

May 8, 2000

EPA SAB-EC-ADV-00-004

Honorable Carol M. Browner
Administrator
U.S. Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, DC 20460

Subject: Advisory on the Agency's "Total Risk Integrated Methodology" (TRIM)

Dear Ms. Browner:

The Environmental Models Subcommittee (EMS), hereinafter referred to as the "Subcommittee", met December 13-14, 1999 to review the "Total Risk Integrated Methodology (TRIM) Status Report", the draft "TRIM.Expo Technical Support Document" and the two volume "TRIM.FaTE Technical Support Document" developed by EPA's Office of Air Quality Planning and Standards (OAQPS). The Subcommittee conducted this advisory in order to provide the Agency with advice and insights on the adequacy of the proposed TRIM approach to predict exposures and risks posed by air pollutants.

In general, we find the OAQPS' ongoing efforts to develop TRIM as a flexible, state-of-the-art system for evaluating multimedia chemical fate, transport, exposure and risk, to be effective and innovative. The OAQPS staff and its consultants have been responsive to our previous advice on components of TRIM.FaTE that required further consideration and improvement. While current knowledge and available methods continue to limit the rigor and accuracy with which Hazardous Air Pollutant (HAP) impacts can be assessed, OAQPS is developing a system capable of recognizing and characterizing these limitations and attendant uncertainties. Much of our review focuses upon ongoing efforts that can help to promote further advancement and reduction of these uncertainties. Specific findings and recommendations are as follows:

The modular design and open architecture of TRIM provide a flexible and appropriate means of accommodating new scientific information. However, significant user guidance and support will be necessary to ensure that appropriate model setups and configurations are selected. Early workshops and beta testing of the integrated TRIM system by the affected user community are recommended to ensure the appropriate level of stakeholder input and a well-designed product.

Proposed plans for addressing uncertainty and variability within TRIM are innovative and consistent with the current state-of-the-art in the risk sciences. Significant user guidance and interface capabilities will be needed to ensure that these tools are utilized in an informed and well-documented

manner. The OAQPS should provide examples where uncertainty analysis and model evaluations are presented within the context of intended regulatory applications, such as the calculation of residual risk following implementation of emission reductions. Additional effort is also recommended to develop methods capable of capturing the effects of local, sub-compartmental variations in landscape properties, chemical concentrations and exposures.

Evaluation plans for TRIM.FaTE, including code validation, mass balance checks, model-to-model comparisons, and comparisons against observed data in field applications are appropriate, though further review of the results of these evaluations in the context of regulatory applications is necessary to ensure proper implementation and inferences. Evaluation plans should consider simultaneous test applications of the TRIM modules (FaTE, Expo and Risk) to ensure that model linkages are properly specified, with outputs from the upstream modules of the appropriate type and resolution for input to the subsequent module(s).

The Subcommittee is concerned that the planned field comparison for mercury may not be effective, because of the high degree of complexity and uncertainty in mercury chemistry, the large number of adjustable parameters that must be fit for the model, and the difficulty in obtaining adequate data to properly test the model. As such, planned field comparisons of mercury should be replaced or augmented by considering sites with other metals that undergo simpler fate and transport processes in the environment, so as to ensure that a successful model specification can be achieved.

Tests of the TRIM system at larger scales, such as for a metropolitan air basin with multiple stationary and mobile sources, are recommended to evaluate the ability of the TRIM system to operate at this scale of application and to utilize emerging electronic/GIS databases with geographic, meteorological, emissions, population and environmental resource information. Evaluation of the TRIM system should be a continuing process that encourages ongoing data collection and evaluation for local, site-specific applications, with iterative updates to the model structure, database and characterization of uncertainty. The application protocol for TRIM should provide incentives for the development of improved data collection methods (with improved sensitivity, accuracy and precision) and improved databases for model input.

Efforts to improve the TRIM.FaTE module to address local-scale atmospheric dispersion through the use of alternative air pollution models, to develop appropriate transport parameters for surface waters and air-soil mass transfer, to include kinetic, reversible reactions among metal species, and to incorporate seasonal effects in biotic processes, are appropriately focused. Specific recommendations are provided in our report to allow further improvements and focus. In each case, we emphasize the need for an effective user-interface that guides users in the selection of alternative modules and input parameters given the chemical(s), landscape properties, and types of exposures and risks addressed.

The design of TRIM.Expo and its use of existing modeling science for inhalation and ingestion exposures are, in general, consistent with OAQPS' programmatic and regulatory needs and the state-

of-the-art of exposure assessment. System flexibility is needed to allow the selection of time-activity patterns and exposure factors consistent with the necessary level of spatial and temporal detail, distinguishing between long-term chronic health endpoints and short-term acute effects.

The design of the TRIM.Risk module appears to be appropriate, though more details and example applications will be necessary for rigorous review. Particular care will be needed to ensure that the time scales for exposure and risk calculation are appropriately matched (in particular, for acute, non-cancer health effects associated with short-term and/or peak exposures, where current knowledge and guidance are lacking) and in providing options for incorporating emerging knowledge on pollutant interactions which may result in non-additive risk. Ecological risk endpoints and metrics are not well defined in TRIM (or in any other risk assessment framework currently available), and further work will be needed to provide appropriate options. The multi-chemical, multi-media design of the TRIM system provides the opportunity to explore methods for addressing new and emerging issues in risk assessment and the risk sciences, including the effects of mixtures, population susceptibility and cumulative risk; as well as metrics for environmental equity and ecological impacts at the population level. OAQPS should take advantage of this opportunity to suggest and illustrate possible approaches to these issues for broader Agency consideration and evaluation.

We thank the Agency for the opportunity to provide technical advice on this important effort at the interface of environmental science, modeling and regulatory need. The Science Advisory Board and its Environmental Models Subcommittee look forward to your response to our report, with a particular emphasis on the points raised in this letter to you, and for the opportunity for further focused reviews in the future.

Sincerely,

/s/

Dr. Morton Lippmann, Interim Chair
Science Advisory Board

/s/

Dr. Mitchell Small, Chair
Environmental Models Subcommittee
Science Advisory Board

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ABSTRACT

The Environmental Models Subcommittee of the EPA Science Advisory Board (SAB) reviewed the Agency's development of the Total Risk Integrated Methodology (TRIM) for predicting multimedia exposures and risks posed by hazardous air pollutants. The Subcommittee found the EPA TRIM model to be an innovative, flexible, state-of-the-art system for evaluating multimedia chemical fate, transport, exposure and risk. Specific recommendations are provided on efforts to improve the TRIM.FaTE module, planned field comparison studies of the TRIM system, and the design and implementation of the exposure and risk modules.

The Subcommittee determined that there is a need for OAQPS to better specify its plans and timeline for use of the TRIM system within the Agency and subsequent release to a broader user community. Early workshops and beta testing of the integrated TRIM system by the affected user community are recommended to help in the development of user guidance and support. The application protocol for TRIM should provide incentives for the development of improved data collection methods and improved databases for model input. For all current risk assessment models, including the TRIM system, new methods are needed to address emerging issues including: the effects of mixtures; population susceptibility and cumulative risk; and metrics for environmental equity and ecological impacts at the population level.

Keywords: TRIM, hazardous air pollutants (HAPs), multimedia environmental models, exposure assessment, risk assessment, validation, sensitivity analysis, uncertainty

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1. EXECUTIVE SUMMARY

The Environmental Models Subcommittee (EMS), hereinafter referred to as the “Subcommittee”, met December 13-14, 1999 to review the “Total Risk Integrated Methodology (TRIM) Status Report”, the draft “TRIM.Expo Technical Support Document” and the two volume “TRIM.FaTE Technical Support Document” developed by EPA’s Office of Air Quality Planning and Standards (OAQPS). The Subcommittee conducted this review in order to provide the Agency with advice and insights on the adequacy of the proposed Total Integrated Risk Methodology approach to predict exposures and risks posed by air pollutants.

The Subcommittee found the OAQPS’ TRIM model to be an innovative, flexible, state-of-the-art system for evaluating multimedia chemical fate, transport, exposure and risk. The Office of and its consultants were responsive to our previous advice on components of TRIM.FaTE that required further consideration and improvement. While current knowledge and available methods continue to limit the rigor and accuracy with which HAP impacts can be assessed, OAQPS is developing a system capable of recognizing and characterizing these limitations and attendant uncertainties. Much of the Subcommittee’s review focused upon ongoing efforts to help promote further advancement and reduction of these uncertainties. Specific findings and recommendations are as follows:

The modular design and open architecture of TRIM provide a flexible and appropriate means of accommodating new scientific information. However, significant user guidance and support will be necessary to ensure that appropriate model setups and configurations are selected. Early workshops and beta testing of the integrated TRIM system by the affected user community are recommended to ensure the appropriate level of stakeholder input and a well-designed product.

Proposed plans for addressing uncertainty and variability within TRIM are innovative and consistent with the current state-of-the-art in the risk sciences. Significant user guidance and interface capabilities will be needed to ensure that these tools are utilized in an informed and well-documented manner. The OAQPS should provide examples where uncertainty analysis and model evaluations are presented within the context of intended regulatory applications, such as the calculation of residual risk following implementation of emission reductions. Additional effort is also recommended to develop methods capable of capturing the effects of local, sub-compartmental variations in landscape properties, chemical concentrations and exposures.

Evaluation plans for TRIM.FaTE, including code validation, mass balance checks, model-to-model comparisons, and comparisons against observed data in field applications are appropriate, though further review of the results of these evaluations in the context of regulatory applications is necessary to ensure proper implementation and inferences. Evaluation plans should consider simultaneous test applications of the TRIM modules (FaTE, Expo and Risk) to ensure that model linkages are properly specified, with outputs from the upstream modules of the appropriate type and resolution for input to the subsequent module(s). The Subcommittee is concerned that the planned field comparison for mercury may not be effective, because of the high degree of complexity and uncertainty

in mercury chemistry, the large number of adjustable parameters that must be fit for the model, and the difficulty in obtaining adequate data to properly test the model. As such, planned field comparisons of mercury should be replaced or augmented by considering sites with other metals that undergo simpler fate and transport processes in the environment, so as to ensure that a successful model specification can be achieved. Tests of the TRIM system at larger scales, such as for a metropolitan air basin with multiple stationary and mobile sources, are recommended to evaluate the ability of the TRIM system to operate at this scale of application and to utilize emerging electronic/GIS databases with geographic, meteorological, emissions, population and environmental resource information. Evaluation of the TRIM system should be a continuing process that encourages ongoing data collection and evaluation for local, site-specific applications, with iterative updates to the model structure, database and characterization of uncertainty. The application protocol for TRIM should provide incentives for the development of improved data collection methods (with improved sensitivity, accuracy and precision) and improved databases for model input.

Efforts to improve the TRIM.FaTE module to address local-scale atmospheric dispersion through the use of alternative air pollution models, to develop appropriate transport parameters for surface waters and air-soil mass transfer, to include kinetic, reversible reactions among metal species, and to incorporate seasonal effects in some biotic processes, are appropriately focused. Specific recommendations are provided in our report to allow further improvements and focus. In each case, we emphasize the need for an effective user-interface that guides users in the selection of alternative modules and input parameters given the chemical(s), landscape properties, and types of exposures and risks addressed.

The design of TRIM.Expo and its use of existing modeling science for inhalation and ingestion exposures are, in general, consistent with OAQPS' programmatic and regulatory needs and the state-of-the-art of exposure assessment. System flexibility is needed to allow the selection of time-activity patterns and exposure factors consistent with the necessary level of spatial and temporal detail, distinguishing between long-term chronic health endpoints and short-term acute effects.

The design of the TRIM.Risk module is appropriate for analysis of human health and ecological risks, though more details and example applications will be necessary for rigorous review. Particular care will be needed to ensure that the time scales for exposure and risk calculation are appropriately matched (in particular, for acute, non-cancer health effects associated with short-term and/or peak exposures, where current knowledge and guidance are lacking) and in providing options for incorporating emerging knowledge on pollutant interactions which may result in non-additive risk. Ecological risk endpoints and metrics are not well defined in TRIM (or in any other risk assessment framework currently available), and further work will be needed to provide appropriate endpoints and options for assessing them. The multi-chemical, multi-media design of the TRIM system provides the opportunity to explore methods for addressing new and emerging issues in risk assessment and the risk sciences, including the effects of mixtures, population susceptibility and cumulative risk; as well as metrics for environmental equity and ecological impacts at the population level. OAQPS should take advantage of this opportunity to suggest and illustrate possible approaches to these issues for broader Agency consideration and evaluation.

2. INTRODUCTION

The Environmental Models Subcommittee (EMS) met December 13 and 14, 1999 to review the “Total Risk Integrated Methodology (TRIM) Status Report”, the draft “TRIM.Expo Technical Support Document” and the two volume “TRIM.FaTE Technical Support Document”. The Subcommittee conducted this review in order to provide the Agency with advice and insights on the adequacy of the proposed Total Integrated Risk Methodology (TRIM) approach to predict exposures and risks posed by air pollutants.

The charge to the Subcommittee contained nine questions. In general the Subcommittee finds that the OAQPS efforts to develop the TRIM system are innovative and effective, given the significant challenges and the relatively new and rapidly evolving state of science for multimedia fate, transport, exposure and risk models potentially applicable to hazardous air pollutants (HAPs) and criteria air pollutants. Indeed, development of the proposed TRIM system demands much more than piecing together existing models for these processes; rather new methods, approaches and advancement of the state-of-the-art are needed to ensure effective predictive capability and linkage of the various components. Given this, current knowledge and methods continue to limit the ability of such models to provide accurate and meaningful predictions of environmental concentrations, exposures and risks for many of the HAPs and criteria air pollutants that are the focus of the TRIM effort. Our report focuses on key issues and concerns for continued development of a scientifically sound and acceptable modeling system that remains cognizant of these limitations and attendant uncertainties, while encouraging further research and data collection to address them.

3. CHARGE TO SUBCOMMITTEE

3.1 Overall TRIM System

Charge 1: Does TRIM's current design and modular approach provide us with an appropriate design for accommodating new scientific information and model flexibility?

Charge 2: Are the proposed plans for addressing uncertainty and variability scientifically defensible? If not, what would you propose?

Charge 3: An important feature of TRIM is its open architecture (e.g., as demonstrated by the inclusion of an "algorithm library" developed for TRIM.FaTE). This architecture allows the user to add new processes, input data, and approaches to the TRIM modules. Given that a User's Guide will be developed to provide guidance on the use of these features, does this provide TRIM, and specifically TRIM.FaTE, with a significant technical asset in the area of user flexibility and model transparency? If not, what would be the preferred alternative?

3.2 TRIM.FaTE Module

Charge 1: In response to specific recommendations by the previous SAB panel, we (OAQPS) have investigated certain issues. As a result, TRIM.FaTE has been modified (item a), below), or the model documentation has been updated to address specific panel concerns (items b) and c), below).

- a) Do the modifications described in items (i) and (ii) below demonstrate an improvement in the ability of TRIM.FaTE to address these two issues? If not, what specific recommendations could you offer to do that?
 - (i) As a demonstration of the capability of TRIM.FaTE to incorporate output from external models, the Agency has developed and implemented methods for TRIM.FaTE to accept air concentrations and deposition output from an air quality model.
 - (ii) TRIM.FaTE is revised with regard to how it addresses certain kinds of chemical mass movement between certain compartments, specifically: (1) dispersive transport between surface water compartments, and (2) diffusion and advection between soil compartments and from air compartments to surface soil compartments.
- b) The incorporation of both horizontal and vertical atmospheric dispersion/diffusion algorithms directly within TRIM.FaTE using both lateral and vertical Pasquill-Gifford plume dispersion coefficients was pursued. After further review and consultation, it was

concluded that incorporating dispersion terms into the TRIM.FaTE air model was not appropriate at this time. Do you concur with this conclusion (discussed more fully in the model documentation)? What alternate methods for incorporating atmospheric dispersion/diffusion directly within TRIM.FaTE would you recommend?

- c) An evaluation plan for TRIM.FaTE has been developed and is being implemented. Is the proposed evaluation plan scientifically defensible? If not, what would you propose?

Charge 2: Do the newly added TRIM.FATE abilities to: a) follow transformation products temporally through the study period and allow for 'reverse transformation'; and b) track metals in a multimedia environment provide notable improvement in TRIM.FATE's usefulness for Agency air pollutant risk assessments? Have we adequately captured the salient technical features in these additions? If not, what should be included?

Charge 3: Does the addition to TRIM.FaTE of certain seasonal processes (i.e., litterfall and changes in plant uptake) represent an improvement to the model's ability to predict different media pollutant concentrations for the time frames of interest for risk assessment? Are there other processes related to seasonality which play an important role in pollutant transfers and resulting media concentrations for relevant time frames, and thus would be a valuable addition to the model?

3.3 TRIM.Expo

Charge 1: Does the proposed conceptual design for TRIM.EXPO capture the salient technical features necessary to characterize inhalation and ingestion exposures given our programmatic and regulatory needs? If not, what salient features are missing and how should they be included?

Charge 2: Have we drawn appropriately from the existing modeling science on inhalation and ingestion exposures and are the specific algorithms structured in a way that is consistent with the modeling framework?

3.4 TRIM.Risk

Charge 1: Does the overall conceptual approach described for the TRIM.RISK module adequately capture the outputs from the other TRIM modules and provide quantitative human health and ecological risk characterization information that is consistent with Agency risk characterization policy?

4. RESPONSE TO CHARGE

4.1 Overall TRIM System

Charge 1: Does TRIM’s current design and modular approach provide an appropriate design for accommodating new scientific information and model flexibility? and

Charge 3: An important feature of TRIM is its open architecture (e.g., as demonstrated by the inclusion of an “algorithm library” developed for TRIM.FaTE). This architecture allows the user to add new processes, input data, and approaches to the TRIM modules. Given that a User’s Guide will be developed to provide guidance on the use of these features, does this provide TRIM, and specifically TRIM.FaTE, with a significant technical asset in the area of user flexibility and model transparency? If not, what would be the preferred alternative?

The Subcommittee concurs that the current design and modular approach provide a flexible and appropriate means of accommodating new scientific information. Furthermore, the open architecture of TRIM, which allows users to add new processes, input data and approaches, is a significant technical asset in promoting user flexibility and model transparency. To help motivate and clarify these features and their advantages, the technical support document (TSD) for TRIM should include a review of alternative options for promoting model flexibility and ease of use, such as the use of existing model-building software systems. The TSD should also elaborate on why the current design was preferred and ultimately chosen over these other options.

Key issues affecting the appropriate level of model flexibility and user-adaptability involve who will be using the model, for what purpose, and when. There is a need for OAQPS to better specify its plans and timeline for use of the TRIM system within the Agency and subsequent release for use by a broader user community. While the Subcommittee recognizes that much further work is needed before the model will be ready for use for OAQPS’s regulatory needs (and that the deadlines for these applications are rapidly approaching), early interactions with, and involvement of, affected stakeholders are essential steps in the process. Early workshops and beta testing by the affected user community will help identify software errors and limitations, and allow the Agency to gather useful information on the user community.

The need for involving a broad range of affected stakeholders in model development, testing and finalization, was emphasized in a previous consultation of the Environmental Modeling Subcommittee. In its review of the Model Acceptability Use Criteria (MAC White Paper), the Subcommittee recommended that “EPA model development can benefit greatly from targeted stakeholder participation...”. In her response to this recommendation Dr. Norine Noonan, the Assistant Administrator for Research and Development, indicated that:

“Follow-up actions in the MAC White Paper include developing and utilizing a model clearinghouse to inform internal and external stakeholders on model evaluation results, availability, and application experience... We have also included the development of a communication strategy for the public and other external model users to provide feedback to EPA through Internet sites in Section 6.” (EPA,1999)

While a flexible modeling system has many advantages, a drawback to this approach is that it may be easy for users to mis-configure or otherwise misuse the program and obtain inappropriate or misleading results. Users may have difficulty integrating new processes, data, and/or approaches within the TRIM framework, unless the TRIM modules are properly designed and the User’s Guide is clear and specific on how to add new elements to the TRIM modules. Good user guidance and an eventual user interface to guide model setup and configuration will thus be necessary. Such an interface would, for example, identify and help facilitate the setup of a “standard regulatory configuration” for specific problem applications and inform the user that alternative assumptions must be justified (e.g., shown to be as good or better than the standard assumptions) when selected for a particular application. Eventually, an expert-system type user interface to help in module selection, configuration, and input data specification would be of great benefit to the users of TRIM to ensure appropriate and consistent application. This need for pre-screening and an effective user interface is identified a number of times in our report in response to specific questions regarding options for alternative fate and transport, exposure and risk assumptions and modules in the TRIM system.

Linking and interfacing the three proposed TRIM modules on fate and transport, exposure, and risk is a major and difficult task. The first module, TRIM.FaTE, and the second module, TRIM.Expo, have thus far been developed in a parallel and while interactions and communication between these efforts have taken place, some degree of mismatch is apparent. The major input data needed by the second module do not in many cases correspond to the output data from the first module. The modules’ reliance on, and use of, data and parameters of differing spatial and temporal scales may create a number of unforeseen problems. With the rapid advance of GIS, it is quite possible that in the near future detailed meteorological data and three-dimensional geographic maps will be available electronically at local, regional and national levels. It is not clear whether TRIM can handle and integrate the large amount of data this will entail at different temporal and spatial scales in an efficient and accurate manner. Early experimentation with model linkage and the use of available data-sets for emissions, meteorological inputs, census information and GIS resource inventories should take place soon, and not await finalization of the individual modules.

Effective presentation of the TRIM components and their interactions is essential to communicate the key elements of this complex modeling system. Further use of conceptual diagrams is recommended for the TSD to demonstrate model calculations, dependencies and logic.

Charge 2: Are the proposed plans for addressing uncertainty and variability scientifically defensible? If not, what would you propose?

The proposed plan for addressing uncertainty and variability is innovative and consistent with the current state-of-knowledge in the risk sciences. The proposed methods for separating variability and uncertainty are appropriate and current. The proposed tiered method for pre-screening the sensitivity of model parameters to eliminate those to which the model is insensitive from consideration in further, more-detailed uncertainty analyses, is appropriate and necessary to provide for feasible and effective model evaluation and insights. However, caution and appropriate user guidance is needed to ensure that important model uncertainties are not eliminated in this pre-screening phase. Users need to be aware that the results of sensitivity and uncertainty analysis are themselves often very sensitive to the methods used and the assumptions adopted. For example, local (or derivative-based) sensitivity coefficients can be highly sensitive to the base-case around which the derivatives are computed. The inclusion of parameter correlations in an uncertainty analysis may cause predicted uncertainties and resulting inferences to change, however, our knowledge of correlations is often very limited. Users should be provided with a number of options (and accompanying guidance) for sensitivity and uncertainty analysis. The assumptions and input functions for any uncertainty analysis (e.g., the distribution of model inputs, assumed correlation structure, etc.) should be clearly presented and documented as part of the model output, allowing the user to check and document their evaluations.

The TRIM.FaTE model utilizes physical compartments for the environment which are often highly aggregated. Local variations in compartment properties (e.g., soil texture, soil pH or redox conditions) may result in smaller-scale variations in chemical concentrations and exposure which are missed with such aggregation. The Agency should explore options for considering and characterizing the effects of local variability of this type in the TRIM model.

A number of the most interesting results of an exposure and risk assessment occur at the “tails of the distributions.” This may occur at the upper tail of the variability distributions, where variations in media concentrations or exposure factors lead to an individual or subpopulation with very high predicted exposure and risk; or at the tails of the uncertainty distributions, where certain possible (though perhaps unlikely) combinations of parameter values or assumptions lead to significant exposure and risk to all or some of the target population. Traditional methods for sampling variability and uncertainty distributions may not provide adequate coverage of these tails. The Agency should thus explore alternative methods, such as importance sampling, the use of mixtures of distributions, or the decomposition of exposure and risk distributions into further subpopulations, for proper characterization of the extremes of the distributions.

The routing and tracking of uncertainty across multiple, linked modules is not a simple task, with few reported examples in either the basic or applied risk literature. Special attention should be given to those uncertain parameters which affect more than one model component or module. Inferences about the relative sensitivity and uncertainty of the fate and transport, exposure and risk modules, and the interactions between their uncertainties, should be an important part of the learning that takes place as a result of TRIM system applications.

A key issue in uncertainty analysis, widely recognized though rarely addressed in a meaningful manner, is that uncertainties in model formulations and conceptual assumptions are often much more significant and important than uncertainties in model input values. To help promote the evaluation of alternative model formulations and assumptions, the flexible architecture of the TRIM system should be exploited to allow alternative formulations to be compared as part of the model sensitivity and uncertainty analysis.

The issues of model uncertainty analysis and model evaluation are highly interrelated. While the Subcommittee addresses specific issues related to plans for TRIM.FaTE evaluation later in this report (see Charge Question 1c under the TRIM.FaTE Module), the more general relationship between model evaluation and uncertainty should be recognized. Model evaluation must acknowledge and lead to a characterization of the uncertainties that remain even after a model is properly formulated, coded, fitted and tested to the fullest extent possible. Model uncertainty analysis can help guide critical needs for further data collection and research to improve the model.

As acknowledged in the TRIM Status Report (p. 3-6), data are not typically measured or collected in a way that allows for the separation of variability and uncertainty for most parameters. Uncertainty is reduced primarily by good measurement methods that minimize and/or adjust bias, increase sensitivity (by lowering detection or quantification limits), and improve precision. Model evaluation and uncertainty analysis should thus be linked to ongoing laboratory- and field-data collection efforts to better specify key model assumptions and input parameter values, both for the model in general and for use in site-specific applications. The Subcommittee encourages the Agency to provide ongoing guidance and support on the experimental and field-data collection efforts needed to execute an effective application of TRIM, and to promote the development of an improved database that can address long-term needs for model improvement and uncertainty reduction. The protocol for use of the TRIM system should include an appropriate mix of requirements and incentives to see that such critical data are collected and utilized. With this, the OAQPS HAPs and criteria air pollution program using the TRIM system could very well serve as a test case for studying the use of regulatory models in applications with complex, rapidly evolving science, and the associated challenges of model evaluation and uncertainty characterization. With the lessons learned, the effort could also serve as a benchmark for other regulatory programs where similarly complex and uncertain models are considered for use.

4.2 TRIM.FaTE Module

Charge 1: In response to specific recommendations by the previous SAB panel, we (OAQPS) have investigated certain issues. As a result, TRIM.FaTE has been modified (item a, below), or the model documentation has been updated to address specific panel concerns (items b and c, below).

- a) Do the modifications described in items (i) and (ii) below demonstrate an improvement in the ability of TRIM.FaTE to address these two issues? If not, what specific recommendations could you offer to do that?
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 - (ii) TRIM.FaTE is revised with regard to how it addresses certain kinds of chemical mass movement between certain compartments, specifically: (1) dispersive transport between surface water compartments, and (2) diffusion and advection between soil compartments and from air compartments to surface soil compartments.
- b) The incorporation of both horizontal and vertical atmospheric dispersion/diffusion algorithms directly within TRIM.FaTE using both lateral and vertical Pasquill-Gifford plume dispersion coefficients was pursued. After further review and consultation, it was concluded that incorporating dispersion terms into the TRIM.FaTE air model was not appropriate at this time. Do you concur with this conclusion (discussed more fully in the model documentation)? What alternate methods for incorporating atmospheric dispersion/diffusion directly within TRIM.FaTE would you recommend?

The ability of TRIM.FaTE to use other air pollution models, better able to characterize near-field (spatial) and short-term (temporal) variations in air concentrations and deposition, will be important for a number of pollutants and applications where these effects are critical. Examples include lead (or other metal or particle-associated chemical) concentrations and deposition near smelters, or chemical plants or refineries where there are steep concentration gradients near the facility, or for which acute impacts from toxic chemical spills, accidental releases or extreme meteorological conditions are of concern. For these types of problems, the large-scale, compartmental mixing of the TRIM.FaTE model is inappropriate. With the typical air-compartment sizes of the multi-media TRIM.FaTE model, local scale diffusion is greatly overestimated; and it is very difficult to represent the smaller-scale spatial and temporal variations that are important. Example calculations to illustrate this are presented in Appendix A. Incorporation of diffusion within the TRIM.FaTE model (by the inclusion of exchange flow between adjacent air compartments) will not address this issue, since the problem is not one of too little local diffusion, but rather too much diffusion due to the inherent assumption of complete mixing within each box of the air model. The use of existing and newer Gaussian-plume based air pollution models, such as the Industrial Source Complex (ISC) family of models and its successors, can address this problem for the air concentration and deposition calculations of TRIM.FaTE, but this approach raises difficult issues of matching mass transfer between media (i.e., between the air and the adjacent water, soil and biotic compartments). There is no immediately clear method for simultaneously fitting

and executing the imported air pollution model and the rest of the TRIM.FaTE program to ensure overall mass balance.

The OAQPS and its consultants have considered the difficult problems and tradeoffs associated with using a separate air pollution model, which may make it impossible to ensure mass balance, versus the use of the current TRIM.FaTE multimedia compartment approach, with its limited ability to represent near-field and short-term concentration gradients. The OAQPS should continue to work this problem from both ends, exploring creative mechanisms for linking separate air models to TRIM.FaTE while providing checks and corrections for mass balance where appropriate, and providing options to use the standard TRIM.FaTE compartment model with finer grid boxes and finer temporal resolution of wind fields. However, assuming that drawbacks will remain with either approach, the ability to prescreen problems, determine which approach is preferable, and guide users on the selection of an appropriate option, or mix of options, is essential.

For now, the TRIM status report should better distinguish between artificial dilution associated with complete mixing assumptions and numerical dispersion that results from discrete treatment of advection. The status report should also distinguish between horizontal and vertical dispersion in its discussion of the treatment of dispersion in traditional photochemical grid models. Many models use fine vertical resolution and treat vertical dispersion relatively well. Horizontal dispersion is more difficult to capture over varying spatial and temporal scales. For long-term model development, user guidance and preprocessing tools should clearly distinguish between alternative problem types. For problems where broad dispersal in the environment and intermedia transfers and partitioning control the predominant pathways of chemical transport and exposure and chronic risks are the focus of concern, the standard TRIM.FaTE module is appropriate. When significant near-source gradients occur, or when short-term temporal concentration excursions in the air result in acute health risks, a separate and more specialized air pollution model will be required. The eventual TRIM system preprocessor should thus screen the chemical and landscape properties as well as the health and ecological effects of concern to recommend to the user the most effective module options and configurations.

The chemical transport and intermedia mass transfer algorithms for TRIM.FaTE can have important implications for the distribution of chemicals in the environment (TRIM.FaTE Module Charge Question 1 (a) (ii)). While the fundamental algorithm for dispersive transport between surface water compartments, tailored after that of the WASP model and based on exchange flow between adjacent compartments, is correct, the TSD lacks adequate guidance for properly differentiating between, and selecting dispersion coefficient values for horizontal and vertical dispersion in the water column and vertical dispersion between the water column and adjacent sediment pore waters. Furthermore, by assigning the same default value dispersion coefficient for surface water to surface water transport (horizontal or vertical) and surface water-sediment exchange, the current documentation is misleading and incorrect. Since the compartment model imparts numerical dispersion even when no exchange flow is included, users also need guidance on the magnitude of this numerical dispersion and its tradeoff with user-assigned dispersion; the model output should include a report on computed values of numerical and total dispersion. More guidance is also needed for selecting appropriate advective flow rates for

surface water systems. The advection and dispersion assumptions/parameters for a surface water system are linked, since finer resolution of the advection field (in time and space) may preclude the need for some dispersion, and because the intensity of mixing and the corresponding magnitude of the dispersion coefficient may be a function of flow rates and water velocities. Finally, the standard compartment mass balance model does not include a continuity calculation or check to ensure that a fluid balance (water for the water compartments; air for the atmospheric compartments) is maintained, and user inputted flows can thus, when in error, be unbalanced. Flow balance calculations should be performed and users alerted when water and/or air balances are violated for model compartments. This feature, along with the guidance noted above on the selection of appropriate, context-specific dispersion coefficients and flow-dispersion relationships, should be a basic part of the user interface and the TRIM.FaTE technical support document (TSD). Citations should also be provided on accepted approaches for determining more detailed and accurate advection and dispersion parameterizations for surface water system, including the use of hydrodynamic models and the use of conservative tracer measurements (such as salinity in coastal areas) to estimate the transport terms. Additional guidance on dispersion coefficients appropriate for use in surface water systems is provided in Appendix B.

The proposed approach for coupling advection and diffusion within soil columns and air-surface soil mass transfer, through the use of an effective penetration depth, is innovative. The method is currently formulated assuming transport from the air to the soil; a similar parameterization should be developed for cases where soil to air transport ensues. The current model does not appear to fully account for impervious soils or the impervious built environment (roads, buildings, etc.). Appropriate inclusion of such a compartment could be important for mass balance calculations in urban areas, and may also allow eventual evaluation of HAP impacts on materials and infrastructure damage.

- c) An evaluation plan for TRIM.FaTE has been developed and is being implemented. Is the proposed evaluation plan scientifically defensible? If not, what would you propose?

The overall evaluation plan for TRIM.FaTE, including code validation, mass balance checks, model to model comparisons, and comparisons against observed data in field applications, is appropriate. The Subcommittee has not yet received detailed reports on the results of these evaluation efforts (some are not yet completed or are only in the planning phase¹), so we cannot as yet comment on whether each of these steps have been implemented in a proper manner and whether the inferences drawn are justified. The Subcommittee looks forward to future presentation of the model evaluation results and findings. In so doing, the OAQPS is encouraged to frame and present their evaluations in the context of specific regulatory applications, e.g., an evaluation of the model in its intended use for estimating residual risks after meeting specific emission reduction requirements. Also, the OAQPS should be very explicit about the hypotheses that are being tested relative to the *a priori* expectations or needs for model performance in these contexts. This will in most cases dictate tests involving

¹ In response to a request from the Subcommittee at the review meeting, OAQPS did subsequently provide a more detailed list of presentations and publications on the TRIM system. This list is provided in Appendix D. The Subcommittee has not had the opportunity to evaluate these presentations and publications.

combined and integrated applications of all three TRIM modules (fate and transport, exposure, and risk), not just a single module or component.

The proposed evaluation tests should also include application of the sensitivity and uncertainty analysis tools of the TRIM systems. The performance of these tools in these applications must themselves be tested and evaluated and, as noted above, sensitivity and uncertainty analyses are (or at least should be) closely integrated with the model evaluation exercise. Sensitivity analysis of model parameters and component assumptions helps to identify where further improvements in model formulation or input data reliability are essential. The model evaluation exercise should not just be viewed as a one-time effort necessary to finalize an “approved” regulatory model. Rather, it should be viewed as an ongoing process of system learning and model improvement. Similarly, many components of the TRIM system model will require location-specific calibration and evaluation when used for site-specific applications. As previously noted, the proposed plans for TRIM model evaluation, sensitivity and uncertainty analysis are predicated on the availability of appropriate (unbiased, sensitive and precise) field measurements and model inputs. The OAQPS should thus endeavor to develop a protocol for “local” model evaluation as a standard and requisite part of these site-specific applications. This protocol will likely include an outline of necessary steps for basic QA/QC of local applications to ensure proper module selection and configuration, and the use of appropriate and justifiable values for input parameters. It should also indicate which site-specific data are necessary for model evaluation and provide an appropriate framework and incentive for collecting data that promotes long-term model development and improvement.

The proposed TRIM.FaTE evaluation effort, for a chlor-alkali plant with mercury emissions impacting its surrounding landscape and ecosystem, provides an opportunity for the development of such an exemplary protocol. As such, the Subcommittee recommends that the plan for TRIM.FaTE evaluation at this or other sites be expanded to include demonstration and testing of TRIM.FaTE linked with the other TRIM (exposure and risk) modules, and the use of sensitivity and uncertainty analysis tools. The Subcommittee notes that selection of a mercury test case for evaluation imparts significant challenges and difficulties. It is unlikely that sufficient field data are available to allow identification and parameter estimation of the complex, kinetic reactions and processes that impact the multiple chemical species of mercury included in the model. If data for other metals which are subject to simpler transport and reaction mechanisms are available for the site, simultaneous model evaluation for these constituents is recommended. If not, another site or sites where such chemicals are present should be added to the evaluation exercise. This will increase the chances that a successful model specification can be achieved, and help to identify the relationship between specific chemicals chosen for assessment, environmental conditions, and the amount and quality of data necessary to calibrate, apply and evaluate the model in a confident manner.

TRIM is intended for application to HAPs and criteria air pollutants evaluation on a variety of spatial scales, ranging from local, plant-specific estimates to large regional airsheds (e.g., the Los Angeles metropolitan area). The prototype case study of the chlor-alkali plant involves only a few emission sources over a relatively small spatial scale. It will be a significant challenge to apply TRIM to

large metropolitan areas such as the LA basin with numerous stationary and mobile emission sources, and planning should be initiated for testing such applications. In all cases, evaluation should include an assessment of whether the TRIM.FaTE output is appropriately scaled and defined for input to TRIM.Expo.

Charge 2: Do the newly added TRIM.FATE abilities to

- a) follow transformation products temporally through the study period and allow for 'reverse transformation', and
- b) track metals in a multimedia environment provide notable improvement in TRIM.FATE's usefulness for Agency air pollutant risk assessments? Have we adequately captured the salient technical features in these additions? If not, what should be included?

While reversible, kinetically controlled reaction processes can be important for some metals, and the inclusion of this capability in TRIM.FaTE should eventually provide a notable improvement in modeling capability, our knowledge of, and ability to specify the parameter values for these processes in real environmental settings is quite limited. As noted above, the metal for which such processes are most likely to be important, mercury, has been the subject of significant study in recent years, but is still poorly characterized. The current version of TRIM.fate incorporates a set of five parallel transformation reactions for mercury oxidation-reduction and alkyl complexation that are described mathematically using first-order rate expressions.

There are two principal issues of concern in the mercury speciation model. First, it is not obvious that a rate-dependent approach is required in all cases. Generally speaking, trace inorganic substances display variable rates of oxidation/reduction (which may be relatively slow), but rather rapid complexation (seconds to minutes). While mercury may be an exception (reported methylation rate constants in the Status Report are around 0.001/day), this is usually because of a rate limiting elementary step in the reaction sequence, such as the generation of the methyl radical (which itself is dependent on its source), rather than in the complexation step itself. Methylation is not especially important for most inorganics (although complexation is), indicating that the current model includes a degree of complexity that is not generally necessary. Since first-order kinetics are used, this issue can be addressed using a straightforward Damkohler analysis, as is done effectively in the Vertical Transport Algorithms (TSD Vol. II). One question the OAQPS may wish to address is whether or not TRIM.fate should contain a generic description of inorganic fate, or instead utilize element-specific submodules (if the uses of TRIM will encompass only a few elements, then perhaps the latter approach preferred).

The rate coefficients presented in the TSD for the transformations between mercury species appear to be chosen independently. In reality, significant interdependencies exist among them (and these interdependencies can and should be evaluated as part of the model sensitivity and uncertainty

analysis). The input table (Appendix C of the Status Report) shows four coefficients for six separate compartments, for a total of twenty-four constants needed to execute the mercury submodel. It seems unlikely that a complete set of such coefficients will ever be available for a given application, creating the danger that users will choose coefficients from many different literature sources that, in aggregate, are neither internally consistent (i.e., consistent with Hg equilibria), nor descriptive of Hg transformation rates at the site of interest. This relates to the problem noted above of the impossibility of being able to establish an unambiguous set of Hg coefficients. Given this, a more parsimonious model is probably called for in this case. While efforts to better characterize reversible reactions for metals such as mercury should continue, similar effort should be exerted in characterizing the simpler, equilibrium partitioning behaviors of other metals and their dependence on environmental conditions and settings related to factors such as pH and redox conditions.

Charge 3: Does the addition to TRIM.FaTE of certain seasonal processes (i.e., litterfall and changes in plant uptake) represent an improvement to the model's ability to predict different media pollutant concentrations for the time frames of interest for risk assessment? Are there other processes related to seasonality which play an important role in pollutant transfers and resulting media concentrations for relevant time frames, and thus would be a valuable addition to the model?

The inclusion of seasonal processes related to plant growth cycles is a valuable addition to TRIM.FaTE, and other seasonal processes may be important as well, especially related to water balances and flows through soils and surface waters. Seasonal variations in precipitation, runoff, infiltration and evapotranspiration can affect soil moisture and subsequently impact air-soil mass transfers and chemical processes in the subsurface. Seasonal (or intermittent) variations in streamflow can affect water column-sediment transport and chemical partitioning, as well as surface water concentrations for uptake by biota and waterborne exposures. At a minimum, user guidance is needed to ensure that seasonal and/or intermittent patterns of soil moisture and streamflow are consistent with inputted values of temperature and precipitation. If temporal variations in soil moisture and streamflow are found to be important for certain chemicals in certain applications, it may be necessary to interface TRIM.FaTE with a water balance model (i.e, a soil and/or stream hydrologic model) to ensure that these inputs are properly specified.

The ability of the TRIM system to interface with, and accept output from, others model should facilitate this approach; OAQPS may wish to begin to identify appropriate water balance models for an application of this type. For seasonal processes of a more fundamental nature, affecting the structure and rate of chemical uptake or transformation processes in specific environmental media or settings (such as nonlinear algal growth or food chain uptake in surface waters, or more complex soil-to-plant uptake), the ability of TRIM.FaTE to interface with more detailed, media-specific models, can be exploited. For example, in cases where surface water processes have an important influence on chemical fate, ecological risk and human exposure, an integrated surface water modeling system, may be appropriate. Again, the ability to prescreen problems and guide users to appropriate component modules and system configurations will be critical.

4.3 TRIM.Expo

Charge 1: Does the proposed conceptual design for TRIM.EXPO capture the salient technical features necessary to characterize inhalation and ingestion exposures given our programmatic and regulatory needs? If not, what salient features are missing and how should they be included? and

Charge 2: Have we drawn appropriately from the existing modeling science on inhalation and ingestion exposures and are the specific algorithms structured in a way that is consistent with the modeling framework?

The Subcommittee finds that the conceptual design of TRIM.Expo and its use of existing modeling science for inhalation and ingestion exposures are, in general, consistent with OAQPS' programmatic and regulatory needs, the overall TRIM modeling framework, and the state-of-the-art of exposure assessment. However, the Subcommittee also notes that the exposure assessment discipline is young and rapidly evolving, and that a "one-size-fits-all" approach (even one that is very flexible) may not work for all chemicals in all exposure settings. Very different approaches may be needed for assessing long-term, chronic exposures vs. short-term acute impacts. These may significantly impact the type and level of detail necessary in characterizing individual and subgroup variability in time-activity patterns and exposure factors. In certain cases, more refined differentiation of cohort characteristics may be appropriate, while in others, greater emphasis is needed on individual-to-individual variation within a cohort. Greater aggregation of time-activity patterns is acceptable when computing chronic exposures, a finer definition of exposure scenarios may be necessary to identify the upper tail of acute exposures and risks. Once again, an effective pre-screening of problem features, including chemical properties, landscape-exposure characteristics, and the time and spatial scales of health impacts, is needed to best specify the level of temporal and spatial aggregation in the exposure model. A mechanism for such pre-screening and user guidance is needed in the TRIM system.

A number of significant challenges and uncertainties remain in collecting the necessary information for a meaningful and reliable exposure assessment. OAQPS and its consultants are clearly aware of these challenges. These include difficulties in extrapolating short-term time-activity studies to estimate longer-term behavior (and exposure); a lack of information on diet source and the relative role of home-grown, local and national or international sources of foods for a given local pollution scenario; and the appropriate chemical concentrations of different food sources to assign, particularly when issues of cumulative risk begin to be addressed. The relative importance of these issues will hopefully be illuminated as evaluation studies of the overall TRIM system (and TRIM.Expo) evolve. Test applications are encouraged for a problem such as mercury or other metal exposure occurring through a variety of environmental pathways, as well as a HAP problem with a predominant air exposure pathway, perhaps using a NHEXAS study area (and its associated data set) for model calibration and evaluation.

4.4 TRIM.Risk

Charge 1: Does the overall conceptual approach described for the TRIM.Risk module adequately capture the output from the other TRIM modules and provide quantitative human health and ecological risk characterization information that is consistent with Agency risk characterization policy?

The overall plan and conceptual approach for TRIM.Risk appears to be appropriate; since it is in the early stage of development, more details and example applications will be necessary for a more rigorous evaluation. There are some issues that the Subcommittee has identified as possible concerns for the ongoing module development. These include:

a) Risk Analysis of Acute Health Effects: For human cancer risk assessment, the time frame is defined as the life span of 70 years. The 70-year risk estimate is divided by 70 to generate the annual incidence rate. For non-cancer acute health effects caused by many hazardous and criteria air pollutants involving short-term or peak exposures, no time scale is defined for performing the risk calculation. It is intended that TRIM.FaTE will generate hourly, daily and yearly concentration estimates. There is currently a lack of guidance on how to integrate short-term and/or peak exposure estimates for calculating the risk of acute health effects.

b) Adequacy of Additive Model: An additive model is chosen to estimate risk for simultaneous exposures to several carcinogens (page 9-8 of the TRIM Status Report).

This is a reasonable and logical choice for general representation. However, there are important cases where synergistic effects are believed to occur when there is simultaneous exposure to two carcinogens. Examples include smokers exposed to asbestos or radon. Flexibility to allow for synergistic or antagonistic effects of multiple contaminants will be important for such cases (see also our more general comments on chemical mixtures and cumulative risk effects below).

c) Interpretation of Hazard Index (HI) and Hazard Quotient (HQ): The HQ is defined as the ratio of computed exposure to a reference level and the HI (for a mixture of compounds) is calculated as $HI = HQ_1 + HQ_2 + \dots + HQ_i$. As such, an additive model is again assumed for multiple chemical effects. Both the HQ and the additive HI have been challenged as appropriate indicators for noncancer risks. As acknowledged on page 9-8 of the TRIM Status Report, if comparisons of HQs across substances may not be valid, then use of the HI, defined as the summation of HQs, is even more questionable.

d) Indicators and Descriptors for Ecological Risks: No general guidance is given in the conceptual TRIM.Risk module to calculate, analyze, express and interpret ecological risks. It is unclear what kind of outputs will be generated by TRIM.Risk to characterize

ecological risks. This problem is not unique to the TRIM system, since (similar to methods for noncancer human health risk assessment) current methods and accepted protocols for ecological risk assessment are limited. It will thus be difficult to define endpoints and metrics of impact and risk that are generally and widely accepted.

The Subcommittee does commend OAQPS' ongoing efforts to link with other multimedia exposure and risk assessment activities in the Agency, such as the Hazardous Waste Information Rule (HWIR) being developed in the Office of Solid Waste and Emergency Response (OSWER) and the Multi-media Integrated Modeling System (MIMS) being developed by the National Exposure Research Laboratory (NERL) in the Office of Research and Development. These collaborations are important to ensure that maximal benefit, consistency and coordination is achieved between these efforts.

The TRIM system provides the opportunity to begin to seriously address new and emerging issues in risk assessment and characterization, including the evaluation of mixtures, cumulative risk, environmental equity and methods for considering more-susceptible subpopulations. This opportunity is especially applicable to the assessment of the residual risk associated with multiple HAPs under different emission control scenarios. While the Agency continues to struggle with how best to address and incorporate these new and emerging ways of looking at risk, OAQPS should be proactive in suggesting and exploring options within its integrated modeling system. Often the efficacy of new ways of addressing problems cannot be judged until they are first tried and illustrated. The OAQPS should utilize this opportunity to see whether the TRIM system in the context of HAP assessment can begin to provide such examples for broader Agency consideration and evaluation.

The framework for ecological risk assessment in TRIM.Risk (and the state-of-the-art in general) is quite new and undeveloped. Clear measures of ecological impact must be identified and evaluated. Currently, these focus on inferences of toxicity and hazard extrapolated from limited tests on individual organisms in isolation. As new knowledge emerges on population-level ecosystem effects, attempts should be made to incorporate this science. To begin to explore such options, OAQPS should review available population-level ecosystem models to see which may be able to utilize output from, or be compatible with, the TRIM system.

5. CONCLUSIONS

The Environmental Models Subcommittee (EMS, or “the Subcommittee”) of the Science Advisory Board’s (SAB) Executive Committee met on December 13 & 14, 1999 to review the Agency’s “Total Risk Integrated Methodology (TRIM) Status Report,” as well as the draft “TRIM.Expo Technical Support Document,” and the two-volume TRIM.FaTE Technical Support Document” developed by the EPA’s Office of Air Quality Planning and Standards. The Subcommittee conducted this review in order to provide the Agency with Advice and insights on the adequacy of the proposed TRIM approach to predict exposures and risks posed by air pollutants.

The Subcommittee concluded that:

- 1) **The Overall TRIM Efforts to Date Have Been Innovative and Effective** - The EPA OAQPS’ efforts to develop TRIM as a flexible, state-of-the-art system for evaluating multimedia chemical fate, transport, exposure and risk, have to date been innovative and effective. The modular design and open architecture of TRIM provide a flexible and appropriate means of accommodating new scientific information;
- 2) **There is a Significant Need for User Guidance and Support** - Significant user guidance and support will be necessary to ensure that appropriate model setups and configurations are selected;
- 3) **There is a Need to Better Specify Plans and Timeline** - There is a need for OAQPS to better specify its plans and timeline for use of the TRIM system within the Agency and subsequent release for use by a broader user community;
- 4) **Early Interactions and Involvement with Stakeholders , Workshops and Beta Testing is Essential** - While the Subcommittee recognizes that much further work is needed before the model will be ready for use for OAQPS’s regulatory needs, early interactions with, and involvement of, affected stakeholders are essential steps in the process. Early workshops and beta testing of the integrated TRIM system by the affected user community are thus recommended to ensure the appropriate level of stakeholder input and a well-designed product;
- 5) **Efforts to Improve TRIM.FaTE Module are Appropriately Focused** - Efforts to improve the TRIM.FaTE module to address local-scale atmospheric dispersion through the use of alternative air pollution models, to develop appropriate transport parameters for surface waters and air-soil mass transfer, to include kinetic, reversible reactions among metal species, and to incorporate seasonal process in biotic processes, are appropriately focused. The planned field comparison study of mercury should be reconsidered or augmented to include metals that undergo simpler fate and transport processes in the environment to ensure that a successful model specification can be achieved;

6) **Testing of TRIM System at Larger Scales is Recommended** - Tests of the TRIM system at larger scales, such as for a metropolitan air basin with multiple stationary and mobile sources, are also recommended to evaluate the ability of the TRIM system to operate at this scale of application and to utilize emerging electronic/GIS databases with geographic, meteorological, emissions, population and environmental resource information.

7) **Design of TRIM.Expo is Consistent with OAQPS' Programmatic and Regulatory Needs and the Current State-of-the-Art of Exposure Assessment** - The design of TRIM.Expo and its use of existing exposure science for inhalation and ingestion modeling are, in general, consistent with OAQPS' programmatic and regulatory needs and the current state-of-the-art of exposure assessment;

8) **Design of TRIM.Risk Module Appears Appropriate, But Needs More Example Applications for Rigorous Review** - The design of the TRIM.Risk module appears to be appropriate, though more details and example applications will be necessary for rigorous review;

9) **Need to Ensure That Model Linkages are Appropriately Evaluated** - Evaluation plans should consider simultaneous test applications of the TRIM modules (FaTE, Expo and Risk) to ensure that model linkages are properly specified; and

10) **Should Motivate Improved Data Collection Methods, Improved Data Bases for Model Input and New Approaches to Emerging Risk Issues** - The application protocol for TRIM should provide incentives for the development of improved data collection methods and improved databases for model input. Because the multi-chemical, multi-media design of the TRIM system provides an opportunity to explore methods for addressing new and emerging issues in risk assessment and the risk sciences, including the effects of mixtures, population susceptibility and cumulative risk; as well as metrics for environmental equity and ecological impacts at the population level, OAQPS should suggest and illustrate possible approaches to these issues for broader Agency consideration and evaluation.

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APPENDIX A - ILLUSTRATION OF POTENTIAL MISREPRESENTATION OF DISPERSION IN TRIM.FaTE

The TRIM.FaTE model is designed to be applied with low resolutions in both space and time, similar to related multimedia compartment models, such as CalTOX and ISMCM. The numerical algorithms effectively employ a first-order upwind finite-difference method with respect to the advective transport. As a result, there is a constraint on the sizes of spatial grids and time steps. The algorithm yields a numerical diffusion coefficient, D_N , given by:

$$D_N = kV \Delta S [1 - \zeta(\Delta\tau / \Delta S)]$$

where k is a constant depending on the dimensionality (for 1-D problems, $k = 1/2$), V = velocity, $\Delta\tau$ = time-step size, ΔS = spatial grid size. Clearly, the mesh Courant number $C_r = V\Delta\tau/\Delta S = T_t$ (where T_t is the transfer factor defined in TRIM.FaTE) must be less than or equal to 1 to make the numerical diffusion coefficient positive. In practice, it should not be much greater than 1 so that the simulation results look reasonable (whether the simulations are accurate or not is another issue). If explicit integration is used, then the Courant number must be less than or equal to 1 to ensure numerical stability. Furthermore, to make numerical simulations close to the mathematical representation of the advective processes, D_N should be less than the physical diffusion/dispersion coefficient. This implies that the users must design the time-step and spatial-grid sizes such that the mesh Courant number is close to 1.0 for all compartments (an extremely difficult, if not impossible task, under space- and time-varying velocity fields).

Consider an air compartment as an example. Assume a typical wind velocity of 10 m/s. If we use a time-step size of 1 year, 1 month, 1 day, and 1 hour, the compartment size must be greater than 310,000 km, 26,000 km, 864 km, and 36 km, respectively. The use of large compartment sizes would yield very large numerical diffusion coefficients, unless the mesh Courant number can be made exactly equal to 1.0 for all compartments (an impossible task). If we are able to design the compartment sizes such that the mesh Courant number on average is 0.5, then the numerical diffusion coefficients would be on average equal to 3,100,000,000 m²/s, 260,000,000 m²/s, 8,640,000 m²/s, and 36,000 m²/s, respectively. Thus, even for a time-step size of one hour, the numerical diffusion would be significantly overestimated (short-term diffusion coefficients in Gaussian plume models increase with spatial distance and scale, but are typically on the order of 100 – 5000 m²/s), yielding simulations that may appear reasonable, yet are very inaccurate (predicting concentrations possibly several orders-of-magnitude smaller than the true solutions in terms of peak concentrations). Faced with this problem, users can either (1) use high resolution in both spatial-grid and time-step sizes to yield accurate simulations (this would require excessive computational resources with TRIM.FaTE); or (2) use a coarse resolution in compartment sizes and time-step sizes as done in CalTox or ISMCM, overlooking the resulting inaccuracy in predicted concentrations.

In summary the inability of TRIM.FATE to numerically produce an appropriate mathematical representation when coarse compartments and large time-step sizes are used is a major limitation. The predicted concentrations in simulations using TRIM.FaTE could be several orders-of-magnitude smaller (with respect to peak concentrations) or higher (with respect to small concentrations) than the true solutions.

APPENDIX B - MORE DETAILED COMMENTS ON THE PARAMETERIZATION OF DISPERSION AND ADVECTION FOR SURFACE WATER COMPARTMENTS IN TRIM.FaTE

The dispersion between surface water compartments in TRIM.FaTE is modeled after the methodology in WASP (Ambrose, 1993). This appears adequate for TRIM.FaTE simulations. The importance of including a physical dispersion process in the exchange between surface water compartments will depend directly on the size (spatial resolution) and type (river vs. estuary) of the compartments and whether they contain external sources (i.e., whether the numerical dispersion overwhelms the physical dispersion). The suggested tiered approach to determining model sensitivity can be used to assess the importance of the contribution of physical dispersion to the overall distribution of mass among the various model compartments.

Dispersion Coefficients in Surface Water Compartments and Between Surface Water and Sediment Compartments:

On pp. 4-9 to 4-11 of Vol. II of TRIM.FaTE TSD, the default dispersion coefficient values for these two processes (i.e., water to water dispersion, and water to sediment dispersion) are the same, listed as 2.25×10^{-4} m²/day. Actually, there are three dispersive processes involved: horizontal dispersion and vertical dispersion in the water compartment and the dispersion between the sediment-water interface. Normally, horizontal dispersion coefficients in the water column are several orders of magnitude greater than the dispersion coefficients in the vertical direction, which in turn are several orders of magnitude greater than the dispersion coefficients across the sediment-water interface. Typical values are:

Horizontal dispersion in water column:	1-300	m ² /s
Vertical dispersion in water column:	10^{-5} - 10^{-3}	m ² /s
Dispersion across sediment-water interface:	10^{-10} - 10^{-9}	m ² /s

Horizontal dispersion coefficients include longitudinal and lateral dispersion. Usually, longitudinal dispersion coefficients are greater than lateral dispersion coefficients.

For the TRIM.FaTE model, we suggest that ranges of dispersion coefficient values should be provided for use as default values.

Derivation of Advective Transport Coefficients:

The TSD document does not indicate how to derive advective transport coefficients such as the bulk transport. In general, two methods can be used: direct field measurements and using a hydrodynamic model. Note that being a box-model, the WASP modeling framework requires the assignment of the mass transport coefficients by the user. Hydrodynamic models are available for 1-D,

2-D, or 3-D configurations of a waterbody to develop mass transport coefficients, however, this results in a significant increase in model complexity and input data requirements.

In estuaries and coastal waters, tidal currents are at least one order of magnitude greater than tidally averaged velocities.

APPENDIX C - SPECIFIC EDITORIAL COMMENTS ON THE TRIM.Expo and TRIM.Risk MODULES

Page 4-3, on one side of equation 4-1 the exposure variable seems to only be dependent on (t, z, and m) while on the other side of the equation the other two variables include a number of other “indices”. Perhaps using the “conditional” notation “|” could clarify?

In Sections 4.1.2 to 4.1.4, how would acute exposure scenarios be described?

See Table 4-1 page 4-13. Is this too ambitious?

Page 4-29: Do we lose the potential dependency between the original parameters and outputs of subsequent modules if the outputs of the intermediate modules are summarized into percentile distributions and used as inputs into the subsequent modules?

Using short-term data to project to longer term: “Blanket statement” at bottom of page 4-29: *“OAQPS believes that these data are the best available and extrapolating to generate long-term factors or creating a longer term sequence of such data is the best approach”* This should be referenced with a description of the studies conducted and any efforts to “validate” this statement.

Page 5-3, different exposure event sequences are selected each day, how about repetitive tasks, (e.g., wake up, shower, breakfast, commute to work, etc...)? Is the same “exposure” used for all people in a cohort?

Chapter 6:

There appears to be some inconsistency in the description of contaminant exposure pathways in the TRIM.Expo module as compared to exposure pathways described in the TRIM.FaTE module description. This probably reflects the earlier stage of development of the TRIM.Expo module as compared to the TRIM.FaTE module. However, it is important that the modules are consistent. Examples include:

Sections 6.2.3 and 6.2.4: In the discussion of ingestion pathways for foodstuffs it is not clear if root-uptake of pollutants, and subsequent translocation to above-ground plant parts is factored into the exposure pathway model. There is a short description of the parameter, K_{ow} , the octanol/water partition coefficient, but is not stated if this parameter is used or not. The implication is that it is not. However, in the TRIM.FaTE Technical Support Document (Volume II) biotic transport algorithms for root-uptake are defined, suggesting this pathway is considered

Page 6-7, Table 6-2: In the taxonomy of food types categorized as fruits, vegetables and grains (Table 6-2), beans are listed as protected, above-ground crops. This is not true for all types of beans. Some commonly eaten beans such as, french beans and mange-tout, are essentially unprotected because the pod is also consumed. Later in section 6.2.3. 1 string beans are listed in the exposed produce category.

Page 6-15: The exposure pathways shown in Figure 6-4, and the descriptions in the supporting text appears somewhat inconsistent. It would be helpful to insert a section that deals with pasture because this is a key component to the livestock and animal produce exposure pathways. Currently, in section 6.2.3.2 on dairy products, pasture is defined as all foodstuffs grown on the farm to feed the animals (e.g., open pasture grass, grain, corn). These are a combination of different food categories that are expected to have different contaminant concentrations. Frequently, there are seasonal differences in the relative contributions of these categories to the livestock's feed. Therefore, it would seem more appropriate to explicitly identify the different categories of fodder in the model.

In Figure 6-4, the exposure pathway for chickens is shown to come from pasture, rather than grains that represent a more realistic exposure pathway. Using the current definition for pasture, pasture may in fact refer to grains, which is confusing because grains are shown as a separate category in the figure and supporting text. A more transparent approach, as described above, is recommended.

APPENDIX D - UPDATED LIST OF TRIM PRESENTATIONS AND PUBLICATIONS

1) Peer Reviewed Publications

Palma, Ted., Amy B. Vasu, and Robert G. Hetes, 1999. "Total Risk Integrated Methodology (TRIM)", Air and Waste Management Association - EM Magazine, March 1999, Pg 30-34.

2) External Scientific Meetings

20th Annual Meeting of the Society of Environmental Toxicology and Chemistry. 14-18 November, 1999. Philadelphia, PA.

Efroymson, R.A., Jones, D.S., Vasu, A. *An Ecological Risk Assessment Methodology for Hazardous Air Pollutants.*

International Life Sciences Institute's "Aggregate Exposure Assessment Model Evaluation and Refinement Workshop". 19-21 October, 1999. Baltimore, Maryland.

Richmond, H., McKone, T. *Total Risk Integrated Methodology (TRIM).*

19th Annual Meeting of the Society of Environmental Toxicology and Chemistry. 15-19 November, 1998. Charlotte, NC.

Vasu, A.B., Hetes, R.G., Palma, T., McKone, T.E. *TRIM: A Multimedia, Multipathway Framework for Assessing Human and Ecological Exposure and Risk.*

91st Annual Conference of the Air and Waste Management Association. 14-18 June, 1998. San Diego, CA.

Palma, Ted, Amy B. Vasu, and Robert G. Hetes. *An Introduction to the Total Risk Integrated Methodology (TRIM).*

Annual Meeting of the Society for Risk Analysis. December 7-10, 1997. Washington, DC.

A.B. Vasu, T.R. Johnson, T.E. McKone, T. Palma, M.G. Dusetzina. *Introduction to the Total Risk Integrated Model.*

T. R. Johnson, G.W. Suter II, T. Palma. *EcoFaTE: A TRIM Module for Linking Multimedia Environmental Systems with Biotic Domains.*

S. Guha T.E. McKone, D.H. Bennett, B.F. Lyon *A Generalized , Mass-Conserving Multimedia Transport and Transformation Model: Development of Transfer Factors.*

B.F. Lyon, S. Guha, T.E. McKone. *TRIM: Mathematical and Numerical Aspects.*

D.H. Bennett, T.E. McKone, M.G. Dusetzina. *Building Uncertainty and Sensitivity Analysis into the TRIM Framework.*

R.A. Efroymson, B.E. Sample, B.F. Lyon, G.W. Suter II, C.T. Hunsaker, A.W. Simcock, and D.H. Bennett. *A Dynamic Model for Terrestrial Ecological Exposure to Toxic Air Pollutants.*

R.D. Zimmer, J.Deer, D.S. Jones. *Predicting Pollutant Mass Transfers within Aquatic Systems using the EcoFaTE Model..*

T.E. McKone, Ted Johnson, G.W. Suter II. Estimating Multi-pathway human and ecosystem exposures within the Total Risk Integrated Model (TRIM).

C.T. Hunsaker, B.F. Lyon, T.E. McKone, V. Kilaru, A. W. Simcock. *EcoFaTE Model Parameterization and Verification.*

18th Annual Meeting of the Society of Environmental Toxicology and Chemistry. 16-20 November, 1997. San Francisco, CA.

T. McKone, S. Guha, T. Johnson, B. Lyon, G. Suter, A. Vasu. A Multimedia Health and Ecological Risk Assessment Methodology for Air Pollutants.

R. Zimmer, J. Dee, D. Jones, B. Sample, G. Suter. *Use of EcoFaTE in Modeling Pollutant Mass Transfers and Subsequent Risks within Aquatic Systems.*

R. Efroymson, B. Sample, C. Hunsaker, B. Lyon, A. Simcock, and G. Suter. *A Dynamic Model for Terrestrial Ecological Exposure to Toxic Air Pollutants.*

APPENDIX E - ACRONYMS

BASIN Better Assessment Science Integrating Point and Nonpoint Sources

CHNHYD Channel Hydrodynamic Model for Simulating Flows and Water Surface Elevation in a Stream River Network

CalTox A California EPA Total Exposure Model for Hazardous Waste Sites

CHNTIN Channel Transport Model for Simulating Sediments and Chemical Distribution In a Stream River Network

C_r Courant Number

D Dimensions (1-D, 2-D, or 3-D) (Configurations for models)

D_n Diffusion Coefficient

EC Executive Committee (U.S. EPA/SAB/EC)

EMS Environmental Models Subcommittee (of the U.S. EPA/SAB/ EC)

EPA Environmental Protection Agency (U.S. EPA, or EPA)

HAP Hazardous Air Pollutant

Hg Mercury

HI Hazard Index

HQ Hazard Qotient

HWIR Hazardous Waste Identification Rule

ICM Integrated Compartment Method

ISC Industrial Source Complex family of models and its successors

ISMCM Integrated Spacial Multimedia Compartmental Model (USCLA/School of Engineering and Applied Science)

km	<u>K</u> ilometer
MAC	<u>M</u> odel <u>A</u> ceptability Use <u>C</u> riteria
MATTUM	<u>M</u> ultidimensional <u>M</u> odel for simulating moisture and <u>T</u> hermal <u>T</u> ransport in <u>U</u> nsaturated Porous <u>M</u> edia
m	<u>M</u> eter
MIMS	<u>M</u> ulti-Media <u>I</u> ntegrated <u>M</u> odeling <u>S</u> ystem
NERL	<u>N</u> ational <u>E</u> xposure Research Laboratory (U.S. EPA/NERL)
OAQPS	<u>O</u> ffice of <u>A</u> ir <u>Q</u> uality <u>P</u> lanning and <u>S</u> tandards (U.S. EPA/OAQPS)
SAB	<u>S</u> cience <u>A</u> dvisory <u>B</u> oard (U.S. EPA/SAB)
S	<u>S</u> patial Grid Size
TRIM	<u>T</u> otal <u>R</u> isk <u>I</u> ntegrated <u>M</u> ethodology (Includes TRIM.Expo, TRIM.FaTE, and TRIM.Risk)
TRIM.Expo	<u>T</u> otal <u>R</u> isk <u>I</u> ntegrated <u>M</u> ethodology <u>E</u> xposure Module
TRIM.FaTE	<u>T</u> otal <u>R</u> isk <u>I</u> ntegrated <u>M</u> ethodology <u>F</u> ate Module
TRIM.Risk	<u>T</u> otal <u>R</u> isk <u>I</u> ntegrated <u>M</u> ethodology <u>R</u> isk Module
TSD	<u>T</u> echnical <u>S</u> upport <u>D</u> ocument
V	<u>V</u> elocity
WASP	<u>W</u> aste <u>A</u> rea <u>S</u> <u>P</u> model (- see TRIM.FaTE discussion)



AN SAB ADVISORY ON THE AGENCY'S "TOTAL RISK INTEGRATED METHODOLOGY" (TRIM)

**Prepared by the Environmental
Models Subcommittee of the
Science Advisory Board**