PEER REVIEW OF EPA'S HAZARDOUS WASTE IDENTIFICATION RULE RISK ASSESSMENT MODEL

Solids Transport Module for EXAMS
HWIR Review Draft

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EPA Contract No. 68-W-99-001
Work Assignment No. 17

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September 13, 1999

NOTE

This report was prepared by Eastern Research Group, Inc. (ERG), an EPA contractor, under Contract Number 68-W-99-001. The report presents comments provided by peer reviewers on the *Solids Transport Module for EXAMS HWIR Review Draft* document that is part of EPA's Hazardous Waste Identification Rule risk assessments.

The comments presented in this report have been compiled by topic and by individual peer reviewer. As EPA requested, this report provides the peer review comments exactly as they were submitted to ERG. Also attached are the original comments submitted by each individual reviewer.

Charge for review of EXAMS implementation for HWIR.

Background

EXAMS is a general surface water fate model for organic chemicals (Burns, L.A., 1997, Burns, L.A., et al., 1992). This compartment model has been used routinely by both EPA and industry analysts for the analysis of expected pesticide concentrations in generically-defined environments, such as farm ponds. It has also been used for site-specific analysis of pesticide concentrations in various water bodies around the world. Recently EXAMS was adopted for use as the surface water module for the multimedia software framework (FRAMES) being developed in support of EPA's Hazardous Waste Identification Rule (HWIR).

FRAMES-HWIR simulations will be based on limited data from some 200 sites around the country, supplemented with regional and national data. The sites to be simulated are approximately 3 km in radius, and include networks of small streams, ponds, lakes, and wetlands. These sites will be repeatedly simulated in the context of an overall Monte-Carlo implementation for 200 to 400 chemicals of concern. Each simulation can last between 100 and 10,000 years, depending upon the source releases and multimedia chemical dynamics. Several modules will be passing annual-average flows, solids loads, and chemical loads to EXAMS; these "upstream" modules represent a waste management unit, the local atmosphere, the surrounding watershed, and a shallow groundwater plume. EXAMS will be run in a quasi-dynamic mode driven by these annual-average loads and flows. Concentrations predicted by EXAMS will be averaged annually and passed to a bioaccumulation module, a human exposure module, and an ecological exposure module. To better fit within this FRAMES-HWIR system, some adaptations and extensions of EXAMS are being pursued. The resulting model should be of similar sophistication as the other media modules, must run with available data, and must be able to complete a simulation within a few seconds.

The present version of EXAMS requires the user to specify solids concentrations in water column compartments and bulk density, water content, and bed load (if any) in benthic compartments. Solids are not simulated, but are used to modify chemical transport and reactivity through partitioning. Chemical exchange between water column and underlying sediment is controlled by a bulk dispersion coefficient. Net deposition and burial of solids and associated chemical are not considered.

A simple conservative solids module is implemented in the EXAMS-HWIR interface program ExamsIO. This interface calculates solids concentrations in each reach from annual watershed erosion loadings and reach flows assuming no settling loss (i.e., washload only). Updated solids concentrations are delivered to EXAMS for each simulated year.

A more detailed solids module is proposed here for implementation within EXAMS, replacing the ExamsIO washload calculations. This new solids module would link internal solids transport and concentrations to external and internal solids loadings. It is not intended to be a predictive sediment transport model. Rather, the objective is to obtain a conceptually complete and internally consistent description of net solids transport in order to better predict chemical fate in water body networks linked with their watersheds. The time scale for this module is months to years. It does not attempt to simulate the short-term dynamics of sediment transport, which would require detailed hydrodynamic data. The solids module will be based in part on measured or inferred site-specific data.

Charge Questions:

In a screening level assessment such as contemplated for HWIR, is the present ExamsIO conservative treatment of solids acceptable? There is no net settling/burial loss pathway for chemicals in the present version of EXAMS. The lack of long-term average settling loss in small upland systems would be conservative for ponds, lakes and wetlands, and perhaps a good assumption for stream networks. Please comment on these issues.

The annual-average solids balance treatment outlined in the review document is designed to make the EXAMS solids concentrations more accurate, and to add a long-term average settling/burial loss for ponds, lakes, and wetlands. Will the gain in internal consistency be worth the extra computational burden?

In implementing the solids balance equations outlined in the review document, we have made choices as to which terms are state variables and which are input parameters. We have tried to calculate the most uncertain variables (i.e., net settling velocity for abiotic solids) based on regional or site-specific input of other variables (i.e., long-term average burial or accretion velocity). Please comment on the choice of state variables versus input parameters, and the availability of data to support this approach.

More mechanistic solids simulation models, of course, exist. The data and computational burdens were considered too severe for implementation in the HWIR program. Please comment on this judgment. If there are better solids models available that could simulate water body networks based on annual flows and loadings within a few seconds (maximum), please let us know.

Reviewer Comments Summary Report for the
Solids Transport Module for EXAMS
HWIR Review Draft

Charge 1: *In a screening level assessment such as contemplated for HWIR, is the present ExamsIO conservative treatment of solids acceptable? There is no net settling/burial loss pathway for chemicals in the present version of EXAMS. The lack of long-term average settling loss in small upland systems would be conservative for ponds, lakes and wetlands, and perhaps a good assumption for stream networks. Please comment on these issues.*

Dr. Aral:

As is described in the relevant, literature [Tetra Tech, 1997], the application of the FRAMES-HWIR model may be required at different levels of detail for different applications. In these applications, the details and accuracy required of the sub-models used in the FRAMES software will be significantly different from one another. For example, for the surface impoundment study described in Tetra Tech [1997], a three-tier modeling effort is proposed with a minimum application of at least the first two tiers. In this case, the complexity of the approach, thus the level of modeling detail required to meet the objectives of the study, increases, as the tier number increases. The level of detail is generally classified as either a screening level study (tier one) or a detailed study (tier two) or a site-specific study (tier three). A key determination of the acceptable level of detail lies in determining the acceptable level of certainty in the analytical results and evaluating the availability and quality of input data.

This observation indicates that the components of the EXAMS model that will be utilized in the FRAMES model, has to provide this flexibility to the user as well. As indicated in the STM/EXAMS, a simple conservative solids module is implemented in the EXAMS-HWIR interface program EXAMSIO. In this interface, the solids concentrations in each reach is calculated from annual watershed erosion loadings and reach flows assuming no settling loss. This approach is suitable for screening level analysis (tier one) and provides a conservative solution to the problem in the absence of data, for ponds, lakes and wetlands. However, this approach will not provide a conservative solution for stream networks since the settling is not the only important mechanism that needs to be considered in this case. Internal solids transport, advection effects and re-suspension of sediments are just a few of the other mechanisms that need to be considered in this case.

The approach provided in EXAMSIO may not be suitable, if a more detailed analysis is the primary objective, as described in tier two or tier three level studies [Tetra Tech, 1997]. For such cases more realistic solids simulation models may be required as attempted in the STM/EXAMS. Thus, both approaches are necessary and should be made available for implementation. The choice between the two approaches should be made by the user, which will be based on the objectives of the study conducted and the availability of the data in the specific study.

Dr. Donigian:

The present conservative treatment of solids in ExamsIO, with no setting/burial pathway for sorbed chemicals, would appear to be acceptable for non-persistent, non-sorptive (i.e. hydrophilic) compounds that do not sorb to sediments/solids, and therefore are not likely to accumulate in beds of streams, wetlands, and waterbodies with the accumulated solids deposition. I also agree with the statement that ignoring a long-term settling loss in small upland systems may be appropriate for ponds, lakes, and wetlands, and might be a good assumption for streams, depending upon the degree of conservatism that is acceptable in a screening level exposure assessment like HWIR. I am not familiar enough with HWIR, (and no HWIR background document was provided with this assignment), to be able to make a judgement as to whether the ExamsIO treatment of solids is acceptable for HWIR assessments.

However, for highly sorptive (i.e. hydrophobic) compounds, ignoring the settling loss pathway may be too conservative. If the compound is non-persistent (i.e. decays relatively rapidly), any deposition losses will effectively remove it from the system, and ignoring this loss may lead to significant over-estimation of exposure concentrations. For persistent compounds that remain in the bed, the opportunity exists for resuspension into the water column, and subsequent exposure, during high flow periods; therefore ignoring the settling loss might be appropriate for long-term screening-level exposure assessments. If (as I suspect) most of the HWIR compounds tend to be in this persistent, hydrophobic category, the ExamsIO conservative treatment of solids may be acceptable.

Dr. Lick:

Solids Balance in Streams and Rivers

3. There is no vertical diffusion or mixing in any of these equations. In particular, there is no diffusive flux from the sediments (mixed benthic layer) to the overlying water.

   By almost any reasonable calculation, there are generally more (often orders of magnitude more) contaminants in the bottom sediments than in the overlying water. These bottom sediments are also generally the major source and/or sink of contaminants to the overlying water. This flux can not be ignored and, more than that, since it is the major source/sink of contaminants, the accuracy of the model predictions depends on the accuracy with which the flux is calculated.

4. The model uses a parameter, V_{B2}, which is undefined in the report but I assume it is the volume of the mixed benthic layer. How will this parameter be estimated? If there is exchange of contaminants between the bottom sediments and the overlying water as suggested above, the parameter will govern the long-term behavior of the contaminants and therefore needs to be known accurately; unless of course you want to assume the answer and deduce V_{B2} from this (a poor approach).

5. The model assumes the presence of a benthic boundary layer. Considering the approximations in the rest of the model, this seems unnecessary and introduces additional parameters whose values are unknown and can not be estimated accurately, e.g., V_{B1}, v_{B1}.

Solids Balance in Ponds, Lakes, and Wetlands

2. In Eqs. (17)-(20), there is no vertical diffusion or flux from the mixed benthic boundary layer to the overlying water. Same comments as in A3 and A4.

3. Is benthic boundary layer necessary? Same Comments as in A5.

General

1. Is treatment of solids acceptable? No, in any present or proposed version of EXAMS.

   To repeat, sediments are the major source/sink of contaminants in rivers, lakes, and other surface waters. This flux must be addressed directly and treated accurately. The accuracy of the description of this process determines the accuracy of the model predictions.

   The model must have mixing (bioturbation, resuspension/deposition) of contaminants in a mixed layer in the bottom sediments and a flux from the bottom sediments to the overlying water. V_{B2} is the crucial parameter and must be estimated accurately since this determines the long-term behavior of a contaminant in an aquatic system.

Charge 2: *The annual-average solids balance treatment outlined in the review document is designed to make the EXAMS solids concentrations more accurate, and to add a long-term average settling/burial loss for ponds, lakes, and wetlands. Will the gain in internal consistency be worth the extra computational burden?*

Dr. Aral:

The procedure outlined in STM/EXAMS is important in view of the tier two and tier three level studies described above. This improvement is necessary in order to gain some internal consistency, if the data is available to implement it. In this improved computational model, the added computational burden should not be the concern nor the criteria for two reasons: (i) the proposed algorithms are very simple and the added computational burden will be minimal even if the model will be used in a Monte Carlo sense; and (ii) ever increasing speed of computational platforms will further eliminate this concern. Having said that, I am of the opinion that the procedures described in STM/EXAMS is mainly suitable for ponds, lakes, and wetlands and may not be applicable to rivers and stream networks. For the latter, if an improvement to the existing code is required, then EXAMS, in its present state or in its improved state through STM/EXAMS, may not be the method of choice.

Dr. Donigian:

I agree that the proposed enhancements to the solids balance in EXAMS, including a settling/burial loss term, should make the overall solids concentrations more accurate by including a representation of settling and burial processes for lentic (ponds, lakes, wetlands) systems. However, I am concerned with its use on an average annual basis, especially in climatic regions that show extreme, or highly variable, seasonal patterns in precipitation and resulting watershed runoff and loadings. Loadings from atmospheric and watershed sources may be too dynamic and variable to be well represented by average annual values, especially in arid or semi-arid areas of the West, Southwest, and portions of the Midwest. Loadings from shallow groundwater and waste management units may be less variable, and thus more appropriate for an annual assessment, but some seasonal variation would still be expected.

I can't really respond to the issue of whether the 'gain in internal consistency ... is ... worth the extra computational burden' from the proposed solids enhancements. No information was provided to indicate what 'computational burden' is likely to result from the proposed code enhancements. Normally, analytical solutions are not often very demanding in terms of computational time; however, any time a methodology involves hundreds of chemicals and multiple decades/centuries of simulation time, any significant increase in runtime for a single run can be a substantial burden.

Dr. Lick:

The above changes [see Dr. Lick's comments below in the General section] should cause negligible change in computer time.

Charge 3: *In implementing the solids balance equations outlined in the review document, we have made choices as to which terms are state variables and which are input parameters. We have tried to calculate the most uncertain variables (i.e., net settling velocity for abiotic solids) based on regional or site-specific input of other variables (i.e., long-term average burial or accretion velocity). Please comment on the choice of state variables versus input parameters, and the availability of data to support this approach.*

Dr. Aral:

In STM/EXAMS document the derivation or the physical principles and reasoning used to arrive at the balance equations (Equations 1 through 19) are not given. Thus, it is not clear to the reader which mechanisms are considered, which mechanisms are ignored, which mechanisms are simplified and included, and which mechanisms are fully implemented without simplification. STM/EXAMS document would have been a more complete document if the details of this aspect of the study were included in the draft document. For example, it is not clear to this reviewer why the terms L_{SBU} and L_{PBU} are included in to the equations as known variables, and L_{SB} and L_{PB} terms are not used in these equations at all, as either known or unknown variables. In the text of the document L_{SB} and L_{PB} are defined as solids loss through the bed load. Does this imply that the solids loss through the bed load is ignored, i.e., considered to be an unimportant mechanism, or does it imply that these terms are inherently considered in other mechanisms and should not be double counted? This reviewer did not find any evidence of possible double counting of these terms in the governing equations, if they were included as explicit variables. Thus, the conclusion is that they must have been ignored, considering that this mechanism is unimportant. If such is the case, the reason behind this assumption should be clearly explained.

Similarly, the terms S_{B1} and S_{B2} are treated as known variables. These terms define the solids concentrations at benthic sediment layers. If one treats these terms as known variables then the assumption is that the solids concentrations in the benthic sediment layers are not changing, based on transfer mechanisms considered. This is not a good assumption since it is more likely that these variables will change based on L_{SBU} and L_{PBU}, L_{SB} and L_{PB} (which is completely ignored as indicated above) and other variables such as solids transport velocities etc. This problem might have been handled by the introduction of another known variable TSS_{B1} and TSS_{B2}, similar to the definition used for TSS for upper layers, representing an observed average solids concentration that will be maintained as a long-term average in the lower layers. Then, given TSS_{B1} and TSS_{B2}, which would be a characteristic value for the region under study, the S_{B1} and S_{B2} could be treated as unknown variables and two interface balance equations could be written to solve these additional unknowns. These interface equations would include L_{SBU}, L_{PBU}, L_{SB} and L_{PB}.

In the charge given above it is indicated that the authors *have tried to calculate the most uncertain variables...based on regional or site-specific input of other variables*. This reviewer is of the opinion that the unknown variables should be selected based upon the physical principles which describe the mechanisms considered and not based on the uncertainty associated with a certain variable. For example the "f" terms represent organic carbon content of solids. F_{G2} and f_{G3} are input values which are assumed to be known. The rate constants "k" are considered to be known which is the most logical choice. Then terms such as f_{G2B1}, f_{G3B1} should be a function of 'k," "S_{PW}" and S_{SW}" variables and not explicit unknowns. These terms are treated as unknowns in the present study. The reason behind this choice should be explained.

In summary, it is not clear to this reviewer how these choices came to be made in the present study. Most probably these points are associated with some physical reasoning and may be explainable. However, as indicated above, the STM/EXAMS document does not include a section in which the details of the derivation or the physical reasoning used to arrive at the balance equations (Equations 1 through 19) are given. This lack of information may be the source of the questions raised above. These points may be clarified during the revision of the STM/EXAMS document.

Dr. Donigian:

In general, the solids enhancements appear to be well-developed and intelligently described, and they are consistent with the overall level of detail in EXAMS. The model formulation, in terms of state variables versus input parameters, appears to be reversed from more traditional dynamic modeling approaches, where the state variables tend to be concentrations and compartment storages and the parameters are usually rate coefficients and physical/chemical/biological characteristics of the system being modeled. I understand the choice of state variables versus parameters was based on the availability of input data, but it is not abundantly clear (to me) that all the required input data is readily 'available', as suggested in the 'Background' section (i.e. 'Must run with available data'). Summary tables of 'required input data' and state variables would make the document (and approach) much easier to review and evaluate.

Dr. Lick:
Solids balance in Streams and Rivers

1. S_{pw1} is determined from Eq. (1). Once this is known, Eq. (2) determines v_{sdep}, which is assumed to be a state variable and therefore depends on and varies with the other input and state variables in Eq. (2). From a physical point of view, I can't imagine why this should be so. By this means, a wide variation in v_{sdep} is possible (even negative numbers?) and these v_{sdep}'s would have nothing to do with a deposition or settling velocity.

   In the usual interpretation, v_{sdep} depends on the settling (deposition) speed (which depends on particle properties, flow rate, bottom roughness, slope angle, and possibly sediment type). More generally, it is used as a net deposition velocity which somehow averages resuspension and deposition. What it is not is a fudge factor which can be used to balance mass balance equations, although it is often used this way.

2. In Eq. (2), I assume the TSS-S_{pw1} is the concentration of suspended abiotic solids in the water column. If this is true and since TSS is an input variable (constant?), then the concentration of suspended abiotic solids is dependent on the concentration of plankton solids and can vary arbitrarily (also possibly negative?). Doesn't seem realistic.

6. Bed load is variable which depends on hydrodynamic conditions. It is not a state variable to be determined by the variation of other state variables.

Solids Balance in Ponds, lakes and Wetlands

1. Eq. (9) contains a term $S_{pw1} E_{w12} / L_{w12}$ which presumably represents vertical diffusion (mixing). But diffusion of S depends on a gradient of S (or a difference between two quantities at different levels), not on an absolute value of a single variable, S. For example, in Eq. (9), the diffusion term should be $(S_{pw1} - S_{pw2}) E_{w12} / L_{w12}$. Same comments for Eq. (10). As written, the diffusion term behaves as a settling, or convection, term and adds to it.

5. v_{pdep} can be calculated from Eq. (9) since it is the only state variable in Eq. (9). v_{pdep} is a variable that depends on size, density, etc. of the particle. Whys should it depend on variables in Eq. (9)? Similar comments to those in A1. Same Comments pertain to v_{sdep} in Eq. (10).

General

2. Choice of State Variables.
   Settling (deposition) velocities are certainly important variables but they are determined by physical quantities and hydrodynamics. They are not dependent state variables that are varied so as to satisfy mass balance equations.

Suspended abiotic solids concentration should not be determined from TSS-S_{pw1}. It does not depend on S_{pw1}.

Bed load is a variable which depends on hydrodynamic conditions. It is not a state variable to be determined by the variation of other state variables.

Charge 4: *More mechanistic solids simulation models, of course, exist. The data and computational burdens were considered too severe for implementation in the HWIR program. Please comment on this judgment. If there are better solids models available that could simulate water body networks based on annual flows and loadings within a few seconds (maximum), please let us know.*

Dr. Aral:

Based upon a literature search I have conducted for this review, it seems there is no suitable model that exists in the literature that would fit to the specifications described in the STM/EXAMS (simplicity and minimal computation time). There are more sophisticated river networks models such as OTIS and RiverNET or other HEC-based simulation tools for rivers, ponds, and lakes. However, these models would not be suitable for limited data and efficient computation applications, such as the one required in FRAMES-HWIR modeling effort. Given this background, it is feasible to proceed in the direction outlined in STM/EXAMS. However, the governing equations used in the STM/EXAMS would be more reliable if differential mass balance equations are used instead of linear mass balance processes described in STM/EXAMS. If differential mass balance equations are used, the governing equations may be expressed in terms of simultaneous ordinary differential equations instead of simultaneous algebraic equations. These simultaneous ordinary differential equations can be solved very easily on desk top computers without much difficulty and with out excessive computation time. The reliability provided in this approach would be more convincing and suitable for the purpose of the effort undertaken in STM/EXAMS.

Dr. Donigian:

I am not aware of any other models/methods that could meet the severe constraints of performing annual solids simulations with a few seconds of runtime, so that repeated Monte Carlo simulations of 100 to 10,000 years could be efficiently performed for 200 to 400 chemicals at 200 sites. These are extremely severe constraints. It would have been helpful to have additional background documentation on FRAMES-HWIR requirements and methodologies to describe the regulatory environment and situation within which the proposed EXAMS changes were developed.

Dr. Lick:

3. Solids Simulation Models

Many people are working on sophisticated sediment transport and fate models. However, this is not what you need in EXAMS, except that anything you do in EXAMS cannot be totally at variance with correct sediment transport and fate processes.

At the very least, a well-mixed benthic layer approximation should be used. This allows the interaction (by bioturbation and resuspension/deposition) and transfer of contaminants between the bottom sediment and the overlying water. A simple model of this type is that developed by Edgington (1993). This concept has been used more extensively and in more detail by many others (see, for example, the text by Chapra (1997) and numerous articles in the literature by Connolly (1991, 1992, and more recent articles), presently at QEA).

In general, the authors should at least be aware that, in many cases, average flows and conditions do not adequately describe fluxes of contaminants. Big events, such as floods on rivers and storms on lakes, may transport more contaminants than the total of all other smaller events (Lick, 1992; Lick et al., 1994). Because of this, flows necessary to satisfy the mass balance equations are probably not the average flows (as defined by averages over time). Same comments pertain to settling and deposition velocities.

General Comments:

Dr. Aral:

The document under review is prepared to provide a conceptually complete and internally consistent description of net solids transports module for the EXAMS model [Burns, L.A., 1997; Burns, L.A., et al., 1992]. The following modifications and/or extension of the study summarized in the STM/EXAMS document are necessary to improve the presentation of the material to a technical audience.

i. It is recommended that the report begin with a clear description of assumptions and limitations of the proposed approach.

ii. It is recommended the report include a section on physical principles implemented in the derivation of balance equations used in the proposed approach.

iii. It is recommended that the authors provide information on which alternative approaches were considered in addition to the model described in the draft document. The criteria used in selecting the model proposed in the draft document should be clearly identified. In its present form the draft document does not provide this information. This section may be included in the final report.

iv. Justification of the assumptions made in the derivation of mass balance equations should be provided in terms of physical, statistical, and conceptual reasoning. In its present form the draft document does not provide this information.

v. A better and more reliable set of governing equations can be developed using differential mass balance approach. The governing equations derived through such a process would be more meaningful and defensible in terms of the identification of the known and unknown variables of the problem.

vi. In its present form, the draft document provided to the reviewers is weak in its technical content and in details of the processes that are considered in the development of the system of equations. To justify the adoption of the proposed model as a new module for the EXAMS software package, more information is needed along the lines of the discussion provided in this review.

Dr. Donigian:

a. A summary of model assumptions, for both lotic and lentic systems, would be helpful to clarify the document. The assumptions are noted in the text, but a summary table would enhance the discussion.

b. Summary tables of input parameters, state variables, units, and typical values would help the overall presentation of the proposed enhancements.

c. Some level of testing should be performed and documented to show how the proposed changes behave under typical application conditions and available data for parameter evaluation.

d. A small '*v*' is used in the text and equations for solid transport velocities, but there is also a capital '*V*' in the equations that I was not able to find defined anywhere in the text; perhaps I missed it. I assumed it was a compartment volume term, but I didn't see it defined anywhere. Also, the figure was a little confusing in how it showed the 'v' term - small or large, e.g. v_{Pdep} looks like a small v meaning a velocity, but all the other 'v's in the figure look like capital 'V's.

e. In the discussion on Lentic reaches, the first sentence in the second paragraph says 'bed load in lotic reaches is neglible' - I assume this should be 'lentic' reaches.

f. Page numbers should be added to the document.

Dr. Lick:

<u>Solids Balance in Ponds, Lakes, and Wetlands</u>

4. In Eqs. (11) and (12), terms with an overline appear. These terms are never defined. The statement "(terms with overline are omitted if this is the bottom water segment)" cannot be understood.

<u>General:</u>

In summary, suggested improvements to the model are as follows.

(a) Redefine state variables.
(b) Flux of chemicals from the bottom sediments (well-mixed layer) to the overlying water must be included.
(c) The benthic boundary layer is unnecessary and adds complexity but not accuracy.
(d) Burial velocity should be included in the river model as well as in the lake model.

The above changes should cause negligible change in computer time.

References:

Dr. Aral:
Ambrose, R.B., Burns, L.A., and Suarez, L.A., 1998. *Solids Transport for EXAMS-HWIR Review Draft*, USEPA document, 15p.

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Tetra Tech, 1997. *Technical Memorandum, Proposed Risk Assessment Modeling Framework for the Surface Impoundment Study*, USEPA Contract No. 68-W6-0061, prepared by Tetra Tech Inc.

Dr. Lick
Chapra, S.C., 1993, Surface Water-Quality Modeling, McGraw-Hill.

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Edgington, D.N., 1993, The Effects of Sediment Mixing on the Long-Term Behavior of Pollutants in Lakes, in "Transport and Transformation of Contaminants Near the Sediment-Water Interface," Lewis Publishers.

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ATTACHMENT A

Peer Review of *"Solids Transport Module for EXAMS HWIR Review Draft"* by:

Mustafa M. Aral
Georgia Insitute of Technology

Review

Solids Transport Module for EXAMS
HWIR Review Draft

by

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During the first week of August 1999, USEPA provided a group of reviewers with a fifteen page technical document entitled "Solids Transport Module for EXAMS - HWIR Review Draft," [November 12, 1998]. In this review, the draft document will be referred to as STM/EXAMS. In addition to STM/EXAMS, reviewers were also given a document entitled "Charge to Peer Reviewers" (CPR). The CPR identified specific topics to be addressed in the review. This chronology constitutes the starting point of this review. The topics identified in the CPR and my response to each topic may be found below.

Charge Questions

Charge 1: *In a screening level assessment such as contemplated for HWIR, is the present ExamsIO conservative treatment of solids acceptable? There is no net settling/burial loss pathway for chemicals in the present version of EXAMS. The lack of long-term average settling loss in small upland systems would be conservative for ponds, lakes and wetlands, and perhaps a good assumption for stream networks. Please comment on these issues.*

Response: As is described in the relevant, literature [Tetra Tech, 1997], the application of the FRAMES-HWIR model may be required at different levels of detail for different applications. In these applications, the details and accuracy required of the sub-models used in the FRAMES software will be significantly different from one another. For example, for the surface impoundment study described in Tetra Tech [1997], a three-tier modeling effort is proposed with a minimum application of at least the first two tiers. In this case, the complexity of the approach, thus the level of modeling detail required to meet the objectives of the study, increases, as the tier number increases. The level of detail is generally classified as either a screening level study (tier one) or a detailed study (tier two) or a site-specific study (tier three). A key determination of the acceptable level of detail lies in determining the acceptable level of certainty in the analytical results and evaluating the availability and quality of input data.

This observation indicates that the components of the EXAMS model that will be utilized in the FRAMES model, has to provide this flexibility to the user as well. As indicated in the STM/EXAMS, a simple conservative solids module is implemented in the EXAMS-HWIR interface program EXAMSIO. In this interface, the solids concentrations in each reach is calculated from annual watershed erosion loadings and reach flows assuming no settling loss. This approach is suitable for screening level analysis (tier one) and provides a conservative solution to the problem in the absence of data, for ponds, lakes and wetlands. However, this approach will not provide a conservative solution for stream networks since the settling is not the only important mechanism that needs to be considered in this case. Internal solids transport, advection effects and re-suspension of sediments are just a few of the other mechanisms that need to be considered in this case.

The approach provided in EXAMSIO may not be suitable, if a more detailed analysis is the primary objective, as described in tier two or tier three level studies [Tetra Tech, 1997]. For such cases more realistic solids simulation models may be required as attempted in the STM/EXAMS. Thus, both approaches are necessary and should be made available for implementation. The choice between the two approaches should be made by the user, which will be based on the objectives of the study conducted and the availability of the data in the specific study.

Charge 2: *The annual-average solids balance treatment outlined in the review document is designed to make the EXAMS solids concentrations more accurate, and to add a long-term average settling/burial loss for ponds, lakes, and wetlands. Will the gain in internal consistency be worth the extra computational burden?*

Response: The procedure outlined in STM/EXAMS is important in view of the tier two and tier three level studies described above. This improvement is necessary in order to gain some internal consistency, if the data is available to implement it. In this improved computational model, the added computational burden should not be the concern nor the criteria for two reasons: (i) the proposed algorithms are very simple and the added computational burden will be minimal even if the model will be used in a Monte Carlo sense; and (ii) ever increasing speed of computational platforms will further eliminate this concern. Having said that, I am of the opinion that the procedures described in STM/EXAMS is mainly suitable for ponds, lakes, and wetlands and may not be applicable to rivers and stream networks. For the latter, if an improvement to the existing code is required, then EXAMS, in its present state or in its improved state through STM/EXAMS, may not be the method of choice.

Charge 3: *In implementing the solids balance equations outlined in the review document, we have made choices as to which terms are state variables and which are input parameters. We have tried to calculate the most uncertain variables (i.e., net settling velocity for abiotic solids) based on regional or site-specific input of other variables (i.e., long-term average burial or accretion velocity). Please comment on the choice of state variables versus input parameters, and the availability of data to support this approach.*

Response: In STM/EXAMS document the derivation or the physical principles and reasoning used to arrive at the balance equations (Equations 1 through 19) are not given. Thus, it is not clear to the reader which mechanisms are considered, which mechanisms are ignored, which mechanisms are simplified and included, and which mechanisms are fully implemented without simplification. STM/EXAMS document would have been a more complete document if the details of this aspect of the study were included in the draft document. For example, it is not clear to this reviewer why the terms L_{SBU} and L_{PBU} are included in to the equations as known variables, and L_{SB} and L_{PB} terms are not used in these equations at all, as either known or unknown variables. In the text of the document L_{SB} and L_{PB} are defined as solids loss through the bed load. Does this imply that the solids loss through the bed load is ignored, i.e., considered to be an unimportant mechanism, or does it imply that these terms are inherently considered in other mechanisms and should not be double counted? This reviewer did not find any evidence of possible double counting of these terms in the governing equations, if they were included as explicit variables. Thus, the conclusion is that they must have been ignored, considering that this mechanism is unimportant. If such is the case, the reason behind this assumption should be clearly explained.

Similarly, the terms S_{B1} and S_{B2} are treated as known variables. These terms define the solids concentrations at benthic sediment layers. If one treats these terms as known variables then the assumption is that the solids concentrations in the benthic sediment layers are not changing, based on transfer mechanisms considered. This is not a good assumption since it is more likely that these variables will change based on L_{SBU} and L_{PBU}, L_{SB} and L_{PB} (which is completely ignored as indicated above) and other variables such as solids transport velocities etc. This problem might have been handled by the introduction of another known variable TSS_{B1} and TSS_{B2}, similar to the definition used for TSS for upper layers, representing an observed average solids concentration that will be maintained as a long-term average in the lower layers. Then, given TSS_{B1} and TSS_{B2}, which would be a characteristic value for the region under study, the S_{B1} and S_{B2} could be treated as unknown variables and two interface balance equations could be written to solve these additional unknowns. These interface equations would include L_{SBU}, L_{PBU}, L_{SB} and L_{PB}.

In the charge given above it is indicated that the authors *have tried to calculate the most uncertain variables...based on regional or site-specific input of other variables*. This reviewer is of the opinion that the unknown variables should be selected based upon the physical principles which describe the mechanisms considered and not based on the uncertainty associated with a certain variable. For example the "f" terms represent organic carbon content of solids. F_{G2} and f_{G3} are input values which are assumed to be known. The rate constants "k" are considered to be known which is the most logical choice. Then terms such as f_{G2B1}, f_{G3B1} should be a function of 'k," "S_{PW}" and S_{SW}" variables and not explicit unknowns. These terms are treated as unknowns in the present study. The reason behind this choice should be explained.

In summary, it is not clear to this reviewer how these choices came to be made in the present study. Most probably these points are associated with some physical reasoning and may be explainable. However, as indicated above, the STM/EXAMS document does not include a section in which the details of the derivation or the physical reasoning used to arrive at the balance equations (Equations 1 through 19) are given. This lack of information may be the source of the questions raised above. These points may be clarified during the revision of the STM/EXAMS document.

Charge 4: *More mechanistic solids simulation models, of course, exist. The data and computational burdens were considered too severe for implementation in the HWIR program. Please comment on this judgment. If there are better solids models available that could simulate water body networks based on annual flows and loadings within a few seconds (maximum), please let us know.*

Response: Based upon a literature search I have conducted for this review, it seems there is no suitable model that exists in the literature that would fit to the specifications described in the STM/EXAMS (simplicity and minimal computation time). There are more sophisticated river networks models such as OTIS and RiverNET or other HEC-based simulation tools for rivers, ponds, and lakes. However, these models would not be suitable for limited data and efficient computation applications, such as the one required in FRAMES-HWIR modeling effort. Given this background, it is feasible to proceed in the direction outlined in STM/EXAMS. However, the governing equations used in the STM/EXAMS would be more reliable if differential mass balance equations are used instead of linear mass balance processes described in STM/EXAMS. If differential mass balance equations are used, the governing equations may be expressed in terms of simultaneous ordinary differential equations instead of simultaneous algebraic equations. These simultaneous ordinary differential equations can be solved very easily on desk top computers without much difficulty and with out excessive computation time. The reliability provided in this approach would be more convincing and suitable for the purpose of the effort undertaken in STM/EXAMS.

General

The document under review is prepared to provide a conceptually complete and internally consistent description of net solids transports module for the EXAMS model [Burns, L.A., 1997; Burns, L.A., et al., 1992]. The following modifications and/or extension of the study summarized in the STM/EXAMS document are necessary to improve the presentation of the material to a technical audience.

i. It is recommended that the report begin with a clear description of assumptions and limitations of the proposed approach.

ii. It is recommended the report include a section on physical principles implemented in the derivation of balance equations used in the proposed approach.

iii. It is recommended that the authors provide information on which alternative approaches were considered in addition to the model described in the draft document. The criteria used in selecting the model proposed in the draft document should be clearly identified. In its present form the draft document does not provide this information. This section may be included in the final report.

iv. Justification of the assumptions made in the derivation of mass balance equations should be provided in terms of physical, statistical, and conceptual reasoning. In its present form the draft document does not provide this information.

v. A better and more reliable set of governing equations can be developed using differential mass balance approach. The governing equations derived through such a process would be more meaningful and defensible in terms of the identification of the known and unknown variables of the problem.

vi. In its present form, the draft document provided to the reviewers is weak in its technical content and in details of the processes that are considered in the development of the system of equations. To justify the adoption of the proposed model as a new module for the EXAMS software package, more information is needed along the lines of the discussion provided in this review.

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Ambrose, R.B., Burns, L.A., and Suarez, L.A., 1998. *Solids Transport for EXAMS-HWIR Review Draft*, USEPA document, 15p.

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Tetra Tech, 1997. *Technical Memorandum, Proposed Risk Assessment Modeling Framework for the Surface Impoundment Study*, USEPA Contract No. 68-W6-0061, prepared by Tetra Tech Inc.

ATTACHMENT B

Peer Review of *"Solids Transport Module for EXAMS HWIR Review Draft"* by:

Anthony S. Donigian
AQUA TERRA Consultants

Review of 'Solids Transport Module for EXAMS HWIR Review Draft'
by R.B. Ambrose, Jr., L.A. Burns, and L.A. Suarez
Draft dated 12 November 1998

Prepared by

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29 August 1999

Prepared for

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The above-cited draft document was reviewed following the general guidelines provided by ERG, Inc in the companion document entitled 'Charge for Review of EXAMS Implementation for HWIR'. Below I have prepared my responses for each of the four major 'Charge' questions included in guidelines, followed by some general recommendations and questions.

1. Comment on the acceptability of the ExamsIO treatment of solids for screening level assessments like HWIR.

The present conservative treatment of solids in ExamsIO, with no setting/burial pathway for sorbed chemicals, would appear to be acceptable for non-persistent, non-sorptive (i.e. hydrophilic) compounds that do not sorb to sediments/solids, and therefore are not likely to accumulate in beds of streams, wetlands, and waterbodies with the accumulated solids deposition. I also agree with the statement that ignoring a long-term settling loss in small upland systems may be appropriate for ponds, lakes, and wetlands, and might be a good assumption for streams, depending upon the degree of conservatism that is acceptable in a screening level exposure assessment like HWIR. I am not familiar enough with HWIR, (and no HWIR background document was provided with this assignment), to be able to make a judgement as to whether the ExamsIO treatment of solids is acceptable for HWIR assessments.

However, for highly sorptive (i.e. hydrophobic) compounds, ignoring the settling loss pathway may be too conservative. If the compound is non-persistent (i.e. decays relatively rapidly), any deposition losses will effectively remove it from the system, and ignoring this loss may lead to significant over-estimation of exposure concentrations. For persistent compounds that remain in the bed, the opportunity exists for resuspension into the water column, and subsequent exposure, during high flow periods; therefore ignoring the settling loss might be appropriate for long-term screening-level exposure assessments. If (as I suspect) most of the HWIR compounds tend to be in this persistent, hydrophobic category, the ExamsIO conservative treatment of solids may be acceptable.

2. Comment on the benefits from the proposed enhancements to the solids treatment in EXAMS.

I agree that the proposed enhancements to the solids balance in EXAMS, including a settling/burial loss term, should make the overall solids concentrations more accurate by including a representation of settling and burial processes for lentic (ponds, lakes, wetlands) systems. However, I am concerned with its use on an average annual basis, especially in climatic regions that show extreme, or highly variable, seasonal patterns in precipitation and resulting watershed runoff and loadings. Loadings from atmospheric and watershed sources may be too dynamic and variable to be well represented by average annual values, especially in arid or semi-arid areas of the West, Southwest, and portions of the Midwest. Loadings from shallow groundwater and waste management units may be less variable, and thus more appropriate for an annual assessment, but some seasonal variation would still be expected.

I can't really respond to the issue of whether the 'gain in internal consistency ... is ... worth the extra computational burden' from the proposed solids enhancements. No information was provided to indicate what 'computational burden' is likely to result from the proposed code enhancements. Normally, analytical solutions are not often very demanding in terms of computational time; however, any time a methodology involves hundreds of chemicals and multiple decades/centuries of simulation time, any significant increase in runtime for a single run can be a substantial burden.

3. Comment on the choice of state variables versus input parameters, and availability of data.

In general, the solids enhancements appear to be well-developed and intelligently described, and they are consistent with the overall level of detail in EXAMS. The model formulation, in terms of state variables versus input parameters, appears to be reversed from more traditional dynamic modeling approaches, where the state variables tend to be concentrations and compartment storages and the parameters are usually rate coefficients and physical/chemical/biological characteristics of the system being modeled. I understand the choice of state variables versus parameters was based on the availability of input data, but it is not abundantly clear (to me) that all the required input data is readily 'available', as suggested in the 'Background' section (i.e. 'Must run with available data'). Summary tables of 'required input data' and state variables would make the document (and approach) much easier to review and evaluate.

4. Comment on overall approach and availability of alternative models/methods.

I am not aware of any other models/methods that could meet the severe constraints of performing annual solids simulations with a few seconds of runtime, so that repeated

Monte Carlo simulations of 100 to 10,000 years could be efficiently performed for 200 to 400 chemicals at 200 sites. These are extremely severe constraints. It would have been helpful to have additional background documentation on FRAMES-HWIR requirements and methodologies to describe the regulatory environment and situation within which the proposed EXAMS changes were developed.

Additional Recommendations, Questions, etc.

a. A summary of model assumptions, for both lotic and lentic systems, would be helpful to clarify the document. The assumptions are noted in the text, but a summary table would enhance the discussion.

b. Summary tables of input parameters, state variables, units, and typical values would help the overall presentation of the proposed enhancements.

c. Some level of testing should be performed and documented to show how the proposed changes behave under typical application conditions and available data for parameter evaluation.

d. A small '*v*' is used in the text and equations for solid transport velocities, but there is also a capital '*V*' in the equations that I was not able to find defined anywhere in the text; perhaps I missed it. I assumed it was a compartment volume term, but I didn't see it defined anywhere. Also, the figure was a little confusing in how it showed the 'v' term - small or large, e.g. v_{Pdep} looks like a small v meaning a velocity, but all the other 'v's in the figure look like capital 'V's.

e. In the discussion on Lentic reaches, the first sentence in the second paragraph says 'bed load in lotic reaches is neglible' - I assume this should be 'lentic' reaches.

f. Page numbers should be added to the document.

ATTACHMENT C

Peer Review of *"Solids Transport Module for EXAMS HWIR Review Draft"* by:

Wilbert Lick
University of California-Santa Barbara

Review of
Solids Transport Module for EXAMS
HWIR Review Draft

Specific comments on details of the model are as follows:

A. Solids Balance in Streams and Rivers

1. S_{pw1} is determined from Eq. (1). Once this is known, Eq. (2) determines v_{sdep}, which is assumed to be a state variable and therefore depends on and varies with the other input and state variables in Eq. (2). From a physical point of view, I can't imagine why this should be so. By this means, a wide variation in v_{sdep} is possible (even negative numbers?) and these v_{sdep}'s would have nothing to do with a deposition or settling velocity.

   In the usual interpretation, v_{sdep} depends on the settling (deposition) speed (which depends on particle properties, flow rate, bottom roughness, slope angle, and possibly sediment type). More generally, it is used as a <u>net</u> deposition velocity which somehow averages resuspension and deposition. What it is not is a fudge factor which can be used to balance mass balance equations, although it is often used this way.

2. In Eq. (2), I assume the TSS-S_{pw1} is the concentration of suspended abiotic solids in the water column. If this is true and since TSS is an input variable (constant?), then the concentration of suspended abiotic solids is dependent on the concentration of plankton solids and can vary arbitrarily (also possibly negative?). Doesn't seem realistic.

3. There is no vertical diffusion or mixing in any of these equations. In particular, there is no diffusive flux from the sediments (mixed benthic layer) to the overlying water.

   By almost any reasonable calculation, there are generally more (often orders of magnitude more) contaminants in the bottom sediments than in the overlying water. These bottom sediments are also generally the major source and/or sink of contaminants to the overlying water. This flux can not be ignored and, more than that, since it is the major source/sink of contaminants, the accuracy of the model predictions depends on the accuracy with which the flux is calculated.

4. The model uses a parameter, V_{B2}, which is undefined in the report but I assume it is the volume of the mixed benthic layer. How will this parameter be estimated? If there is exchange of contaminants between the bottom sediments and the overlying water as suggested above, the parameter will govern the long-term behavior of the contaminants and therefore needs to be known accurately; unless of course you want to assume the answer and deduce V_{B2} from this (a poor approach).

5 The model assumes the presence of a benthic boundary layer. Considering the

approximations in the rest of the model, this seems unnecessary and introduces additional parameters whose values are unknown and can not be estimated accurately, e.g., V_{B1}, v_{B1}.

6. Bed load is variable which depends on hydrodynamic conditions. It is not a state variable to be determined by the variation of other state variables.

B. Solids Balance in Ponds, Lakes, and Wetlands

1. Eq. (9) contains a term $S_{pw1} E_{w12} / L_{w12}$ which presumably represents vertical diffusion (mixing). But diffusion of S depends on a gradient of S (or a difference between two quantities at different levels), not on an absolute value of a single variable, S. For example, in Eq. (9), the diffusion term should be $(S_{pw1} - S_{pw2}) E_{w12} / L_{w12}$. Same comments for Eq. (10). As written, the diffusion term behaves as a settling, or convection, term and adds to it.

2. In Eqs. (17)-(20), there is no vertical diffusion or flux from the mixed benthic boundary layer to the overlying water. Same comments as in A3 and A4.

3. Is benthic boundary layer necessary? Same Comments as in A5.

4. In Eqs. (11) and (12), terms with an overline appear. These terms are never defined. The statement "(terms with overline are omitted if this is the bottom water segment)" cannot be understood.

5. v_{pdep} can be calculated from Eq. (9) since it is the only state variable in Eq. (9). v_{pdep} is a variable that depends on size, density, etc. of the particle. Whys should it depend on variables in Eq. (9)? Similar comments to those in A1. Same Comments pertain to v_{sdep} in Eq. (10).

Charge Questions

Many of the charge questions are indirectly addressed above but will be specifically answered here for completeness.

1. <u>Is treatment of solids acceptable?</u>
No, in any present or proposed version of EXAMS.
To repeat, sediments are the major source/sink of contaminants in rivers, lakes, and other surface waters. This flux must be addressed directly and treated accurately. The accuracy of the description of this process determines the accuracy of the model predictions.
The model must have mixing (bioturbation, resuspension/deposition) of contaminants in a mixed layer in the bottom sediments and a flux from the bottom sediments to the overlying water. V_{B2} is the crucial parameter and must be estimated accurately since this determines the long-term behavior of a contaminant in an aquatic system.

2. Choice of State Variables.

Settling (deposition) velocities are certainly important variables but they are determined by physical quantities and hydrodynamics. They are not dependent state variables that are varied so as to satisfy mass balance equations.

Suspended abiotic solids concentration should not be determined from TSS-S_{pw1}. It does not depend on S_{pw1}.

Bed load is a variable which depends on hydrodynamic conditions. It is not a state variable to be determined by the variation of other state variables.

3. Solids Simulation Models

Many people are working on sophisticated sediment transport and fate models. However, this is not what you need in EXAMS, except that anything you do in EXAMS cannot be totally at variance with correct sediment transport and fate processes.

At the very least, a well-mixed benthic layer approximation should be used. This allows the interaction (by bioturbation and resuspension/deposition) and transfer of contaminants between the bottom sediment and the overlying water. A simple model of this type is that developed by Edgington (1993). This concept has been used more extensively and in more detail by many others (see, for example, the text by Chapra (1997) and numerous articles in the literature by Connolly (1991, 1992, and more recent articles), presently at QEA).

In general, the authors should at least be aware that, in many cases, average flows and conditions do not adequately describe fluxes of contaminants. Big events, such as floods on rivers and storms on lakes, may transport more contaminants than the total of all other smaller events (Lick, 1992; Lick et al., 1994). Because of this, flows necessary to satisfy the mass balance equations are probably not the average flows (as defined by averages over time). Same comments pertain to settling and deposition velocities.

In summary, suggested improvements to the model are as follows.

(a) Redefine state variables.
(b) Flux of chemicals from the bottom sediments (well-mixed layer) to the overlying water must be included.
(c) The benthic boundary layer is unnecessary and adds complexity but not accuracy.
(d) Burial velocity should be included in the river model as well as in the lake model.

The above changes should cause negligible change in computer time.

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