Laundry detergents should use Henry's Law, but that was not mentioned on p. 21 (see also question #13). Solid air fresheners are unlikely to emit at a constant rate throughout their life unless they are actually removed by the user according to a schedule based on the manufacturer's test data showing when it will deviate from a constant "permeation" rate. A full analysis of the evaporation model used in each scenario and their possible differences in outcome would take more time (and perhaps more information) than was available.

9. User-Defined Inhalation Scenario

See question #13.

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10. Exposed Population Assumptions

OK

11. Inhalation Inputs

Some guidance for User Defined scenarios would be useful.

12. Day of Use and Day After Use Activity Patterns

OK

13. Physical/Chemical Property Information

I presume that somewhere it should be made clear that this input vapor pressure value is for the pure chemical compound if my understanding is correct that the computer will calculate a reduced vapor pressure using Raoult's Law for ideal mixtures for non-aqueous mixtures and Henry's Law for aqueous mixtures. That could be clarified on p. 18 of the text if not on the screen.

One small point: you might also list "mmHg" along with torr as the units for vapor pressure; they are equivalent (it is probably arguable which is more commonly understood).

With regard to milliequivalents, rather than have the user divide the molecular weight by the valance number, it would seem much easier for the user to input just the valance number [default = 1] and have the computer do the calculation.

See also question #21 for inputs and uses for the Weight Fraction. Because the default weight fraction estimates were not easily accessible for all scenarios, I did not have time to review them all or to compare them to other sources, but I did notice that 0.013 for enzymes in laundry detergent seems exceedingly high; I would expect that might be more in the range of 10^{-4} to 10^{-6}.

14. Estimated Indoor Air Concentration

OK

15. Inhalation Exposure Calculations

OK

COM Peer Reviewer COMMENTS

16. Inhalation Exposure Descriptors

See question #3.

17. References

OK

18. Scenario-specific or Other Comments

OK

DERMAL EXPOSURE REVIEW COMMENTS

19. Default Dermal Scenarios

Liquid Laundry Detergent events per year (from professional judgement) seemed unclear. I presume the median was for users of liquid detergents and that each event was a washing cycle. Under inhalation, there were 312 events (6 washings per week) each lasting about 20 minutes; that sounds OK. But why only 52 dermal events? Is spillage, dispenser leakage, or water immersion assumed? Spillage may occur one out of six washes, but contact with a contaminated dispenser or water immersion is likely to be much more frequent, perhaps approaching 312 events. It looks like both hands (1120 cm^2) of skin contact is assumed. I doubt that one would get detergent on both hands from spillage; from the dispenser, maybe so but still not commonly from immersion (assuming we are talking about automatic washers and not ringers). Some of this variation in the exposure scenario may be taken into account by the Amount Retained on the Skin, but if so, it is obscured (see question #21).

20. User-Defined Dermal Scenario

See comments regarding the Surface Area to Body Weight Ratio in question #21.

21. Dermal Inputs

The Surface Area to Body Weight Ratio seems needlessly obscure. Why not input the exposed skin area for the average person? These values can be obtained by multiplying the current defaults by the nominal 71.8 kg or from values in the Exposure Factors Handbook. It would be easy to add a drop-down list of the areas of body parts or some series of subjectively selected default body areas that would yield the current default Ratio values. Similarly, one could much more easily interpret the assumed exposure scenario from the default body areas. And any variation in these areas could be calculated in proportion to other than default body weights input

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on the Inhalation screen. In a related mater, the single asterisk footnote is not correct; for instance, the Ratio values have nothing to do with Frequency of Use but do appear to correspond to the exposed part of the body, which is only the whole body for the Bar Soap users. As written, a better footnote might be "These values equate to exposed skin surface area divided by the body weight." If changed to exposed area, a footnote is probably not needed.

Amount Retained on Skin is really confusing (even more than the above Ratio). Density is supposedly used but it is not entered via any scenario (default or otherwise). Dilution is supposedly used and it would seem is input via the Weight Fraction on the PChem screen. As near as I can tell, changing the Weight Fraction does affect the output but does not affect the Amount Retained on the Skin. Thus, it appears that Amount Retained is really driven by Film Thickness (as it should be). It would seem that asking for the user to input Film Thickness or to select a value from a list would be a lot simpler and more understandable than asking for the Amount Retained. At the very least, a much better explanation of Amount Retained is needed. There is an unexplained wide (huge) difference in the g/cm²/event for Laundry Detergent and Bar Soap versus the other dermal scenarios.

22. Exposed population assumptions

OK

23. Physical/Chemical Property Information

See questions #13 and #21.

24. Dermal Potential Dose Rate

OK

25. Dermal Flux Rate Equation

Didn't have time to evaluate this one.

26. Dermal Exposure Calculations

Didn't have time to evaluate this one.

Comments by
W. Popendorf

COM Peer Reviewer COMMENTS

27. Dermal Exposure Descriptors

As I mentioned in question #2, there should be an equivalent High End Bounding for Dermal doses. Based on my experimental field survey data, Dermal doses are even more variable than are Inhalation doses. This high variability is also consistent with the mechanisms involved, if you think about how people get dermally dosed.

28. References

Didn't have time to evaluate this one.

29. Scenario-specific or Other Comments

OK

Appendix F

PEER REVIEW COMMENTS
SUBMITTED BY BRAD SHURDUT

Comments by:
Brad Shurdut

COM Peer Reviewer COMMENTS

The primary objective of this model should be to provide an initial screening of potential exposures to products used in the residential environment. As many of the critical defaults used in the exposure algorithms are determined via *professional judgment*, it is unclear whether all the available data was considered as part of the process. It appears that the dearth of information currently available for a number of the parameters relevant to residential assessments precludes such development of relatively simplistic algorithms to describe rather complex exposure scenarios in many of the cases. However, having said that, the model can and does provide conservative assessments useful for the preliminary evaluation of exposures when actual measurements are not available. Exposure estimates derived from this model can subsequently be used to further identify and prioritize chemical specific data needs to refine exposure estimates as needed.

General Comments:

- Although the introduction to the model states that the model may be used for the assessment of exposures to pesticides, no scenarios related to pesticide use are present in model.

- Potential exposures to chemicals used in the residential environment may result in exposures to the individual handling the products as well as those in the home post-application.

- The model does not adequately provide for the assessment of acute toxins. Based on the toxicity of a chemical, it may be appropriate to evaluate daily exposures if a chemical is associated with acute toxicity. Furthermore, in the case of air fresheners that are placed inside the home, air concentrations would likely be transient in nature with a rapid decrease in indoor air concentrations post-application or spray. Amortization of chemical risks would only be relevant for chemicals that exert there toxicity based on cumulative or chronic exposures (e.g, carcinogenic effects). Calculation of daily exposures following the use of a product in the home may be relevant for comparison with acute NOELs or endpoint derived for the acute toxin. This is typically done for urban pesticides which tend to decrease rapidly from the home environ shortly after application. Consistent with this policy, the EPA-OPP has provided guidance to evaluate exposures lasting from 1-7 days in light of an acute NOEL .

- Since 'best professional judgment' is typically used to fill in essential parameters in the exposure algorithm, there are a number of instances where better empirically based estimates should be used (inhalation defaults: duration of use of fabric protector liquid laundry detergent, solid air freshener). These values are critical to the estimation of potential exposures which are generally described as

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concentrations multiplied by durations of exposure. Durations associated with the use of consumer products should be available through surveys conducted by registrants and consumer groups. Numerous contracted surveys have been completed by registrants that may provided meaningful input for this exercise (i.e, Proctor and Gamble, etc.).

- The "mass of product used" descriptor should be omitted and/or supplemented with the volume of product used (especially in the case of liquid based products such as liquid detergent, general purpose cleaner). Since concentrations of a product being used may vary greatly from one product to another, the amount of product likely to be used per event would be more generalizable between different products than the mass of product used. If this change were to be made, then it would also require that the algorithm incorporate a default concentration factor as a multiplier.

- The Exposure Factors Handbook was recently updated and re-published. As a result, the default factors assimilated into this model from the 1996 Version of the handbook should be updated to reflect any changes.

- The inhalation bounding estimates seem reasonable for all the use patterns. The bounding estimate for the laundry detergent seems to be particularly high. Although it may take an individual several hours to complete his/her laundry, it is highly unlikely that an individual would be handling the detergent (pouring into machine) for almost 40 minutes a day. Even if an individual completed several washes a day, the pouring event is somewhat transient and should be measured in the order of seconds/event rather than minutes. Perhaps the scenario of washing manually should be removed from this assessment and included as a new, distinct use pattern to be assessed.

- The model is generally easy to use. The 'day of use' and 'days after use' screens are somewhat confusing for the user. It is unclear unless you have an advanced understanding of the underpinnings of this model as to the actual incorporation of these inputs into the exposure assessment. In addition, the NOTE on the 'day of use' screen further confuses matters and does not clarify anything for the user as probably intended. It is also not clear why this screen is only associated with inhalation exposures. Although this is intuitive, potential dermal exposures may also be dependent on the room of occupancy. For example, assuming that this model is developed to evaluate pesticides used in the home (as indicated in the program's introduction), if a pesticide directly applied to carpeted surfaces in a specific room, then dermal exposures are very dependent on whether there is activity in that room.

Comments by:
Brad Shurdut

COM Peer Reviewer COMMENTS

SPECIFIC COMMENTS

- The model relies exclusively on the 'film thickness' model where it is assumed that an amount of material may be retained on the skin following use which is subsequently absorbed into the body (i.e, body burden or dose). Although this may be appropriate in some instances, generally only the monolayer contacting the skin would subsequently be absorbed percutaneously unless the residue was present for a longer duration. Therefore, it would likely be more appropriate to assume that an exposure would occur to the area-equivalent of the exposed body surface. For example, when using a bar of soap, surface residue would be equivalent to the surface area of the hand. Upon calculating the concentration of the chemical of interest in the soap, one can assume that the concentrated material would coat the surface area of the hands. A dermal penetration factor may then be used to ascertain the amount of chemical subsequently absorbed through the skin. Alternatively, a flux rate method may be used for this step as proposed.

- For products applied to surfaces, exposures may be generally split into two distinct categories: exposures during application to surfaces and subsequent exposures following contact with treated surfaces. If the product is applied to a surface, then exposure upon subsequent contact with that surface could be determined as a product of dislodgeable residues from that surface (DR) and area contacted. For example, studies have shown that less than 10% of an applied pesticide to either smooth or carpeted surfaces may be removed upon contact. Therefore, the application rate of a product multiplied by 10% would result in an upper bound estimate for dislodgeable residues. The amount of material dislodged would also be proportional to the area contacted. The sprayed area contacted (m2) multiplied by the dislodgeable residue fraction (ug/m2) would yield the potential dermal loading for a resident contacting the treated area which would then be corrected for dermal absorption to determine potential dermal dose.

- Activity and use patterns are critical parameters to the evaluation of exposures. The dearth of information related to a number of the these parameters critical to the assessment of exposures compromises the utility and relevance of these proposed guidelines. To optimize the utility of this model, data currently available and currently being developed within a number of efforts should be considered. The development of information, such as use and usage information and activity patterns, is an iterative, ongoing process. Given the importance of these parameters in these assessments, OPPTS should continue to collect and/or develop data to refine many of the 'professional judgment' assumptions included in the default values describing use frequency, etc. The longer term development of questionnaires or surveys refining these default values should continue to be a

COM Peer Reviewer COMMENTS

focus of OPPTS as it is now becoming a focus of the EPA Office of Pesticide Programs for implementation of the Food Quality Protection Act of 1996. In fact, intra-industry efforts, such as the Outdoor Residential Exposure Task Force (ORETF) and the CSMA sponsored Indoor Residential Exposure Joint Venture (IREJV) are both developing data on use and usage information, as well as on activity patterns as it relates to potential pesticide exposures in the urban environment. Such collaborative efforts should be considered for development of similar data with general applicability to the COM model.

- The somewhat unique feature of linking exposures with activity patterns within the home is an extremely useful feature. In the case of exposures following either the painting or spraying of surfaces, the location of the resident in relation to the application is critical to evaluate exposures. Although this seems to add a level of complexity to the model for the user, recognition of the relationship between potential airborne concentrations over time and room of occupancy is integral to a more refined exposure assessment.

Given my cursory review of this model, the overall strength of this model is the 'user-friendliness' and organization of the screens. In addition, the added complexity of activity-based assessments is also extremely useful when conducting product specific evaluations. On the other hand, the potential weaknesses or problems with this model is the widespread use of estimates and default values based upon 'professional judgment'. As mentioned previously, many of these estimates seem to be overly conservative and, in many cases, beyond reality. Understanding that bounding estimates must represent extreme values at the tail of the distribution for the sake of calculating conservative risk estimates, extreme estimates beyond the tails of a distribution should not be used for screening assessments. Although 'professional judgment' is often used as a temporary gap-filler for exposure algorithms, they often become rebuttable presumptions which the regulators often construe as fact over time. Consequently, an effort should be made to verify some of the default values included in the model (i.e, frequency of use, etc.).