

US EPA ARCHIVE DOCUMENT

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

**Testing of the Sampled Chronological Input Model (SCIM) Option in the
Enhanced ISCST3 Model for Use in the Hazardous Waste Identification Rule.**

Prepared for:

David Bartenfelder
Office of Solid Waste
U.S. Environmental Protection Agency
2800 Crystal Drive
Arlington, VA 22202

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Prepared by:

Eastern Research Group, Inc.
2200 Wilson Boulevard, Suite 400
Arlington, VA 22201-3324

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NOTE

This report was compiled 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 *Testing of the Sampled Chronological Input Model (SCIM) Option in the Enhanced ISCST3 Model for Use in the Hazardous Waste Identification Rule* document that is part of EPA's Hazardous Waste Identification Rule risk assessments. The actual review was performed in 1998 under Contract Number 68-W5-0057.

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.

1. Introduction and background

The Office of Solid Waste (OSW) is developing a proposed amendment to its regulations under the Resource Conservation and Recovery Act (RCRA) by establishing constituent-specific exit criteria for low-risk solid wastes that are designated as hazardous because they are listed, or have been mixed with, derived from, or contain listed hazardous wastes. The constituent-specific concentrations under development are to be protective from both human health and ecological effects. The Agency proposed this amendment on December 21, 1995. In addition to public comments (RCRA docket #F-95-WHWP-FFFFF), separate reviews of the risk analyses supporting the rule were conducted by the Science Advisory Board (SAB) and the Office of Research and Development (ORD). The Agency is currently evaluating the impact of these reviews and is modifying the technical information and analyses required to support the next phase of the rule development.

The goal of the exposure and risk assessment is to generate risk-based exit constituent concentrations supporting the management goal to identify low-risk listed wastes. Listed waste with concentrations below the exit concentrations would no longer be regulated by RCRA Subtitle C. The methodology under development will estimate risks through an integrated multi-media, multiple pathway, and multiple receptor assessment that characterizes potential human health and ecological exposure and risk. The assessment will calculate risk to receptor types from simultaneous exposures to a single chemical by adding exposures from potentially contaminated air, ground water, surface water, soil, and biological media. The characterization of exposures and risks are intended to provide a national distribution of individual risk from individual constituents released from the following types of waste management units: industrial landfills, waste piles, land application units, surface impoundments, and tanks. The assessment will be based on a "regional site-based" approach - a tiered design that ensures plausible scenarios are modeled and relies on actual site and receptor data, when available, rather than hypothetical site and receptor descriptions. The approach allows for maintaining correlations among dependent parameters such as climatic, hydrologic, and geologic parameters as a function of site location.

In addition to analyses to support the risk-based constituent exit levels, analyses will include: a systematic evaluation of parameters and uncertainties; understanding the part of the distribution that is above potential exit levels to see if any specific sub-populations or regions have been systematically excluded; verification of model results against existing, more rigorous scientific models; validation of components of the model, where data are available, to compare to background media concentrations and other naturally occurring levels; and several technical analyses described in the consent decree.

The air model selected for use in HWIR98 is the Industrial Source Complex - Short Term (ISCST3) model. ISCST3 is a steady-state Gaussian plume model. The model provides estimates of pollutant concentration, dry deposition (particles only) and wet deposition (particles and gases) for user specified averaging periods (e.g annual).

Two modifications have been made to the regulatory version of the model to create a version to be used in the HWIR assessment. The first revision involves a change in the plume depletion algorithm for dry deposition. The regulatory version of the model includes a depletion algorithm that is computationally expensive. A new algorithm was developed that greatly reduces runtimes, while providing results that are consistent with more intensive computational models. The second modification involves allowing the model

to sample from a file of hourly meteorological data at regular intervals and thus only model a fraction of the hours for the period of record (e.g. 30 years). This enables the model to execute more quickly while producing long-term averages comparable to those obtained from the full data set. This method is referred to as the Sampled Chronological Input Model (SCIM).

ISCST3 will be run for the period of record using normalized emissions and a long-term average particle size distribution in conjunction with sampled meteorological data and will be annualized by multiplying the normalized annual average concentration and annual deposition predictions by an annual emission rate. Very few scavenging coefficients are available for vapors. Additionally, using chemical specific scavenging coefficients adds additional runtime burden to the air module. Therefore, the scavenging coefficients used for modeling the wet deposition of gases will be the same as for small particles. Although the new depletion algorithm is faster than the previous version, it is still fairly computationally expensive. It is likely that the effects of depletion due to dry deposition will not be included in the model runs for HWIR.

2. Materials provided for review

The following materials are provided to provide more detail about the ISCST3 model and the HWIR specific modifications and should assist the peer reviewers in answering the questions posed in the charge.

- a. User's Guide for the Industrial Source Complex (ISC3) Dispersion Models. Volume II - Description of model algorithms. Draft 8/98.
- b. contractor report on SCIM approach

3. Charge to reviewers

A. The plume depletion algorithm in ISCST3 has been replaced with an algorithm that offers greater execution speed while providing results that are close to the full numerical solution.

1. Is the new depletion algorithm scientifically sound?
2. Is the new depletion algorithm appropriate for HWIR type sources (area sources)?
3. In the event that runtime prohibits the use of the depletion algorithm for dry deposition, will the concentration and deposition estimates made for HWIR be defensible?

B. To speed execution of ISCST3, a methodology was implemented to sample from the meteorological data at regular intervals specified by the user.

1. Will the sampling method provide defensible estimates of concentration, dry and wet deposition?
2. Is the sampling method appropriate for the HWIR assessment (screening-level, site-based approach)?

C. Due to runtime considerations, ISCST3 will be run using several simplifying assumptions. We are interested in the potential effects of these assumptions on the final risk numbers that will be calculated.

1. Will the use of annual average estimates calculated by multiplying a long term annual average values and annualizing by the emission rate provide us with a plausible estimate of air impacts?
2. Is the use of the small particle assumption in place of chemical specific scavenging coefficients appropriate for this assessment?

4. Criteria for selecting reviewers

1. Expertise in the area of air quality modeling
2. Expertise in the area of deposition modeling

General Comments

Dr. Mogolesko: The ISCST model is based upon generally accepted physical modeling concepts and attempts to model local and long-distance phenomena. To the extent possible, they are benchmarked by experimental and field data. They are not a new and untried modeling capability, but an outgrowth of a series of gradual modeling improvements that reflect a better understanding of the factors impacting the dispersion and deposition process in the real-world. Each evolution in the model enhancement tries to more completely account for real-world processes, but is in itself only an approximations. In an attempt at completeness, some uncertainties are recognized and minimized, while other may have been included.

In general, I believe the model is scientifically sound [Charge A.1.] and the depletion algorithm is appropriate for HWIR area type sources [Charge A.2.]. The model is basically sound, but it must be used responsibly by qualified practitioners who can keep track of limiting assumptions and uncertainties. As with other professionally documented modeling tools, the authors have identified what I like to call "cautions".

For example, see pages 1-15, 1-1-24, 1-33, 1-34, 1-39, 1-42, 1-46, 1-49, 1-63, 1-64, etc. of the User's guide to support this observation.

Although I generally have a comfort level with the model, I have some concerns. According to general knowledge and information learned from open literature reviews some concerns need to be highlighted. When at a loss to bound the usefulness of concepts, I typically return to basic principles. We can all agree that individual aerosol particles and gas molecules have a finite residence period in the atmosphere. The dominant removal processes include precipitation scavenging, dry deposition, and physical/chemical transformation. The dominance of these processes is related to existing meteorological variables and the specific pollutant. The open literature suggests a strong influence of residence times with precipitation scavenging. Since meteorological data are typically incomplete and subject to a degree of uncertainty, it is easy to conclude that precipitation scavenging estimates may be uncertain. This is especially true for short-term estimates where results may only be good to within a factor of ten. Taking these basic thoughts a bit further, suggests that the resultant risk assessments can't be better than the limitations just suggested.

These concerns won't go away overnight because similar state-of-the-art models are similarly questioned. The significance of the concerns is often dispositioned by comparing model results with field data, and completing parametric experiments with the model. Some of these specific concerns and observations follow:

- ! Wet deposition estimation methods indicate the results for individual precipitation events are UNCERTAIN by several orders of magnitude.

- ! Inherent UNCERTAINTIES in the deposition modeling process are related to underlying meteorological processes such as the exact nature and location of each rain event in relation to the model grid.
- ! Some public domain models estimate scavenging coefficients for a family of rainfall intensity ranges independent of rainfall amount. The ISCST3 appears to use measured rainfall amounts, irrespective of rainfall intensities (EPA plans to use hourly precipitation amounts). Hence, EPA appears willing to accept that scavenging is affected only by RAINFALL AMOUNT.
- ! EPA assumes deposition rates vary linearly with precipitation rate. The ISCST3 model assumes that the same amount of scavenging will occur in a short, intense rain event as in a longer period of moderate rain, as long as the same amount of rain is collected. This is contrary to theoretical and experimental determinations of scavenging coefficients which appear to be STRONGLY INFLUENCED BY DROPLET SIZE DISTRIBUTION OF THE RAIN.
- ! How does the modeling approach affect the model projections for a variety of particle sizes and weather types? SCAVENGING can be viewed as a strong function of PARTICLE SIZE.
- ! Deposition value varies with distance in all models. This is especially pronounced for coarse size particles who decay at a greater relative rate than small particles. At long travel times, only small and medium particles continue as part of the deposition pattern.
- ! Implications for risk assessments due to different contaminants having varying particles size classes need to be understood. Scavenging of large particles is a potential concern since, in reality, it could result in a tight deposition pattern around sources for large particles. For small particles, ISCST3 probably won't change the deposition pattern, but could decrease the deposition amount for all locations.
- ! ISCST3 is likely to produce less conservative results than some older models (Bowman coefficients based models may prove to be unnecessarily conservative), but validation may be a problem.
- ! Wet deposition results will need to be used with care, bearing in mind that individual results may be orders of magnitude in error.

Much of the debate about using this code in a structured risk assessment must fall on the concepts used for scavenging. It is observed that the greatest problem is associated large particles. In lieu of the availability of an accepted database representing all chemical-specific scavenging coefficients, the use of the small particle assumption is reasonable [Charge C.2.].

Although state-of-the-art methods are employed in the development of the ISCST model, uncertainty can't be avoided. A perspective is that uncertainties can be referred to as parameter uncertainty, model uncertainty, and completeness uncertainty. To fully clarify this perspective, definitions of these uncertainties are provided:

1. Parameter uncertainties are those linked with the values of the fundamental parameters of the ISCST model. Parameter uncertainties can be explicitly represented and propagated through the ISCST model, and probability distributions of the relevant metrics can be

generated. Typically, these distributions can be used to assess the confidence with which guidelines are met. Determine whether the tails of the distributions are being determined by uncertainties on a few significant parts of the model. If yes, these components can be highlighted for their potential impacts on the decision making process.

2. Model uncertainties relate to how certain physical issues are modeled. The effect of model uncertainty is to introduce some type of bias into the model results. Particularly, some model uncertainties arise in the modeling of the dispersion and depletion progression. It is useful to understand the impact of a specific assumption on the predictions of the model. The impact of using alternate assumptions or models can be addressed by performing sensitivity studies.
3. Completeness uncertainty is not in itself an uncertainty, but a reflection of ISCST scope limitations. The reality of completeness uncertainty is an uncertainty about where the true risk lies. Since it represents an unanalyzed contribution, it is very hard to estimate its magnitude.

The real question is: what do all of the uncertainties mean with respect to decision making? Decision making can become stable and credible if assurance can be offered that:

- ! the parameter and some model uncertainties that are quantified in the model do not produce a probability distribution on the estimated output values that results in a low sense of confidence that the goal is met (model uncertainty);
- ! the adoption of specific modeling does not overly bias the results in favor of the consideration, but reasonable modeling assumptions would not alter the decision;
- ! the contributions to risk that are modeled would not alter the decision significantly (completeness uncertainty)

The five sources selected for the study are reasonable HWIR sources. The limitation on particle size distribution is understandable if EPA is only interested in impacts far downwind. Assuming the data were input properly, the modeling results using the SCIM option vs, the non-SCIM option are encouraging. As shown in Appendix A:

- ! plots for dry deposition fluxes were similar to those for concentrations (the basis for their agreement, that concentrations are calculated at the ground-level and dry deposition fluxes are calculated by ISCST3 as ground-level concentration times deposition velocity, is reasonable);
- ! wet deposition fluxes vary from concentration plots, especially when comparing SCRIM vs. Non-SCRIM options;
- ! SCRIM agreement for concentration is best at short distances from the source and highlights a sense of uncertainty
- ! uncertainty is certainly noted for the dry city where the sampling scheme may not have adequately described the actual rainfall history.

The idea of separating the sampling scheme for wet deposition from that of concentration and dry deposition fluxes is prudent. As in the use of models in general, knowing and accepting the fragilities of the model enhance the likelihood that a selected sampling method will produce defensible results. The sampling methods presented are reasonable, especially when the model user is sensitive to the concerns of applying the model at specific locations (dry vs. wet areas)[Charge B.1.]. Again, awareness of uncertainty in wet deposition must be strong. Utilization of the models for screening level assessments should also be reasonable in light of the above comments [Charge B.2.].

The Appendix B results are also encouraging. Less frequent sampling creates its own uncertainty contribution (less frequent sampling results in larger uncertainties). It seems that certain locations will require utilization of the full database to produce representative model output with minimized uncertainty. As shown in Appendix B, comparisons were made for no wet hour sampling vs. 4 and 8 wet hour sampling frequencies. The error bars are large for the wet deposition fluxes when there is no separate wet hour sampling, while they almost vanish when doing the separate wet hour sampling. The average of the 24 samples, when doing the separate wet hour sampling agrees with the No SCIM results as compared to not doing the separate wet hour sampling.

The results from the modeling runs to generate error bars were used to generate frequency distributions of SCIM to No SCIM ratios to determine the general shape of the distributions. These distributions are approximately normal for all distances, but the distributions for individual distances vary somewhat with distance from the sources and don't define a standard shape. They are narrower and taller for short distances and tend to be wider and flatter as distances increase. A logical conclusion was structured forcing frequency distributions to be based on ratios of impacts that are paired in space and not just on maximum impacts by distances.

For concentrations, no significant differences exist between 4 and 8 day skipping and are not affected by separate wet hour sampling. Concentration estimates seem reasonably well founded close to the source, but as was shown, the error bars increase as distance from the source increases. The issue of defensibility is difficult, but the results, when displayed in a parametric sense, allow the decision makers and the general public to understand the strength or weakness of their conclusions, and they provide a basis to debate the quality of the decision [Charge A.3.].

Regarding wet deposition fluxes, the 8 day skipping sample frequency is presented as typical and indicates that doing a separate wet hour sampling increases the likelihood of accurate estimates and minimization of uncertainty.

In summary, the results of applying the ISCST model must be considered in an integrated manner. It is hoped that decisions won't be driven solely by the numerical results of the ISCST model. They are just one of several inputs into the decision making process and support development of an overall snapshot of the implications of the consideration on risk. Areas which have a low precipitation frequency require increased sampling frequency to reduce uncertainty. This fact is especially true for wet deposition fluxes and only of minor importance regarding concentrations.

Tank sources are generally a modeling problem due to their relatively small size. More frequent sampling is probably needed for small area sources and point sources.

No information was provided to this Peer Reviewer concerning the cost and level of effort associated with runtime decisions. The integrity of any risk assessment lies in its completeness and minimization or understanding of uncertainties. From my perspective, the use of risk assessments as a decision support tool is a giant leap forward when used in the regulatory process. Since many of the decisions being made have substantial environmental and emotional impacts, the costs associated with runtime need to be considered as a key point in an effort to build trust. Computer time gets less expensive from day to day and it should not become a driver that inhibits the integrity of a properly structured decision process [Charge C.2.].

From a personal perspective, I prefer using risk assessment tools in a so-called delta mode. I strive to understand the benefits and limitations of the models and databases, and then use them in a relative manner. I don't believe the strength of these tools lies in the absolute values they produce. I think their strength lies in their use in assessing change from a so-called base.

Dr. Turner: My expectation related to this review was to be provided proposed guidance with relation to the modeling that would be required to satisfy the requirements of this rule and the technical documents related to the guidance. However no information on proposed guidance was furnished.

The information furnished consisted of the following:

- A. two and one-half pages:
 - 1. Introduction and background.
 - 2. Materials provided for review [list].
 - 3. Charge to reviewers.

And

- B. Two documents:
 - User's Guide for Industrial Source Complex (ISC3) Dispersion Models, Volume II- Description of Model Algorithms – Draft 8/98

Testing of the Sampled Chronological Input Model (SCIM) Option in the Enhanced ISCST3 Model for use in the Hazardous Waste Identification Rule (HWIR)

[However, there was some mix-up in furnishing the proper ISC3 document. The document originally furnished had missing symbols in many of the equations. The first replacement apparently was an earlier version of the document. (Although all three ISC3 - Volume II documents had a title page dated: September 1995.) The last document received on December 2, 1998 was indicated by cover letter that it was the correct document (although the cover of this document also was dated September 1995).]

I would have liked to see some examples of anticipated run times for typical types of modeling simulations that are expected to be required. I expressed this in a fax to Nicole Schubert on November 25, 1998. With the rapid progress being made in the processing speed of personal computers, what was impossible yesterday, is feasible today and routine tomorrow.

Whether it is feasible to model for all hours or resort to SCIM procedures to do the modeling required is a question that needs to be answered. This will certainly be affected by the period of record to be simulated.

A period of 30 years is mentioned in the “Introduction and background” furnished. This seems rather excessive. However, there may be good reason to use a period longer than “the latest five years’ data” required by most regulatory modeling to date.

Period of record considerations could be handled in something like the following: **It is normally expected that a period of record of xx years will be used. For periods of record less than this recommended length the concentration values calculated shall be scaled upward using the factor corresponding to the specific period of record used.** (These factors would have to be specified in the guidance.)

Since the report furnished on the use of SCIM in accomplishing analyses is very encouraging, it does indicate (as one would expect) that error bounds increase with the length of time interval selected for the SCIM analysis. With regard to whether SCIM is being used or not the following could be the form of the guidance: **It is normally expected that all hours will be simulated in the modeling runs used to make the supporting calculations. If it is necessary to employ SCIM (Sampled Chronological Input Model) procedures the resulting concentration values calculated shall be scaled upward using the appropriate factor from tabular values furnished with this guidance.** (An initial determination of these factors by those writing the guidance can be made from the contractor report and should not only be a function of the SCIM interval but also be a function of source type and size as well as distance from the source.)

By having the guidance in the above form, it would be possible to make calculations using both less data and employing less computer time than that thought necessary by the writers of the guidance, **but** a penalty would be paid by the use of the specified factors if shortcuts are taken. Therefore, there would not be a requirement to rush out and buy the most recent fastest computer, although this might be an added incentive. Of course, a separate set of factors would be needed to be specified for the handling of wet deposition. It would seem that the percent of hours with precipitation would be one of the determining factors in the specification of these.

Responses to Charge Questions

A. *The plume depletion algorithm in ISCST3 has been replaced with an algorithm that offers greater execution speed while providing results that are close to the full numerical solution.*

19. *Is the new depletion algorithm scientifically sound?*

Dr. Hanna: The new depletion algorithm is described in a sketchy manner in six pages in Section 1.1.6.3 of the revised ISC document. It is based on a derivation by Venkatram, which is allegedly discussed in more detail in a recent EPA report that the Peer Review group requested, but was not provided by the EPA. While the theoretical equations in Section 1.1.6.3 look reasonable and are consistent with current scientific knowledge, I am not able to respond positively (or negatively) to EPA Question A.1 without looking into the following issues:

Issue 1 – Other similar surface depletion models were proposed 10 or 20 years ago by Horst (1979) and others. Yet there are no references to this related research. The new algorithm should be compared and contrasted with these similar models.

Issue 2 – What is the justification for the selection for the constant “2” in the formula $h = 2 \sigma_z$?

Issue 3 – What is the justification for the selection of the square function in the vertical profile shape?

Issue 4 – Are there comparisons of the predictions of the new model with the previous ISC deposition model, with other alternate surface depletion-type deposition models, and with observations?

Issue 5 – Are there results of sensitivity tests available, to demonstrate that the new algorithm does not occasionally exhibit odd extreme behavior?

Dr. Mogolesko: see comments above.

Dr. Turner: It would have been useful to have been furnished the 1988 or 1998 Venkatram report (referred to as 1998 in text and 1988 on page 3-5 in References) to provide additional information on the development of the algorithm. Based on the information furnished in the ISC3 Vol. II, the algorithm appears to be sound.

20. *Is the new depletion algorithm appropriate for HWIR type sources (area sources)?*

Dr. Hanna: Yes, the vertical diffusivity (K_z) approach is most appropriate for ground-level area sources, such as HWIR-type sources. This conclusion is stated in most texts, such as Pasquill’s (1973) book. The K_z approach would be less appropriate for elevated point sources.

Dr. Mogolesko: see comments above.

Dr. Turner: This new depletion algorithm should work well for area sources and therefore be appropriate for HWIR type sources.

21. *In the event that runtime prohibits the use of the depletion algorithm for dry deposition, will the concentration and deposition estimates made for HWIR be defensible?*

Dr. Hanna: I have a two-part response to this question. Firstly, I would like to know why the EPA is concerned about runtime and what their criteria are for “acceptable” runtimes for ISC. These days, computers are so fast and ubiquitous that people seem to not be worried as much about runtimes. There are groups running MM5 and Models-3 in a forecast mode every day. Other groups are running huge CALMET/CALMET applications for multiple sources and long time periods. A large ISC run can be started on a PC at 5 pm and will be finished when the person arrives at work the next morning. The EPA should define and justify what they would consider to be excessive runtime. Secondly, if the depletion algorithm is not used, the predicted deposition could be in error by a large factor during light-wind stable conditions. This is because during stable conditions, strong concentration gradients can form near the surface as the hazardous substance right at the surface is deposited and the flux of material from aloft is minimal and insufficient to maintain the concentrations at their “undepleted” levels at the surface. Of course, the error would be on the side of underpredictions, which may be acceptable to the EPA. Nevertheless, use of the depletion algorithm would lead to more technically-credible risk assessments.

Dr. Mogolesko: see comments above.

Dr. Turner: Since both concentrations and the quantity of dry deposition (which is dependent upon the ground-level concentration in the air) are greater (at locations near the source) if the depletion is not included, these estimates would tend to overestimate (be conservative) these quantities and therefore should be satisfactory and defensible.

B. To speed execution of ISCST3, a methodology was implemented to sample from the meteorological data at regular intervals specified by the user.

1. *Will the sampling method provide defensible estimates of concentration, dry and wet deposition?*

Dr. Hanna: As I point out in my specific comments on the report, the EPA's approach to the sampling method is not justified in any way, such as by reference to standard statistical procedures as described in statistics texts. The sampling problem is encountered in many studies, including the U.S. census, and statisticians have spent many man-years determining the best way to sample. The EPA employs many statisticians and has had several international statistical experts under contract on various air quality issues (e.g., S. Hunter, P. Switzer, and J. Tukey). However, the EPA sampling method described in the SCIM report is very arbitrary and subjective. Furthermore, the report contains improper usage of many statistical terms (e.g., use of the word "significantly" with no connection to standard statistical usage concerning 95 % confidence levels). The sampling method that was chosen is systematic rather than random. I recommend that the EPA have their SCIM method reviewed and revised by professional statisticians in order to place the method on a sound footing. However, despite these limitations, I suppose that the current arbitrary sampling method will provide reasonable results.

Dr. Mogolesko: see comments above.

Dr. Turner: If suggestions made above are adopted that will multiply estimates made with the SCIM procedure by a factor greater than 1.00 to account for greater uncertainty, the sampling methods should be defensible.

2. *Is the sampling method appropriate for the HWIR assessment (screening-level, site-based approach)?*

Dr. Hanna: This question is very similar to the first part of question B. As I stated in my answer to that question, the sampling method is arbitrary and systematic and needs to be supported by standard statistical references. The EPA should have the method and the report reviewed and possibly revised on the advice of professional statisticians. Nevertheless, the current subjective EPA method is one way to approach the problem and may produce reasonable results for screening-level analyses.

Dr. Mogolesko: see comments above.

Dr. Turner: Here, again, if the use of an appropriate multiplier factor is included (as discussed in the last Response above) calculations made employing sampling should be appropriate.

C. Due to runtime considerations, ISCST3 will be run using several simplifying assumptions. We are interested in the potential effects of these assumptions on the final risk numbers that will be calculated.

1. *Will the use of annual average estimates calculated by multiplying a long term annual average values and annualizing by the emission rate provide us with a plausible estimate of air impacts?*

Dr. Hanna: First it is necessary for EPA to define their criteria for acceptable runtime. Once this number is decided upon, then plans can be made for how best to simplify the runs. In response to this specific question, the average of a product will equal the product of the averages only for smooth distributions of the original variables. If the original variables have odd skewed distributions, then there can be a large difference between the average of a product and the product of the averages. The importance of this issue can be determined by running some actual test cases both ways.

Dr. Mogolesko: see comments above.

Dr. Turner: The way in which I am interpreting this question is that a multi-year period of record is used to determine a multi-year concentration. Then, emission rates which are changing year by year are then used to presumably obtain year by year annual concentrations. These individual annual concentrations would be an approximation to annual impacts. What would not be included would be the actual variations caused by the year to year meteorology. If what is actually desired is the long term impact, the varying annual emissions can first be averaged. Then this set of emissions can then be used in the long-term modeling.

2. *Is the use of the small particle assumption in place of chemical specific scavenging coefficients appropriate for this assessment?*

Dr. Hanna: This seems like a poorly-thought-out assumption. Has anyone checked this out with some calculations using these alternate ways of treating the topic of scavenging? I can think of some obvious problems, since there are large differences in the scavenging coefficients for gases, depending on the chemical properties of the gases (solubility in water, Henry's constant, presence of other chemicals, etc.) and the characteristics of the atmosphere and the surface. This assumption should be reviewed by scavenging experts such as George Slinn.

Dr. Mogolesko: see comments above.

Dr. Turner: Of course, the appropriateness of using small particle assumptions in place of an appropriate removal rate for a specific chemical will depend upon how much the specific rate deviates from that for small particles. Of course, the direction of error due to the use of the small particle assumption will depend upon whether the actual rates of scavenging are faster or slower than that due to the small particle assumption.

Miscellaneous Comments

Dr. Hanna: Comments on PES September 1998 Report on EPA Contract No. 68D70002, Work Order No. 1-001, entitled "Testing of the Sampled Chronological Input Model (SCIM) Option in the Enhanced ISCST3 Model for Use in the Hazardous Waste Identification Rule"

Cover Page – It would be useful if the authors of the report were listed. It seems illogical to list the EPA contract monitor’s name and not the people who actually did the work.

p. iii, Preface - Nothing is said about the subject of the report – the SCIM methodology. The preface should describe the objectives of the work and give an overview of the contents of the report. The phrase “long term pollutant impacts” should be defined.

p. v, Table of Contents – The Headings for the Appendices should be listed. At present, none of the appendices have a name and none of the figures in the appendices have adequate descriptive legends.

p. 1-1 – Section 1, Introduction – This section currently reads like an executive summary rather than an introduction. The problem should be described, the objectives listed, and the methodology outlined. For example, the justification for wanting to improve the run-time should be given. With the speed of computers (even PCs) these days, it is hard to believe that run-time is an issue any more. This entire report seems to be solving a problem that may have been true 10 years ago, but is not true now.

p. 1-1, line 1 – This is the first use of the word “significant”, which appears many times in the remainder of the text. This word has statistical connotations (e.g., 95 % confidence intervals) related to statistical hypotheses and brings up the single major problem with the report –

The work that is described is a basic straightforward statistical exercise that should be have been treated with standard textbook statistical procedures. Instead, the authors have carried out a series of ad hoc arbitrary calculations and subjective sensitivity tests. However, the authors then state their conclusions in statistical terminology (i.e., ‘significantly different’) which has no mathematical basis.

p. 1-1, SCIM Interval (also applies to Wet Sampling Frequency) – The method used to select the subset of hours is systematic rather than random. Is there a reference that justifies this method?

p. 2-1, par. 1 – Reference should be made to standard statistical texts. The problem described here is faced by many other studies (the most current example is the census) and there are thousands of pages of references on the topic. The authors of this report appear to be attempting to reinvent a wheel that has been worked on and refined countless times. Furthermore, there are analytical solutions available.

p. 2-2, top par. – receptor spacing – It seems that, by placing only one receptor at the center of a 22.5 degree sector, the authors are causing interpretation problems later on. Many of their statistical results are caused be combinations of incomplete receptor coverage and the sampling procedure. It would have been better to increase the receptor coverage (say every 5 degrees) so that the results could have been interpreted as being wholly due to the sampling method.

p. 2-2, line 5 from bottom – By substituting concentrations for dry deposition (the plots were “very similar”), the authors have made moot any investigations of the effects of the new Venkatram surface depletion model. The words “very similar” should be backed up by quantitative results. I would expect the ratio of dry deposition to concentration to vary with ambient stability and with underlying surface type (e.g., grass, desert, bay, city).

p. 2-2, line 4 from bottom – By “significantly”, do you mean that you have done statistical tests of 95 % confidence intervals? If not, don’t use the word.

p. 2-2, line 3 from bottom – Define “reasonable”. Are there any criteria for your decisions? Who made them up? A group of modelers, users, and regulators?

p. 2-3, first word – Who “decided” and what was their quantitative argument?

p. 2-3, line 6 - As I stated before, please define “reasonably well”.

p. 2-3, lines 7-8 – The increase with distance does not look like much to me. These two sentences (the first concluding that there is a variation and the second concluding that there is little variation) should be supported by data and statistical tests.

p. 2-3, line 1 of last par. – Same comment as above concerning “significantly”.

p. 2-3, line 5 of last par. – “the probability is high” – Please give a number for the probability.

p. 2-3, line 3 from bottom – What was the quantitative criterion for deciding “the uncertainties were deemed to be unacceptably large for all cities”? What uncertainty would you have accepted and who decided that value?

p. 3-1, line 2 – “significantly” – same comment.

p. 3-1, line 4 – What were the criteria for “limitations on model run-time”? Same comment applies to the last line on this page (“considerably increasing the model run-time”).

p. 3-1, lines 11-12 from bottom - This is a statistical problem that should be treated by standard textbook methods. Words like “remarkable” and “significant” should not be used without backing them up with hard numbers.

p. 3-1, line 2 from bottom – “significantly”! This conclusion depends on the number of “wet hours” and can be addressed using methods in statistical texts.

p. 3-1, bottom – Please comment on why the concentrations are different in the plots in Appendices A and B.

p. 3-2 – A recommendation should be made concerning the best way to set the sampling intervals, etc.

p. 4-1 – This error analysis addresses only one component of the total error. As I mentioned in an earlier comment, it may be better to randomly sample rather than use this systematic sampling method.

p. 4-1, lines 7, 8, 10, and 12 from bottom - Again, there is unjustified use of the terms “significantly”, “remarkable” and “rather large”.

p. 4-2, lines 2-3 – There is confusion concerning the meaning of the term “SCIM to NoSCIM ratios” This term should be clearly defined and qualified.

p. 4-2, line 13 from bottom – The Kolmogorov-Smirnov test should be applied to determine whether the distributions can indeed be considered to be normal, within 95 % confidence bounds.

p. 4-2, lines 3, 17, and 19 from the bottom, and line 10 from the top – “significantly”.

p. 4-3, lines 3 and 4 – The terms “greatly increased” and “greatly reduced” should be justified with quantitative statistical calculations.

p. 4-3, conclusion at the end of section 4.3 – Define “considerably decreases”.

p. 5-1 – The wet hour sampling interval could also be randomly selected, with the means used here.

p. 6-1 – This issue appears to have been investigated by arbitrary sensitivity studies rather than by looking at the model physics assumptions. Also, why not simply use more receptors, since the main purpose of this report is the study of the SCIM method.

All Appendices – Headings are needed for all appendices. Complete descriptive captions are needed for all figures. Currently the “appendices” consist of nothing but printouts of computer-drawn figures with brief legends, which I suppose are understandable to PES and to the EPA contract monitor. However, new readers (such as this reviewer) must flip back and forth between the text and the figures to try to understand them, and, even so, many of them are unintelligible. For example, it would help to show where the edge of the source appears on the x-axis. Also, I suspect that some of the figures were originally in color, because often two lines appear to be labeled the same when copied in black and white (e.g., appendix E).

Comments on EPA Report No. EPA-454/B-95-003b entitled “User’s Guide for the Industrial Source Complex (ISC3) Dispersion Models; Volume II – Description of Model Algorithms”

It should be noted that, although this version of the ISC report is labeled “1995”, it is in fact a 1998 update, containing a new surface depletion model (Section 1.1.6.3).

The review panel has been charged to address their comments only to the new section 1.1.6.3 - “The Vertical Term with Dry Deposition” (pages 1-34 through 1-39). This new section is based on a recent report by Venkatram (1998: A Simple Model for Dry Deposition and Particle Settling, Subcontractor Progress Report 2 (including addendum), EPA Contract No. 68D70002, Work Assignment No. 1-001). This crucial report was requested from both Dr. Venkatram (who said to get it from the EPA) and Mr. Wilhelmi (the project manager of the current review exercise). The four page document plus a handwritten page entitled “New Integration Scheme” was faxed to me the day before the current review was due.

The problem is that, although the equations for the new formulation seem reasonable, they are presented in a sketchy manner in Section 1.1.6.3 with little justification. I have the following questions:

Question 1 – Other similar surface depletion models were proposed 10 or 20 years ago by Horst (1979) and others. Yet there are no references to this related research. The new algorithm should be compared and contrasted with these similar models.

Question 2 – What is the justification for the selection for the constant “2” in the formula $h = 2 \sigma_z$?

Question 3 – What is the justification for the selection of the square function in the vertical profile shape?

Question 4 – Are there comparisons of the predictions of the new model with the previous ISC deposition model, with other alternate surface depletion-type deposition models, and with observations?

Question 5 – Are there results of sensitivity tests available, to demonstrate that the new algorithm does not occasionally exhibit odd extreme behavior?

After quickly reviewing the Venkatram (1998) document, which was provided at the last minute, it appears that there is little new in that document. The document appears to have been reproduced nearly verbatim in Section 1.1.6.3 of the ISC document. There is a reference to Horst (1977) in Venkatram’s report, but there is no justification or comparisons with other models or data.

Specific Comments on Section 1.1.6.3:

p. 1-35 – It should be stated why the previous algorithm was deficient and why there was a need to develop a new algorithm. Was there a concern with model runtime? Were there errors with the old algorithm that were seen in comparisons with observations? More importantly, does the new algorithm eliminate these errors?

p. 1-36 – figure and text – References should be provided to other surface depletion models (e.g., Horst, 1979).

p. 1-37, line after eq. 1-57b – The prescription of the height, h , may be the most sensitive part of the algorithm. Is the choice of the constant, 2, (see the bottom of p 1-38) based on observations? Has it been tested with data and against other models? Have the effects of alternate choices for the constant (e.g., 1 or 3) been investigated?

p. 1-37, eq. 1-58 – There are other simple formulas which also meet the zero gradient criterion. Why was this particular formula selected over the others?

p. 1-38, line above eq. 1-62 – If the choice of this formula is a “starting point”, what is the ending point? Why were no other formulas or constants tested? Why not simply use the 20 year-old Horst surface depletion model?

p. 1-39 – Unless I am missing something, the section ends without doing any comparisons between the old and new depletion algorithms and without carrying out any evaluations with deposition observations. If these comparisons are in the back-up reports by Venkatram, they should have been provided to the review panel. (Last-minute note – the Venkatram (1998) report provided at the last hour does not provide these details).

Dr. Turner: With regards to the SCIM report, it would be much more understandable to the reader if the cause for undertaking the contract work is explained in a preface to this document. It is probable that some long run times were encountered in making some runs involving calculations of dry and wet deposition. If descriptions of these examples could be stated including a description of the processor used so that the need for such research is more clearly understood, it would place the results of the work summarized in the report in much better perspective.

For the purpose of this peer review, it was only necessary to review the following of the ISC- Vol II: pages 1-34 through 1-39; pages 1-54 through 1-60; and pages 1-62 through 1-64. As noted above there are citations on page 1-35 and page 1-54 to “Venkatram (1998)” in the text. In the Reference section on page 3-5 there is a reference: Venkatram (1988). Correction needs to be made. On page 1-63 there is a citation of Radke et al. (1980). This is not given in the references.