November 9, 2004

MEMORANDUM

SUBJECT: Transmittal of Minutes of the FIFRA Scientific Advisory Panel Meeting Held August 26-27, 2004: Fumigant Bystander Exposure Model Review: The Fumigant Exposure Modeling System (FEMS) Using Metam Sodium as a Case Study

TO: James J. Jones, Director
Office of Pesticide Programs

FROM: Paul I. Lewis, Designated Federal Official
FIFRA Scientific Advisory Panel
Office of Science Coordination and Policy

THRU: Larry C. Dorsey, Executive Secretary
FIFRA Scientific Advisory Panel
Office of Science Coordination and Policy

Joseph J. Merenda, Jr., Director
Office of Science Coordination and Policy

Please find attached the minutes of the FIFRA Scientific Advisory Panel open meeting held in Arlington, Virginia from August 26-27, 2004. These meeting minutes address a set of scientific issues being considered by the U.S. Environmental Protection Agency regarding fumigant bystander exposure model review: the fumigant exposure modeling system (FEMS) using metam sodium as a case study.

Attachment

cc:

Susan Hazen
Margaret Schneider
Adam Sharp
Anne Lindsay
Janet Andersen
Debbie Edwards
Steven Bradbury
William Diamond
Arnold Layne
Tina Levine
Lois Rossi
Frank Sanders
George Herndon
William Jordan
Douglas Parsons
Karen Chu
Dayton Eckerson
Enesta Jones
Vanessa Vu (SAB)

<u>FIFRA SAP Members</u>
Steven G. Heeringa, Ph.D.
Kenneth Portier, Ph.D.

<u>FQPA Science Review Board Members</u>
Daniel C. Baker, Ph.D.
Mr. Paul W. Bartlett
Adel F. Hanna, Ph.D.
Michael S. Majewski, Ph.D.
Li-Tse Ou, Ph.D.
James N. Seiber, Ph.D.
Frederick Shokes, Ph.D.
Thomas O. Spicer, III, Ph.D.
Dong Wang, Ph.D.
Eric D. Winegar, Ph.D.,QEP
Scott R. Yates, Ph.D.

SAP Report No. 2004-07

MEETING MINUTES

FIFRA Scientific Advisory Panel Meeting, August 26-27, 2004, held at the Holiday Inn-National Airport, Arlington, Virginia

A Set of Scientific Issues Being Considered by the Environmental Protection Agency Regarding:

Fumigant Bystander Exposure Model Review: The Fumigant Exposure Modeling System (FEMS) Using Metam Sodium as a Case Study

NOTICE

These meeting minutes have been written as part of the activities of the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA), Scientific Advisory Panel (SAP). This report has not been reviewed for approval by the United States Environmental Protection Agency (Agency) and, hence, the contents of this report do not necessarily represent the views and policies of the Agency, nor of other agencies in the Executive Branch of the Federal government, nor does mention of trade names or commercial products constitute a recommendation for use.

The FIFRA SAP was established under the provisions of FIFRA, as amended by the Food Quality Protection Act (FQPA) of 1996, to provide advice, information, and recommendations to the Agency Administrator on pesticides and pesticide-related issues regarding the impact of regulatory actions on health and the environment. The Panel serves as the primary scientific peer review mechanism of the EPA, Office of Pesticide Programs (OPP) and is structured to provide balanced expert assessment of pesticide and pesticide-related matters facing the Agency. Food Quality Protection Act Science Review Board members serve the FIFRA SAP on an ad hoc basis to assist in reviews conducted by the FIFRA SAP. Further information about FIFRA SAP reports and activities can be obtained from its website at http://www.epa.gov/scipoly/sap/ or the OPP Docket at (703) 305-5805. Interested persons are invited to contact Paul Lewis, Designated Federal Official, via e-mail at lewis.paul@epa.gov.

In preparing these meeting minutes, the Panel carefully considered all information provided and presented by the Agency presenters, as well as information presented by public commenters. This document addresses the information provided and presented within the structure of the charge by the Agency.

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August 26-27, 2004, held at the Holiday Inn-National Airport, Arlington, Virginia

A Set of Scientific Issues Being Considered by the Environmental Protection Agency Regarding:

Fumigant Bystander Exposure Model Review: The Fumigant Exposure Modeling System (FEMS) Using Metam Sodium as a Case Study

Mr. Paul Lewis
Designated Federal Official
FIFRA Scientific Advisory Panel
Date: November 9, 2004

Steven G. Heeringa, Ph.D.
FIFRA SAP Session Chair
FIFRA Scientific Advisory Panel
Date: November 9, 2004

Federal Insecticide, Fungicide, and Rodenticide Act
Scientific Advisory Panel Meeting
August 26-27, 2004

Fumigant Bystander Exposure Model Review: The Fumigant Exposure Modeling System (FEMS) Using Metam Sodium as a Case Study

PARTICIPANTS

FIFRA SAP Session Chair
Steven G. Heeringa, Ph.D., Research Scientist & Director for Statistical Design, Institute for Social Research, University of Michigan, Ann Arbor, MI

FIFRA SAP Members

Kenneth Portier, Ph.D., Associate Professor, Statistics, Institute of Food and Agricultural Sciences, University of Florida, Gainesville, FL

FQPA Science Review Board Members

Daniel C. Baker, Ph.D., Senior Consultant, Environmental Computing, Shell Global Solutions US, Houston, TX

Mr. Paul W. Bartlett, Research Associate, Center for the Biology of Natural Systems, Queens College, City University of New York, New York, NY

Adel F. Hanna, Ph.D., Research Professor, Carolina Environmental Program, University of North Carolina at Chapel Hill, Chapel Hill, NC

Michael S. Majewski, Ph.D., Research Chemist, US Geological Survey, Sacramento, CA

Li-Tse Ou, Ph.D., Scientist, Soil & Water Science Department, University of Florida, Gainesville, FL

James N. Seiber, Ph.D., Director, USDA/ARS/Western Regional Research Center, Albany, CA

Frederick Shokes, Ph.D., Director and Professor of Plant Pathology, Virginia Tech, Tidewater Agricultural Research and Extension Center, Suffolk, VA

Thomas O. Spicer, III, Ph.D., Professor and Head, Department of Chemical Engineering University of Arkansas, Fayetteville, AR

Dong Wang, Ph.D., Associate Professor, Department of Soil, Water & Climate, University of

Minnesota, St. Paul, MN

Eric D. Winegar, Ph.D., QEP, Applied Measurement Science, Fair Oaks, CA

Scott R. Yates, Ph.D., Interim Research Leader, USDA/ARS, GEBJ, Salinity Lab., Soil Physics & Pesticides Research Unit, Riverside, CA

PUBLIC COMMENTERS

Oral statements were made by:
William Feiler, Ph.D., representing Amvac

No written statements were provided.

INTRODUCTION

On August 24-25, 2004, August 26-27, 2004 and September 9-10, 2004, the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA), Scientific Advisory Panel (SAP) held three separate open Panel meetings to consider and review three fumigant bystander exposure models. The FIFRA SAP met on August 24-25, 2004 to review the Probabilistic Exposure and Risk Model for FUMigants (PERFUM), using iodomethane as a case study and on September 9-10, 2004 to review the SOil Fumigant Exposure Assessment system (SOFEA), using telone as a case study. These meeting minutes focus on the FIFRA SAP's August 26-27, 2004 review of the Fumigant Exposure Modeling System (FEMS) using metam sodium as a case study**.** Minutes from these other FIFRA SAP meetings are available from the FIFRA SAP website at http://www.epa.gov/scipoly/sap/ or the OPP Docket at (703) 305-5805.

Advance notice of the meeting was published in the *Federal Register* on July 23, 2004. The meeting was chaired by Steven G. Heeringa, Ph.D. Mr. Paul Lewis served as the Designated Federal Official. Mr. Joseph J. Merenda, Jr. (Director, Office of Science Coordination and Policy, EPA) and Ms. Margaret Stasikowski (Director, Health Effects Division, Office of Pesticide Programs, EPA) offered opening remarks at the meeting. Mr. Jeffrey Dawson (Office of Pesticide Programs, EPA) highlighted the goals and objectives of the meeting. Mr. David Sullivan (Sullivan Environmental Consulting) provided a summary of the fumigant emissions modeling system.

SUMMARY OF PANEL DISCUSSION AND RECOMMENDATIONS

Documentation

The FEMS documentation seems complete and well organized with good flow from one part to another, although some sections are a little wordy. The model developers followed the Agency's guidance documents, made linkages to existing literature and included full references with an easy-to-read glossary and definitions of acronyms. The descriptions of the model components were sound. Between the technical documentation and the program files, one can quickly gain an understanding of how the program was operating. The Panel had no problem running the program with the documentation provided. TOXST seems to be appropriate and within it documented capabilities.

System Design/Inputs

Although the actual field emission fluxes are dependent on a variety of factors such as the application method, injection depth, tarp material type and thickness, and the physical/chemical properties of the degradation product of metam sodium, methyl isothiocyanate (MITC), the model-estimated flux values appear to be independent of these variables and dependent only on the measured field emission flux estimates. The Panel had some concern that the different application parameters do have an effect on volatilization fluxes and that data from similar studies should be used to estimate buffer zones for each particular application method.

The model developers need to demonstrate that over the full term of the simulation, fumigation will start on every day of the year. In addition, there is uncertainty as to whether the method of generating the pseudo time series data using actual yearly meteorological measurements (with minor perturbations) maintains the temporal persistence that is typically found in actual weather time series. If such bias doesn't exist, the approach is appropriate. It is not clear if the Monte Carlo methodology uses sampling with replacement (e.g. bootstrap sampling) or some other selection method.

The indirect flux method suffers from the fact that field measured concentrations have associated errors due to measurement difficulties, which can bias toward either the high or low side of physical reality depending on the experimental methods employed and input data used in calculations. Using log-transformed concentrations for the indirect flux method tends to give more importance to lower concentrations in the fitting process. With regard to the metam sodium case study, there were many problems with applying a single flux study to other parts of the country.

Concerning the consideration of multiple emission sources, FEMS seems capable of correctly handling such scenarios inasmuch as the ISCST3 model is capable of correctly handling these scenarios. Regarding the issue of whether a threshold r^2 value should be enforced when regressing measured and modeled concentrations in flux rate determinations, no particular value was recommended by the Panel.

The NWS (National Weather Service) data are available nationwide, are consistent, have good quality control, and are released as complete data sets. These qualities make NWS data valuable for FEMS. Meteorological regions should be chosen according to common climate, terrain, topography, and customary planting times. Meteorological data consistent with the rural farming areas is preferred. Measurement of most data points at the same height above the surface is important to consistently evaluate the dispersion and estimate the emission by the method of back calculation for ISCST3. The height of 1.5-2 meters has the advantage of being the height of human exposure in a rural area, whereas 10 meters is the more customary height for meteorological data, and is more representative of regional conditions. The Panel recommended that measurements be taken at both heights.

The "assumed distributions" method has the advantage of carrying through uncertainty from meteorological inputs to the results. This method also requires further evaluation in regards to meteorological data to be assured that a systematic bias is not introduced that affects boundary conditions and estimated buffer zones.

The Panel believed that the specific inputs into ISCST3 were generally appropriate and that any concern was primarily regarding other aspects of the overall FEMS model structure. The Panel believed that the capability to examine the alternate scenarios was valuable to potential users given the lack of understanding of how low wind speed and high concentrations at the surface are rigorously assessed. The Panel believed that the documentation on computing endpoint distances was sparse and needed to be more thoroughly discussed. The Panel concluded that the capability to model different field shapes is a useful and appropriate function of the modeling system as it presents a more realistic representation of the physical configurations of actual fields.

Results

FEMS can be further proven to have generic applicability to other fumigants. FEMS has the capabilities of (1) estimating emissions from field data, (2) using ISCST3 to account for dispersion under a realistic range of meteorology, (3) post-processing with TOXST to account for the batch nature of the fumigant application, and (4) probabilistic treatment of model inputs. This overall approach is valid, and therefore, FEMS can identify and estimate airborne concentrations of soil fumigants from treated fields.

The FEMS model incorporates uncertainty (i.e., bounds and distribution types) by using values published in the literature and determined via expert elicitation. This approach is reasonable given the lack of empirical data. However, the manner in which the uncertainty should be applied is neither straightforward nor obvious. Efforts have been taken to produce highly realistic meteorological emission inputs in an effort to better simulate uncertainty and to provide reasonable and robust assessments. The sensitivity analysis did not include any quantitative measure of the change of the output variable with change of the input variable. This type of information would be valuable to users of FEMS so that more emphasis is placed on the important input parameters. The Panel recommended conducting a numerical sensitivity analysis.

PANEL DELIBERATIONS AND RESPONSE TO THE CHARGE

The specific issues to be addressed by the Panel are keyed to the Agency's background documents, references and Agency's charge questions.

<u>Critical Element 1: Documentation</u>

Question 1: The background information presented to the SAP panel by the FEMS developers provides both user guidance and a technical overview of the system.

A) Is this document sufficiently detailed and understandable?

Panel Response

The FEMS documentation seems complete and well organized with good flow from one part to another, although some sections are a little wordy. The model developers followed the Agency's documentation guidance. The documentation provides linkages to existing literature and includes full references with an easy-to-read glossary and definitions of acronyms. The documentation had insufficient discussion of how the 5-year NWS data are restructured to create a 200-year climate time series. The approach intends to capture the uncertainty, which is very desirable. The planned use of the AERMOD will remedy some of the ISCST3 model shortcomings, especially those related to incorporating stability for the scales of modeling used. Documentation for the TOXST module in FEMS was missing. Apparently the Agency has removed the on-line documentation to TOXST and as a result necessary documentation is hard to find. Better description of the case studies used in the documentation should be provided. Members of the Panel appreciated the fact that reprints of published papers were provided with the documentation. Documentation of the back calculation method should be moved from the appendix into the main body of the documentation. The Panel also suggested that a rewrite of the documentation should concentrate on explaining how the model operates, describing the methods, theory, and applications. Side issues should be moved to the discussion section or deleted. Finally, the Panel suggested adding sections on model limitations, user pitfalls and plans for future improvements.

B) Are the descriptions of the specific model components scientifically sound?

Panel Response

To be scientifically sound it was understood that the documentation must enable a knowledgeable user to recreate everything discussed in the document. By this definition the descriptions of the model components are sound.

C) Do the algorithms in the annotated code perform the functions as defined in this document?

FEMS uses a series of FORTRAN executable programs, batch files, and base modeling files, interacting with the user through an input dialog within a DOS prompt. The FORTRAN code was easy to read and seemed to perform as expected. However, there were some problems with documentation of the FORTRAN code. A number of the files had very little documentation, with no description of their function included in the code file. Descriptions were provided in the supporting technical documentation and the appropriate comments should be added to the code. Most of the logic of the program is incorporated in the batch (BAT) files. The BAT fields were also sparsely documented in the code set with slightly more documentation in the technical report. The use of a *.BAS file extension for the base modeling files was initially confusing because the system identified these as Visual Basic code sets. One quickly comes to understand the nature and function of these files, although there is again very little documentation inside the files. In conclusion, between the technical documentation and the program files one can quickly get an understanding of how the program is operating.

The FEMS system comes with precompiled FORTRAN modules. The batch files need no modifications to run the test case. The base files are used as input to some of the FORTRAN programs that subsequently output .BAT files. For example the RANDOM.BAT script referred to in the PROGRAM.BAT script is created from the RANDOM.BAS file. This process is not documented in the text nor commented on in the FORTRAN code. Because of this it was difficult to track the program flow with the documentation provided.

This raises a more general concern about the current structure of the FEMS system. As it now stands, the user progresses sequentially through the process with the ability to look at intermediate results along the way. Steps that produce output that does not look correct can be re-run without having to start from the beginning. This is an advantage in a process that can take up to eight hours to complete. Composed as it is of many interlocking parts, the FEMS program system would be very difficult to manage if there were a fairly large user base. There would need to be some consolidation of functions, resulting in fewer but larger files. For example, everything in the nine batch files could be put in one file. This could, with careful planning, reduce some of the current inflexibility of the program.

Other problems were observed when running the program with different options. The Panel believed that the addition of a detailed flow chart of program flow to the documentation, with a second flow chart detailing (input/output) I/O need, would help clarify user options.

D) Were the panel members able to load the software and evaluate the system including the presented case study?

Panel Response

Members of the Panel had no problem running the program with the documentation provided. The program spends a lot of computational time in ISCST3, performing computations for the full 200 years in one step. Then in subsequent steps TOXST only selects part of the ISCST3 output. It was noted that the program can be run with and without added variability to the wind data.

<u>Critical Element 2: System Design/Inputs</u>

Question 2: In *Section 2.1: Overview of Conceptual Model* of the background document, a series of flowcharts (Figures 2, 3, and 4) are presented that detail the individual processes and components that are included in FEMS. The key processes include (1) emissions processing, (2) 200-year weather inputs and how they are used for longer-term Monte-Carlo sampling; and (3) TOXST analysis. What can the panel say about these proposed

processes, the nature of the components included in FEMS and the data needed to generate an analysis using FEMS? Are there any other potential critical sources of data or methodologies that should be considered?

Panel Response

(1) Emissions Processing

The FEMS system is composed of an interface that couples ISCST3 and the TOXST post processor to allow a Monte Carlo analysis of emission and down-wind transport of fumigants, and potentially other volatile organic chemicals. The modeling system provides several types of information on the frequency of exposure and can address the development of buffer zones. ISCST3 and TOXST have been evaluated and recommended by EPA and the California Department of Pesticide Regulation (CDPR). The use of ISCST3 and TOXST is appropriate for determining fumigant exposure, and FEMS doesn't alter either program in any manner. The relative accuracy (in a regulatory context) of the back-calculated emission source flux estimates are the order of 40-50%, as reported by the model developers. However, the Panel would appreciate references to support that conclusion.

The FEMS system was used to model a "worst case" scenario only for the test fumigant MITC (i.e. the field and environmental conditions result in the high emission fluxes and high down wind air concentrations after a fumigant application was used). This scenario is the starting point for the evaluation process, and other environmental conditions can be investigated as the need arises. Actual field data were used to calibrate the model. The field tests were conducted at only one location, but included several different application and sealing methods. The fields, both actual and modeled, were restricted to square or rectangular shapes, but the Panel was assured by the model developers that the model had the capability of providing results for irregularly shaped fields and variable application time lengths (in custom runs), in addition to multiple field/sequential application scenarios, although no examples were provided. The potential for FEMS to be used to assess downwind concentrations from more than one application is an advantage of FEMS. But again no examples were given in the documentation of FEMS. Model runs can also be restricted to seasonal application periods using the appropriate meteorological data.

Although the actual field emission fluxes are dependent on a variety of factors such as the application method, injection depth, tarp material type and thickness, and the physical/chemical properties of MITC, the model-estimated flux values appear to be independent of these variables and dependent only on the measured field emission flux estimates. The Panel had some concern that the different application parameters do have an effect on volatilization fluxes and that data from similar studies should be used to estimate buffer zones for each particular application method.

Period emission estimates were only obtained from an indirect method (i.e., scaling a nominal emission value used in ISCST3 and obtaining a scaling factor through a regression analysis). There is a real need to verify the modulated values of source emission flux data.

There needs to be a means for assessing, or at least expressing the confidence in the accuracy of the back calculation emission method. No comparison was shown between modeled values and established direct (i.e., aerodynamic or gradient) field methods. Even comparisons with other soil emission models would help to provide an independent check and allow for concentration data to be estimated at adjacent receptor sites and increase the confidence in model output.

Using various other approaches to estimate source fluxes and down-wind air concentrations will allow the accuracy/reliability of this critical information to be explored. Results from an alternate estimation method will also increase the confidence in the FEMS results. The chosen method should result in a single, standardized and robust period-emission value.

Some Panel members raised issues related to the chemical's stability in the environment. MITC has a reported atmospheric half-life on the order of one to four days. Under the "worst case" scenario (i.e., full sunlight, midsummer heat, high ozone levels, etc.,) the downwind samplers may show lower MITC concentrations than the model predicts, due to atmospheric degradation or surface deposition of MITC between the field and the downwind samplers, particularly the farther downwind locations. Deposition processes were not considered to be important in estimating downwind concentrations, but this is an assumption and the impacts of alternative assumptions were not examined.

These environmental fate concerns, however, may be secondary to the estimation of when and where the concentrations exceed the exposure threshold values as established by EPA. Differences in the time scales of plume movement as it applies to human health end points versus environmental fate are probably on a much smaller time frame but again, experimental proof of this is desirable.

The regression model used to calibrate emissions is forced through the origin (i.e., there is no y-intercept). This is made possible by changing the field sample no-detect (ND) results to 0.1, i.e., one half the analytical limit of detection for transformational purposes. The arguments presented for this transformation are sound, but more detailed discussions on these points are presented by the Panel in response to other questions.

The Panel discussed the relationship between the mass balance and the period flux rates for MITC. The issue is the ability to estimate the percent of fumigant volatilized as a function of the amount applied and the estimated period flux rates. This method typically overestimates the volatilized percent for soil fumigants. The back calculation method used either with or without log transformation does not seem to directly address this mass balance issue.

The model developers mentioned that they were thinking about expanding the 4-hour sampling periods to six hours to decrease the chances that the wind direction will be from only one direction, i.e., concentration hits at only a few downwind samplers. The Panel disagreed with this as the 6-hour periods will provide less information about emission trends, and an anomalous value, either high or low, may have an unwarranted influence on the emission trends.

Several Panel members suggested that information on the vertical component of the plume spread, in addition to the horizontal component, would be valuable in estimating the source emissions.

The flow chart shown in Figures 2-4 of the model documentation appears appropriate. If a new approach for obtaining period emission values is adopted, however, a slight change to the flow chart (Figure 2) may be required.

2) 200-year weather inputs and how they are used for longer-term Monte-Carlo sampling to show variability and uncertainty

The Monte-Carlo variables for a model run include the application start time, emission rates, and meteorological parameters. A 200-year weather data set was created based on 5 years of weather measurements obtained in the Fresno, California area. Sampling from the simulated set of 200 years of NWS weather data allows variability in meteorological data to be incorporated into the risk assessment analysis. The emission data are temporally matched to the meteorological data regardless of start time in each four day model run. However, there is some concern that using ISCST3 to analyze emission events in a sequential manner may introduce a bias into the results. The model developers need to demonstrate that over the full term of the simulation, fumigation can start on any day of the year (i.e., it is not the case that the actual weather data have a number of records that are divisible by 4, and only the 1, 5, 9, … days will be sampled as start points in each of the 200 years). In addition, there is uncertainty as to whether the method of generating the pseudo time series data using actual yearly meteorological measurements with minor perturbations maintains the temporal persistence that is typically found in actual weather time series. If such bias doesn't exist, the approach is appropriate.

It is not clear if the Monte Carlo methodology is utilizing sampling with replacement (e.g. some form of bootstrap) or some other selection method. It would seem possible to convert all the FEMS input data to probability distributions and conduct the analysis by sampling these distributions. Such an approach might allow adjustment of the probability distribution to allow investigation of rare events under hypothetical conditions. If the approach creates probability functions that are sampled repeatedly during the analysis, the model developers need to emphasize this. They may want to include graphs showing examples of the probability functions. This would help the reader to better understand the methodology.

The model developers appear to use a truncated range for sampling from distributions (i.e., 2.5%-97.5%). This may limit a user's ability to investigate rare events with FEMS. FEMS places no restriction on stability class change with time. This increases the ability to match on-site conditions. ISCST3, however, restricts changes in stability class to one class change per hour.

If more than one NWS meteorological station containing the required 5-year data sets is in the application area, they should be used in the model. This will better capture the variability of weather in the region. There is still an issue of the representativeness of using far distant, airport NWS data to represent climate for simulating emissions in an open field.

3) TOXST analysis

TOXST is used as a post processor in the FEMS system. It starts the application process using the input meteorological information from ISCST3 to estimate hourly acute downwind air concentrations at various receptor sites for the duration of the study period, usually four days. TOXST seems to be well documented and used appropriately.

4) Other Data and Methodologies

One of the Panel members offered an alternative approach for calculating the period emission rates. The method would require application of ISCST3 with an arbitrary emission rate to determine the position of the plume. At each sample location that resides inside the plume, a flux value is calculated that produces exact agreement between ISCST3 and measurement, producing a set of flux values. The average of this set of flux values should be equivalent to the slope obtained from the regression method. The list of flux values could also be used to develop a probability distribution as a measure of uncertainty/variability. This process would be repeated for each period. It has been suggested that this is equivalent to applying the regression approach with a fit through the origin and, if so, may provide justification for adopting a through-the-origin approach. It would also indicate that the intercept is caused by the model's inability to match non-zero measured values that reside outside the plume, that is, where the wind direction was pointed outside the wind direction range, $u_\theta \pm \sigma$ for some portion of the time period, or that other processes occurred which ISCST3 cannot simulate.

The nature of the spacing of the receptor grid can also be used to check the model output. Other Panel members suggested using the sampling points close to the source to estimate the concentration at sampling points further away or conversely, using the distant points to estimate the concentration at near-field sampling locations as a method for calibrating or verifying the model. It would also be possible to use the extensive California Department of Pesticide Regulation (CDPR) database on methyl bromide (around 35 studies) for this purpose. FEMS could use the methyl bromide field data to back calculate the emission fluxes as well as the concentrations at select down wind receptor sites and the results could be compared to those of CDPR. Data from an alternate source could be used to compare with back-calculation data, thus increasing confidence in the back calculation method. Utilizing data from an alternative source is useful for comparison purposes, increasing confidence in the method.

Question 3: The determination of appropriate flux/emission rates is critical to the proper use of the FEMS model as these values define the source of fumigants in the air that can lead to exposures. There are different methods of determining flux/emission rates from empirical data including direct measurements and what is referred to as the "indirect" or "back-calculation" method. Direct measurement of flux is not that common in the available data because of the difficulties and expense associated with generating these types of data. The "indirect" method is most commonly used and involves fitting monitoring data with ISC to determine flux/emission rates. Upon its review of how flux rates can be calculated, the Agency has identified a number of questions it would like the panel to

consider. The emission fitting procedures used in FEMS are based on least squares analyses of log-transformed, dispersion modeling and field monitoring data.

A) What, if any refinements are needed for this process?

Panel Response

The choice of concentration sampling methods for the metam sodium case study raised some questions. Samplers measured concentrations on 4-hour averages. It was mentioned during the presentation that 6-hour average samples were being considered. While this will smooth out concentration data, there are disadvantages. Variations in meteorological data would be smoothed out (calms may be less important), but when the flux data are used for predictions, the meteorological data would have to be comparable to replicate the emission behavior. Using longer averaging times will also reduce the predicted maximum concentration exposures.

Samplers were located at 150 meters from the field edge in recent tests. At this distance, the vertical concentration distribution may be more uniform so that making vertical concentration measurements may be less important. At this distance, there may be a trade off in that more horizontal concentration measurements may need to be made to avoid a condition where only 2 or 3 sampler stations measure concentrations.

For the indirect method determination of the flux, the assumption has typically been made that the flux rates determined by the method will "calibrate" the dispersion model to predict the correct downwind concentrations when used in a predictive mode. This assumption ignores the uncertainties in dispersion modeling. Two of the most important issues include: variability of dispersion coefficients for a particular atmospheric stability and assigning the atmospheric stability class.

Changing stability class in the model results in a step change in distribution coefficients (hence concentrations), while in reality, the distribution coefficients are continuous variables depending on stability parameters. So that if stability is determined to apply to two periods during flux measurement experiments, that does not mean that the distribution coefficients in those two time periods are the same.

Atmospheric stability changes rapidly near sunrise and sunset. Most troublesome is the period after sunset because increased atmospheric stability near ground level (which affects the flux) may go undetected at even slightly higher elevations, and stable stratification will develop from ground level and become deeper with time. Stable conditions should generate the largest concentrations at the same location, all other things being equal. The Panel referred to Figures 19, 20, and 22 in the model documentation for further explanation. Figure 19 shows that the highest measured values generate the largest residuals (shown in the box in the figure). These same points can be followed to the other figures to show that they are at the lowest windspeeds, but the estimated stability for these points is not the lowest atmospheric stability. It is possible that the stable transition may be missed in the analysis. These points could also be a consequence of a calm period where the concentration can build up over the source and then be advected downwind when the windspeed increases (related to the issue of how ISCST3 treats calm conditions).

Modeled concentrations that are zero at locations where measured concentrations are non-zero give rise to the non-zero intercept in the regression equation used to calibrate model emissions. When it is concluded that such measured concentrations are not background concentrations, such a situation indicates that the real plume extends outside the predicted plume behavior. This behavior is likely caused by inadequately predicting the plume direction or the dispersion coefficients. Regardless of the cause of the discrepancy, there is a flux of material in the real plume unaccounted for by the modeled plume even if the modeled concentrations are fit to the measured concentrations within the modeled plume boundary. Thus, having a non-zero intercept indicates that the flux will be underestimated because there is a flux (i.e. mass) of material in the real plume that cannot be captured in the modeled plume.

B) Is it appropriate to log transform these types of data for back-calculation purposes and to use a least-squares regression analysis, which implicitly assumes that the fitted line passes through the origin?

Panel Response

For the indirect flux method, the use of log-transformed concentrations has been debated as to its appropriateness. The FEMS presentation and documentation provided a rationale for using the log-transformed concentration procedure based on statistical arguments. On the other hand, the argument is straightforward that the model concentrations are proportional to the flux so the slope on a modeled versus measured concentration plot (without log transform) reports how the assumed flux should be modified to fit the observed concentration data. Using a log transformation results in a nonlinear relationship. The point made by the model developers was that the resulting flux estimates may differ between methods (log transformed concentrations versus raw concentration data) as to the flux values at specific times, but the overall trends are in agreement for both methods.

Using log-transformed concentrations for the indirect flux methods tends to give more importance to lower concentrations in the fitting process. The importance of this effect may be compounded by setting concentrations to one-half of the minimum detectable limit when no gas concentration is measured. It may be worthwhile to simply leave out sensors that do not detect gas and would not be expected to do so.

As has been previously discussed, one way to begin to address the question of the appropriateness of the log transformation is to check the sensitivity of the assumed flux basis of 1 $\mu g/m^2s$. A problem would exist if the log transformed procedure estimates significantly different fluxes if a different flux basis is assumed (e.g., 100 $\mu g/m^2s$).

C) How appropriate is it to use a flux/emission factor from a single monitoring study (or small number of studies) and apply it to different situations such as for the same crop in a different region of the country?

Panel Response

With regard to the metam sodium (i.e. MITC) case study, there were many problems with applying a single flux study to other parts of the country. Soil types and atmospheric conditions are significantly different so that the intermittent plastic tarp seal used in the present study would not be used in some other parts of the country. Water sealing methods may not work as well under other conditions even if used.

While the flux model used in FEMS could be applied to other fumigants, the Panel raised concerns about the flux model used in FEMS that could also be important for other fumigants in addition to metam sodium as noted below.

The flux model is only aligned for applications within an hour of sunrise because that is when the single study was conducted. One cannot assume that applications beginning later in the day will automatically have shorter buffer zones.

The time series smoothing is not guaranteed to be mass conservative. There also seems to be considerable uncertainty about conversion efficiency of metam sodium to the biologically active compound MITC and the extent of MITC degradation (chemical and biological) in soil. Consequently, it is not certain how much material should be counted as emission even though the application rate is known.

The documentation recognized the importance of other factors such as ambient temperature. Soil flux models also indicated that local meteorological conditions affect the flux. Soil chemistry may also be important. Because FEMS used a single study compound (MITC), it is not clear how the effect of these parameters can be included in the model without applying the model to compounds of differing physicochemical properties.

The stated reason for basing the flux estimates on a single study at the Bakersfield site is that it will be conservative when applied to other geographic regions. However, no supporting research or other information was given. Assuming that the flux measurements from the Bakersfield area tend to be of high value, it is possible that repeated measurements will produce even higher flux values. Even so, conducting additional tests at the Bakersfield site is recommended. The question that would follow would be how to treat multiple data sets for the same location. Furthermore, if Bakersfield fluxes are so much higher than would be expected in other regions, then the resulting buffer zones based on these values may be unrealistically conservative, which would argue for conducting validation studies, with measured downwind concentrations, at other locations and under different conditions.

The FEMS flux estimate, taking into account variability based on the Bakersfield site, is constrained so that all of the applied mass cannot be emitted in the first four hours (it is recognized that the emission will occur over four days at this site). If it is necessary to constrain the emission in such a way (to guard against such drastic overprediction), then it seems reasonable to consider that at the opposite end of the distribution, the emission may be dramatically under predicted when estimating buffer zones.

A single rogue data point may significantly change the character of a flux dataset, and detection of such a misleading value is made more difficult when a single data set is used. Validation of the flux by an independent method would be helpful. This could also be presented as an alternative approach for consideration in response to part G of this question.

The Panel recognized that the FEMS flux model might be acceptable without capturing some of the detail. However, the agricultural community may be reluctant to support such an approach since a single study under possible worst case conditions may be perceived as overly conservative when applied to other regions.

D) Does the panel believe that FEMS could adequately consider multiple, linked application events as well as single source scenarios?

Panel Response

With regard to the consideration of multiple emission sources, FEMS seems capable of correctly handling such scenarios inasmuch as the ISCST3 model is capable of correctly handling these scenarios. An example for acute exposures which field measured data are matched to FEMS would be a helpful addition to the documentation. Based on the presentation, such a scenario may be difficult to simulate, but still possible based upon published data for methyl bromide and telone (1,3-D).

E) Does FEMS appropriately address situations where data are missing (i.e., is the data filling procedure appropriate)?

Panel Response

The effect of missing data can be considered by taking a complete set (which exists for metam sodium) and deleting measurements. The data set with the missing data can be filled in by the proposed procedure, and its efficacy can be studied. Alternative methods such as interpolation prediction based on a weighted spline smoothing method may also prove effective (Hastie and Tibshirani 1990).

F) Should there be a threshold r^2 value below, which a regression of measured versus modeled air concentrations should not be used in flux rate determinations?

Panel Response

Regarding the issue of whether a threshold r^2 value should be enforced when regressing measured and modeled concentrations in flux rate determinations, no particular value was recommended by the Panel although some felt that such a threshold might be helpful. Experience with methyl bromide was that r^2 values ranged from .5 to .95 with typical values of .75. Lowest correlations typically occurred at low windspeeds. The Panel suggested that instead of considering a threshold for r^2, it is more appropriate to consider a statistical significance test such as reporting the P-value (confidence) characteristic of the fit. Some measures may improve the fit (and P-value) between observed and measured concentrations.

Some Panel members have recommended sorting modeled values so that the largest measured values are matched with the largest predicted values since it is generally accepted that the ISCST3 and other Gaussian plume models predict maximum concentration values more reliably than the location of the maximum concentration. Sorting data will improve the fit between modeled and predicted values, but there is some concern that using this approach to simply improve the fit may not be the best practice. In the metam sodium case study, concentrations were measured at different downwind locations, and it was recommended that such sorting was a reasonable approach if the sorting is restricted to measurements at the same downwind distance.

Finally, as discussed above, leaving out non-zero points where no emission value was measured may be appropriate, and such a procedure would improve the fit.

G) What are possible alternative approaches?

Panel Response

Possible alternative approaches were recommended for consideration when determining the flux. Instead of considering the measured and predicted concentrations to infer a consistent flux that matches the data, ISCST3 could be used to calculate the flux necessary to predict the measured concentration. This would produce a set of flux values for a set of concentration measurements. Statistical properties of the set of flux values could then be calculated. For such a procedure, non-zero measured concentrations which were recorded at locations where model predicted concentrations are zero would be excluded since no flux in ISCST3 could change the predicted concentration from zero.

Fluxes determined by the indirect method could be compared with a mechanistically-based soil fumigant fate and transport model. Such models could be used in conjunction with an air dispersion model to predict downwind concentrations. Although expensive, direct flux measurements could be made for comparison with method values.

Question 4: The integration of actual time-base meteorological data into ISCST3 is one of the key components that separates the FEMS methodology from that being employed by the Agency in its current assessment. The Agency has identified several potential sources of these data including the National Weather Service, Federal Aviation Administration, California Irrigation Management Information System (CIMIS), and the Florida Automated Weather Network (FAWN). The Agency is also aware that there are several approaches that can be used to process meteorological data and acknowledges that FEMS used PCRAMMET which is a standard Agency tool for this purpose. Upon its review of the meteorological data that are available and how it can be processed for use in an

assessment such as this, the Agency has identified a number of questions it would like the panel to consider.

A) The test case example in FEMS is based on the National Weather Service ASOS meteorological monitoring station in Fresno, California. What are the SAP's thoughts on the use of National Weather Service / Federal Aviation Administration meteorological data sets in comparison with either CIMIS or FAWN for this type of application?

Panel Response

The NWS data are available nationwide, are consistent, have good quality control, and are released as complete data sets. These qualities make NWS data valuable for FEMS. A single consistent data source is important for comparability between meteorological regions.

Quality control is important since the identification and understanding of the rare meteorological events that require the largest buffer zones are the objective of the FEMS project. Poor quality control could result in events that either underestimate or overestimate buffer zones. If data sources other than NWS are used, the problems of data quality need to be identified and evaluated, especially upon how they affect boundary conditions. Regardless of the data source, error and warning routines need to be written into the code that identify impossible and unlikely meteorological data. These irregularities ought to be reported in the results.

The FEMS methodology requires complete meteorological data sets. State data may not have important meteorological variables, like cloud cover, which compromise stability calculations, or the data may have missing periods. State data source locations, however, may be located in areas more representative of agricultural regions. NWS stations are usually located at airports, which are often uncharacteristic of agricultural regions.

FAWN data sets have a significant amount of missing data often due to equipment failure caused by lightning strikes and other problems inherent to research stations. The FEMS methodology requires missing data to be replaced, presumably by either interpolation or reconstruction with climatic data and the aid of other nearby station data. This can be done, but can be time consuming and can conceivably create false weather events that either underestimate or overestimate the buffer zone.

CIMIS stations are in rural areas but have other limitations. Overall, when data are available from different sources, it is recommended to identify the error properties of each data set compared to other available alternatives and choose the meteorological data that is highest in quality and most relevant to the site that is being modeled (see Panel response to question 4b).

B) What criteria should be used to identify meteorological regions for analysis and how should specific monitoring data be selected from within each region?

Panel Response

Meteorological regions should be chosen according to common climate, terrain, topography, and customary planting times. Meteorological data consistent with the rural farming areas are preferred. Some regions may have a wide variety of local conditions that could result in a range of emission and dispersion characteristics.

For some agricultural regions, micro-meteorological data are necessary to estimate the fumigant buffer zone. For complex topography and terrain, micrometeorology can predominate over regional, upper air layer meteorology; the application of boundary conditions determined from flat land will not likely apply. Modeling data such as the Regional Atmospheric Modeling System (RAMS) at Colorado State University (http://rams.atmos.colostate.edu/) and the NCAR Mesoscale Model version 5 (MM5) can overcome these limitations. In general, RAMS includes more physics on land surface and micrometeorological modeling characterization than MM5.

In some parts of the country, local meteorological data can be very different between small locations. For instance in a nine county region in Virginia, peanut disease forecasting requires 10 weather stations to get good information. Finally, the impacts of localized showers can be important.

Soil emission measurements and modeling have identified variables that affect fumigant emissions but are not directly accounted for in the FEMS approach. Application of FEMS results from one region to the next will have to account for these factors, especially differences in soil chemistry and soil climate. Carbon content, soil moisture, prior history of chemical fumigant use and pesticides and degradation are all-important factors. Historic use of metam sodium has been found to affect degradation rates of MITC in soil.

In order to evaluate the applicability of the derived emission data from one region to the next, it is advisable to conduct field studies.

C) Anemometer sampling height has been identified as a concern by the Agency in preparation for this meeting. For example, some data are collected at 2 meters while others are collected at a height of 10 meters. What are the potential impacts of using either type of data in an analysis of this nature?

Panel Response

Measurement of most data points at the same height above the surface is important to consistently evaluate the dispersion and estimate the emission by the method of back calculation for ISCST3. The height of 1.5-2 meters has the advantage of being the height of human exposure in a rural area, whereas 10 meters is the more customary height for meteorological data, and is more representative of regional conditions. Below 10 meters, local micrometeorological conditions can prevail. It is preferable to have vertically resolved air concentrations, and to have meteorological data for 1.5-2 meters and 10 meters during the testing period. Thus, the Panel recommended that measurements be taken at both heights.

D) FEMS uses “assumed distributions” to account for uncertainty in the meteorological data based on Hanna, 1998 [as referenced in the FEMS background paper]. Is this an appropriate technique?

Panel Response

The “assumed distributions” method has the advantage of carrying through uncertainty from meteorological inputs to the results. The technique also enables the creation of 200 years and more meteorological data sets out of the 5-year data set from Fresno. This method also requires further evaluation in regards to meteorological data to be assured that a systematic bias is not introduced that affects boundary conditions and estimated buffer zones.

The introduction of independent random disturbances at each time step has drawbacks when applied to meteorological data. This method may distort meteorological time series patterns and produce inconsistent meteorological variables, which would change the distribution of upper bound cases.

Time persisting weather patterns (prevailing and cyclical) can be lost by the perturbations. For example, when a low speed prevailing wind produces a high boundary condition for air concentration, this random disturbances method can artificially dilute the MITC air concentration by either varying wind direction or increasing wind speed. The countervailing case is less likely to be constructed. A set of random disturbances is less likely to produce a prevailing wind speed and direction period to period. The net result could be underestimating the upper bounds and consequently underestimating the buffer zone.

The importance of this example to boundary conditions can be evaluated by conducting a comparative run with and without the perturbation applied to wind direction. Other possibilities need to be tested. A comprehensive sensitivity analysis needs to be done with the perturbations. The objective of putting uncertainty in the bounds should not be lost.

The FEMS probability approach is similar to what has been done with other risk models that have come before the FIFRA SAP (e.g. Lifeline, Calendex, SHEDS, etc.). The difference here is that the addition of perturbations may have the impact of destroying temporal patterns in the parameter, for example wind speed, and hence reduce persistence.

In the model, stability is not allowed to vary. Perturbing other variables like wind speed may result in a mismatch with the stability resulting in an inconsistent set of meteorological variables for some periods.

The efficacy of the method to create 200-1000 years of meteorological data out of five years of data needs to be further evaluated. There may be a variety of ways of evaluating the approach with additional meteorological data and different statistical techniques. The perturbed constructed data series can be compared with a longer-term data series of actual meteorological data.

The meteorological conditions that produce the extreme boundary conditions from experimental computer runs, (the highest impact and the lowest impact) should be retained, characterized and evaluated. This information would be valuable for evaluation of the realism of the conditions from the perturbed data set, and the range of applicability within and between regions. The data could also be used as guidance on the best weather conditions for reducing the area impacted by the application of the fumigant.

It may turn out to be preferable to use actual meteorological data rather than perturbed data when possible. A larger data series could be constructed out of actual data by pooling meteorological data from a set of representative regional stations, and/or by making use of the long-term data sets that have been constructed for long distant transport hemispheric modeling and climate modeling.

E) Does FEMS treat stability class inputs appropriately, especially the quantitative manipulations of these data that have been completed?

Panel Response

According to the model developers, PCRAMMET, an Agency approved method, was used to construct the stability classes for use in ISCST3 from the Fresno NWS station data. There is an inherent problem with using a meteorological data source from a distant location since local conditions may be different, but this problem is not readily overcome. Application of meteorological data from other regional stations would facilitate sensitivity analysis and better evaluation of the influence of applied stability classes.

ISCST3 does not permit the utilization of all meteorological data relevant to stability that can be measured locally during field experiments. Replacement of ISCST3 with AERMOD will allow for more customization to local stability conditions and higher resolution, temporally and vertically. ISCST3 limits stability to one class for one hour, preventing the use of continuous field gathered stability variables. Hopefully, AERMOD will allow stability factors at finer temporal resolutions (shorter model time steps). AERMOD uses measurements at more than one vertical level (sigma values) and inputs for local surface conditions roughness. This may help in better capturing the turbulent and dispersion processes.

F) Is the concurrent use of emissions and meteorological conditions in FEMS useful in identifying concurrent upper-end conditions that could lead to peak exposures for bounding exposure events?

Panel Response

Overall, the approach described is promising in that to understanding the probabilities and uncertainty to peak exposure events. The uncertainty of the approach itself to meteorological data needs to be reduced, as does the generalization of emission distributions from one field study.

This question is discussed in more detail in the sections above. There are two specific areas that were not answered above that will be addressed here: time scales and the use of TOXST to select random starting periods of application.

It is essential to maintain short time scales because that is when drifts and spikes occur. The hourly data and diurnal data should be preserved in results. Twenty-four hour averages, while an Agency standard, are difficult results to evaluate, do not provide information necessary to reduce exposure, and may not be useful for assessment of shorter periods of acute exposure that may be important in our understanding of the exposure to fumigants.

The FEMS results showed significant peaks of emissions on days following the first day of application. Results for the four days may be useful in identifying significant exposure probabilities after the first day.

The applicability of TOXST to agricultural fumigant use in the same manner as to intermittent industrial sources is questionable. The objective of producing a distribution of start times is worthwhile to pursue. The application of fumigants in many regions are not random throughout the year as TOXST is currently applied, but seasonal, and the planting times are determined by specific weather patterns, typically within a very short period in each locale. Moreover the time of day of application is not random, but is distributed throughout the day, (metam-sodium is most commonly applied at sunrise). FEMS is fully capable of using a seasonal approach, and a more representative distribution of start times. An alternative to TOXST may have the additional advantage of not requiring the lengthy computing runs that FEMS currently requires. Annual meteorological data may not be needed with an alternative to TOXST; seasonal data may suffice.

Question 5: The Agency model, ISCST3 is the basis for the FEMS approach. This model has been peer reviewed and is commonly used for regulatory purposes by the Agency. FEMS also uses other Agency systems such as PCRAMMET and TOXST.

A) Are there specific recommendations that the panel can make with regard to any parameter that should be altered to optimize the manner that they are used in FEMS?

Panel Response

The air dispersion model ISCST3 has been thoroughly evaluated by many users and is used across the country in a wide variety of applications. In addition, one of the preprocessing steps for data input into ISCST3 is the use of PCRAMMET for formatting and determining stability classes, etc., and therefore it is a de facto part of ISCST3 modeling. It is also an EPA-approved, peer-reviewed and validated procedure. Therefore, the incorporation of these models into the FEMS system can be viewed with confidence.

The model TOXST also has some level of evaluation and acceptance, given that it is an EPA-accepted model, though it is not used as extensively as ISCST3. The Panel believed that the lack of documentation of TOXST did not allow for a full evaluation of its use or for understanding how input parameters might affect the output.

The Panel believed that the specific inputs into ISCST3 were generally appropriate and that any concern was primarily about other aspects of the overall FEMS model structure. However, there was a question regarding how to deal with low emission periods characterized by high stability where the concentrations at the surface would be high and the wind speed low or below the measurement threshold of the sensing equipment. This type of scenario could be handled potentially by using alternate dispersion coefficients, particularly sigma z. While the dispersion coefficients cannot be directly modified as an input value, it is possible to incorporate site-specific coefficients via modification of the program code.

In addition, it was suggested that an examination of the model sensitivity to vertical and horizontal dispersion parameters be performed by looking at grid data or by adding various multipliers to sigma y and sigma z. Uncertainty related to horizontal and vertical dispersion may be included in model formulation by randomly selecting a multiplier to sigma-y and sigma-z in the ISCST3 model code. The multiplier can be introduced on an hourly or daily basis. This multiplier is based on a cumulative distribution function representing the uncertainty which is based on the difference between measurements at field experiments and the model-calculated sigmas.

A potential way to more easily perform this evaluation is to use the new model AERMOD when it is released for use and perturb the sigma y and sigma z, as is done with FEMS currently.

B) ISCST3 can treat "calm" (i.e., periods where the windspeed in essentially 0) in one of two ways including the concentration is set to (0) and an approach that uses the last non-calm wind direction/concentration. FEMS uses the first approach. Does the panel concur?

Panel Response

The Panel believed that the capability to examine the alternate scenarios was valuable to potential users given the lack of understanding of how low wind speed and high concentrations at the surface are rigorously assessed.

However, the true impact of calms is difficult to determine. If wind speed was observed to be zero for a 4-hour period does this mean that there was no flux? This question arises because setting concentrations to zero results in zero flux via the back calculation procedure. However, the alternative approach results in the flux for the zero wind periods being exactly that of the previous period.

When the wind speed is set to zero, it means that material may pile up at the source, in which case the real discrepancy will occur in the next time period and lead to uncertainties in the overall flux calculations. In analogy to water flow models, as the speed goes to zero, the importance of dispersion increases.

In addition, the question of the effect on how calms should be handled is difficult to answer because of code and measurement sensor limitations. Calm winds may not be really "calm" since observational networks consider winds less than a certain threshold to be calm. The PCRAMMET preprocessor automatically converts any value less then 1 m/s to 1 m/s. Therefore, the low wind speeds that might occur during periods of high stability are automatically scaled to 1 m/s.

Commonly used meteorological sensors have wind speed thresholds on the order of 1m/s, although wind direction sensors are generally more sensitive. It was suggested that the use of sonic wind speed sensors with "virtually zero thresholds " (www.vaisala.com) be investigated for future flux measurements. However, the sensitivity of the model to this factor is unknown.

Although it is not a standard feature of ISCST3, the Panel thought that there should be a third option within the model to allow for some wind speeds below 1 m/s. In those cases where no data exist below that threshold, they thought consideration should be given to an alternative formulation of some detectable value, analogous to the methods used in analytical chemistry, in which either one-half the detection limit is used or a randomly selected value from an arbitrary probability distribution function should be considered. It is expected that such an option would provide better agreement between predicted and observed flux.

The question of calms in an area source scenario is somewhat unresolved, as the limitations noted above are built-in and not easily modified. Further research is needed to understand the implication of the current mode of calms processing on high stability area source emissions.

C) In *Section 2.2 Specific Technical Considerations With Regard To The Design Of FEMS* of the background document, there is a section entitled *Computing Endpoint Distances*. Please comment on the procedures included in this section?

Panel Response

The Panel believed that the documentation on this procedure was sparse and needed to be more thoroughly discussed. The user is asked to take the model developers' assurances that this procedure works correctly. No data or depictions were provided to support the statement of the method. In addition, very little documentation on the TOXST program was available to understand how the TOXST output was logarithmically interpolated. Other than the documentation of adequate performance of this method, the Panel has no conceptual disagreement with this type of approach.

D) The FEMS analysis is based on a single field being treated once per year. On this basis, ISCST3 files include 200 full years of hour-by-hour sequential data. Application start times are randomly selected to match the user-supplied application frequency. For example, if a model user entered 10,000 simulations, there will be approximately 10,000 randomly selected start times with batch modeling treatment of 4 days duration for each application. In addition, FEMS allows for more than one application per year to be

modeled. Does the panel view this as an appropriate process? If not, can it make suggest recommendations or modifications that may improve this process?

Panel Response

If one considers 200 years of hourly data, there were 1,752,000 potential starting points in the output file generated by ISCST3. Each 4-day period consists of 96 hours. Dividing 1,752,000 by 96 yields 18,250 potential non-overlapping study periods. Hence, choosing 10,000 randomly selected start times should not produce too many overlapping study periods. If one chose to do many more start times, one would begin to see a large fraction of repeat study periods, or mostly repeat study periods, and the resulting distributions might not be truly representative of the population to be described.

E) Can the panel comment on the source geometry used in FEMS and the implications of this choice?

Panel Response

The Panel concluded that the capability to model different field shapes is a useful and appropriate function of the modeling system as it presents a more realistic representation of the physical configurations of actual fields. It was suggested that the geometry and orientation of the treated fields be included in future sensitivity analyses and that the geometry of the sources be more general to include other shapes apart from just rectangles or squares. In addition, it was suggested that the directional orientation be allowed to vary from primary north-south configurations.

<u>Critical Element 3: Results</u>

Question 6: Soil fumigants can be used in different regions of the country under different conditions and they can be applied with a variety of equipment.

A) Does the SAP believe that the methodologies in FEMS can be applied generically in order to assess a wide variety of fumigant uses?

Panel Response

FEMS' basic methodology and mechanics appear to be applicable to use with other fumigants and other geographic regions. But because the physicochemical properties, including volatility, water solubility, Henry's constant, degradation rates in soil and air, can vary considerably between fumigants, FEMS should incorporate air and soil degradation processes as standard features in addition to the volatility/downwind dispersion characteristics which have received primary consideration in the development of FEMS. To the extent that a chemical breaks down (chemical and biological) in soil, it is less available to the air. Likewise, the extent that a chemical breaks down in air (chemical and photochemical), or is deposited from the air to downwind vegetation and soil surfaces, it is less available for transport to downwind receptors.

The FEMS model was developed for MITC, which is a moderately volatile fumigant. A high volatile fumigant such as methyl bromide can be used to test the applicability of FEMS to other fumigants. Therefore, FEMS can be further proven to have generic applicability to other fumigants (the California DPR model was developed mainly for methyl bromide).

Enhanced degradation rates for MITC in soil should be considered to be a parameter. If the half-life for MITC were shortened to 1 day or 2 days, the system would be automatically triggered to include degradation rates for estimation of buffer zones. The Panel encouraged the model developers to develop models for input flux rates that incorporate degradation and other factors described above.

Regions of the country will also vary considerably in such features as terrain, cropping systems and cultural practices, 'obstructions' (foliage cover, trees as windbreaks, forests, hills, valleys, mountains, etc). FEMS will need to accommodate such locale-specific features to the extent possible. More attention needs to be given to field shape, and the probability that irregular shapes (e.g., center pivot irrigated fields may be circular) may exist due to an irrigation system or terrain requirements.

Regions will also vary in weather, soil type, soil microbial activity, air quality, and typical or frequent field geometry deviations. It will be important for FEMS to be 'calibrated' to different growing regions and cropping situations with field experiments. Such experiments should include: determination of flux by both back calculation and one or more alternative methods, and validation of sampling tools for use in air with differing humidity and temperature and particulate loads. An adsorption tube sampling method might be particularly sensitive to such features as humidity.

FEMS appears to be a very flexible model but five years of regional or local weather data and real regional emissions data are needed to give a reasonable estimate of concentration exceedances and buffer zones. The limitation seems to be developing real, replicated data sets of accurate emissions measurements. These data should be developed in the region or locale where the fumigant application is to be regulated, under local conditions that are typical of those that occur during fumigation. One Panel member questioned the appropriateness of moving the model from one location to another. It is likely appropriate to move the model provided that the data that is input into the model is appropriate for the location, climatic conditions, etc. If the model handles the data appropriately, this should be acceptable. Only validation runs conducted at different locations, times, data sets, etc., will determine this.

Regions will also vary in climate variables that might directly affect the volatilization and downwind dispersion behavior of MITC. These include the frequency and duration of rain, which can act to wash out residues from the air, as well as affect the rate of volatilization. In addition, the frequency and duration of fog that can act to move MITC from the vapor phase to the condensed phase in air can affect both the dispersion characteristics and the manner in which individual down-winders might be exposed. Fog is an important consideration in coastal regions, the California central valley in winter, and in other parts of the country for certain regions and times of the year. People who are outdoors during fog and downwind from use of metam sodium may be exposed to MITC as aerosols rather than vapor, and possibly by dermal as well as inhalation routes.

FEMS documentation included indoor versus outdoor air concentrations downwind. However, it is not clear how that can be modeled since it varies so much from structure to structure and personal preferences (air conditioned homes versus those that rely on open windows in the summer, etc.). This is an area where more experimental data should be collected before applicability can be assessed.

FEMS allows for multiple field applications via custom runs. This may be more important in some regions of the country than others, particularly with differing farm and field sizes and frequency of fumigant use. The Panel suggested that the developers of FEMS consider making this a standard feature rather than a custom use and at some future time that it is validated with field data. The Panel also suggested the Agency review research by Honaganahalli and Seiber (2000) for an example of this approach.

The Panel gained an appreciation for modeling of this type and the information that can be obtained. There was general support to continue the research into methods of incorporation of uncertainty into a model of this type. There was some suggestion that this work (FEMS model development) be coordinated with that of other groups working with the ISCST3 and AERMOD code who are also looking into the issue of uncertainty in model inputs.

There was interest among the Panel as to how the FEMS model (and the other similar models being considered for fumigant modeling) are going to be used and how they might be used in the near term for the six fumigants the Agency is currently considering for registration.

The Panel recommended that some emphasis be placed on developing methods for validating these models. In addition, there was some discussion of the potential for using these models to develop and assess best management practice for agricultural fumigants.

Finally, the Panel asked the Agency about the anticipated role of the AERMOD code and its potential for use in FEMS and other soil fumigant assessment models. The Agency indicated that the expectation is that the ISCST3 model will be used in the near term, at least for the next six months.

B) What considerations with regard to data needs and model inputs should be considered for such an effort?

Panel Response

The Panel identified several data needs. Guidance should be given as to inappropriate use of the model. Information should be provided with potential methods for reducing emissions. High-density polyethylene film for example is highly permeable to MITC. Surface water on the field during the day may affect local meteorology, e.g., changes in atmospheric conditions from unstable to stable over the field. Water condensing on the underside of a tarp does not appear to have an effect on retaining MITC in soil, so is likely not a factor.

Question 7:

A) Does FEMS adequately identify and quantify airborne concentrations of soil fumigants that have migrated from treated fields to sensitive receptors?

Panel Response

FEMS has the capability of (1) estimating emissions from field data, (2) using ISCST3 to account for dispersion under a realistic range of meteorology, (3) post-processing with TOXST to account for the batch nature of the fumigant application, and (4) probabilistic treatment of model inputs. This overall approach is valid, and therefore, FEMS can identify and estimate airborne concentrations of soil fumigants from treated fields. Specific sensitive receptors (i.e., day care centers, nursing homes, schools, hospitals, etc.) were not discussed in the report or presentation. However, once these are identified, FEMS should have the capability to identify and quantify the airborne concentrations of fumigants that have migrated from treated fields to these sensitive receptors. One possible method is to run FEMS for the delineation of a "buffer zone" for MITC dispersion to these sensitive receptors.

It appears true that FEMS can identify and quantify off-site airborne concentrations of soil fumigants, but it is not clear how accurate the concentration predictions are and how efficient the program is. Results are presented but not discussed. One Panel member commented that if the FEMS model has real data from sensors in the fields or out from the fields at appropriate locations downwind, it could identify and quantify the airborne concentrations. However, it is doubtful that the quantification of airborne concentrations would have any meaning apart from the input of fairly accurate field measurements.

The FEMS model did show reasonable comparison between predicted emission fluxes and measured concentrations with an r^2 value of 0.65 (Fig. 19 in the report for chemigation application) and an $r^2=0.53$ (Fig. 24 in report for the shank injection). The FEMS model also showed strong dependence of airborne concentrations with wind speed (Fig. 20). However, this may be a result of the "calm" option being used in the ISC simulations.

The difficulty for the Panel to provide a definitive answer to this question is related to the lack of independent validation for the FEMS model. Independent modeling or field studies would help determine the adequacy of the FEMS model for identifying and quantifying the airborne concentrations. One is not supposed to calibrate the model but to validate the model using soils models for emission predictions or direct field measurements. As FEMS goes forward, it would be good to validate the model to increase its confidence among potential users.

B) The Agency is particularly concerned about air concentrations in the upper ends of the distribution. Are these results presented in a clear and concise manner that would allow for appropriate characterization of exposures that could occur at such levels?

Panel Response

The FEMS model incorporates uncertainty (i.e., bounds and distribution types) by using values published in the literature and determined via expert elicitation. This approach is reasonable given the lack of empirical data. However, the manner in which the uncertainty should be applied is neither straightforward nor obvious. The developers applied uncertainty to each of the hourly values of selected meteorological parameters to produce 40 versions of a 5-year dataset. What is missing in the present model layout is that the 40 datasets are treated randomly to characterize the distribution of hourly meteorological input. One way to address the upper end uncertainty is to produce some extremes in the hourly meteorological values that were not present in the original records. However, statistically they cannot be excluded as possible realizations in the environment during the 5-year record. When processed through ISCST3 and TOXST, hourly concentration extremes may possibly be encountered (i.e., sampled) via the random selection period for fumigant application. In the case study, this was 96-hour blocks of time. If only 1-hr health endpoints are of risk management concern, this approach for applying uncertainty is fully defensible since it produces extremes in 1-hr concentrations (to the extent that they occur through both temporal variability and uncertainty). If other time-averaged health endpoints are of risk management concern, this approach may not be adequate.

To elaborate more on temporal averaging, questions that have yet to be resolved are on the duration of exposure and toxicology studies. Acute versus repeated exposures should be considered of equal importance, especially for shorter intervals such as minutes to hours and longer than 24-hour exposures. Individual hourly extremes in meteorological values may not have any significant influence on the upper end of downwind concentrations for an annual-average time scale. More likely, signals in the meteorological records, like persistence in wind direction and preferential wind direction for low wind speeds, would have a significant influence. By perturbing each hour within the allowed uncertainty bounds, these signals are not being tested (i.e. strengthened) as distinct and real signals for their influence on the upper end concentrations. In fact, the original signals in the original records are probably weakened to some unknown extent due to the Monte Carlo technique for incorporating uncertainty.

Analysis of the base case, using the original unperturbed meteorological files may reveal which signal is most important (i.e., directional preference for low wind speeds, etc.) and then an alternative approach to incorporate uncertainty could be developed for the signal of interest. The same concepts would apply for any averaging time greater than 1 hour (though the influence may diminish with smaller averaging times). Thus it appears that the method of incorporating uncertainty, and incorporating uncertainty as a concept, is more complex than the developers envisioned or were prepared to allow for. In addition, as explained previously, such methods were likely dependent on the averaging time relevant to the health data of interest.

The model developers reported a case study in a so-called ”worst case” situation where the field experiment was conducted at Bakersfield, California. That particular locale represents one of the extreme cases that favor fumigant emissions and off-site transport. A related, but interwoven, matter is processing of calm conditions. By setting all calms to 1 m/s wind speed and by assigning a direction that is the most frequent to occur for low wind speeds, one is likely doing what is outlined above (i.e., strengthening the signal that very likely is driving the upper end concentrations). In that regard, the claim on capturing the upper bounds is appropriate, but how this may be transferred to other locales remains debatable, and this may not necessarily be the worst case for other areas. Until several experiments have been conducted, this remains to be proven.

While 5-year temporal variability was captured in FEMS, the other concern the Panel had was geographical variations in climate (i.e. local, regional, or national meteorological variability), and to keep separate variability and uncertainty.. Uncertainty is introduced on an hourly basis during the simulation. Is it only the hourly extremes that drive the exposure standard? The uncertainty is based on the NWS stations. Thus, if other data (FAWN) is to be used, further uncertainty analysis is needed. Uncertainties at low wind speed should be considered because low wind speed is also important.

Another Panel member commented on the transferability of results from locales within a given terrain to other locales where there are marked terrain differences. In the case of an inversion condition plus elevation variability, density driven flow (where the dispersion model breaks down) may occur on the land surface. FEMS would not be able to address this issue at the present time.

Several Panel members discussed the variability in sampling and measurement of emission fluxes as it relates to detecting the "true" peak fluxes that would produce upper bound concentrations. A short sampling duration would increase the probability of capturing the maximum concentrations or upper bounds. There is uncertainty with all measurement methods that have to be kept in mind. One Panel member showed field validation/comparison results with error bars associated to each data point at very high intervals (30 -100%). Such a relationship was also high for the aerodynamic method (Majewski 1996). The accuracy of the back-calculated emission flux estimates is on the order of 40-50% according to EPA reports. However, no references were provided. Thus, all the verification/ validation/comparison methods seem to have similar uncertainties associated with each other.

Another Panel member indicated that in a bedded system, most emission losses were found from the center of the field beds and an insignificant amount from the shoulders of the beds. Emission measurement with flux chambers in Florida experiments showed that much of the emission came from the center of the field where the fumigant was applied. The FEMS model assumes homogenous sources and does not separate the rows from the beds. Thus, this could have an impact on the estimated emission flux.

Finally, the Panel raised concern about measurement accuracy during transition times, particularly at sundown or sunrise in desert areas when there are rapid temperature changes. The Panel concluded this is probably more of a sampling problem than a problem with FEMS.

Question 8: A sensitivity analysis has been conducted and is described in the FEMS background document.

A) What types, if any, of additional contribution/sensitivity analyses are recommended by the panel to be the most useful in making scientifically sound, regulatory decisions?

Panel Response

Efforts have been taken to produce highly realistic emission meteorological inputs in an effort to better simulate uncertainty and to provide reasonable and robust assessments. Even so, the model developers recognized that there will always be sources of uncertainty in a FEMS analysis.

The report included an appropriate discussion of the sensitivity of various input parameters. A correlation matrix between model inputs was developed. In general, a low correlation was observed between input parameters with the exception of a high correlation between emission and concentration, as was expected. In addition, graphics were presented showing the correlation/uncertainty (i.e., scatter) between the input variables.

Large uncertainties can often be found in the estimated emission fluxes. The Panel suggested comparisons of estimated fluxes with predictions using soils-based transport models (such as CHAIN_2D) that deterministically compute, in a forward fashion, emission fluxes using mainly soils (and dosage) information. These transport models can also be run simultaneously with a parameter generator in a stochastic fashion, thus providing an assessment of uncertainties in the output such as the emission fluxes.

B) What should be routinely reported as part of a FEMS assessment with respect to inputs and outputs?

Panel Response

The sensitivity analysis did not include any quantitative measure of the change of the output variable with change of the input variable. This type of information would be valuable to users of FEMS so that more emphasis is placed on the important input parameters. Conducting a numerical sensitivity analysis was recommended. Also, the Panel questioned how sensitive the results are to down-wind distance. The results should be presented to show the set of parameters that will most affect the buffer zone, i.e., causing the largest or shortest buffer zone distances.

C) Are there certain tables and graphs that should be reported?

Panel Response

In general, the scatter plots of input parameter versus concentration showed more-or-less expected behavior: (a) correlation and some scatter with emission, (b) little correlation and higher scatter at low wind speed, (c) little correlation with wind direction, and (d) a higher scatter of certain stability classes. These examples are specific to the studies described in the Agency's background document.

A detailed analysis was provided showing how the buffer zone is affected by stochastic treatment of input parameters. Several cases were provided ranging from one stochastic input variable to all variables treated as stochastic. These runs were compared to the cases where none of the input parameters vary (i.e., the benchmark). These analyses are useful and produce results that appear correct.

D) What types of further evaluation steps does the panel recommend for FEMS?

Panel Response

No information was given to the accuracy, reliability or suitability of using the expert elicitation survey (Hanna, et al., 1998) to produce probability distributions that represent the variability in ambient meteorological conditions. If Hanna et al. (1998) reported this information; some mention should be made in the technical document.

In addition, no information was provided on the uncertainty that results from using FEMS in a predictive mode, that is, at locations where there are no on-site flux or meteorological measurements. This could be done if data sets are available for similar fumigation systems at other locations. The emission data at one site could be used to predict buffer zones at the other site, and then compared to the actual measured air concentration data. The experiments include samples at distances appropriate to test buffer zone predictions. Also, jackknifing could be employed as a way to test the model's ability to provide protective buffer zones, although this would not be as comprehensive a test as using an independent data set.

There is a need to investigate the mass lost over the 4-day period based on 2.5%, 50% and 97.5% sampling of the probability distribution. At the high level, the total mass loss should be less than 100%. If greater, the probability distribution should be changed to limit mass loss to 100% (an unreasonably high number). In the current formulation, the probability distribution only represents variability due to single-site measuring/modeling errors. It is unlikely that the cumulative flux error would be 3-4 times of the measured cumulative flux (i.e., if the mean flux is 20%, it would be unlikely that uncertainty would result in cumulative flux values of 80%). A value of 10-30% would be more likely. A range of 4-day cumulative emissions ranging from 10-80% may be appropriate for a suite of studies conducted in the same region and climatic conditions, but at different locations and times. Williams et al. (1999), Wang et al. (1997) and Yagi et al. (1993, 1995), Yates et al. 1996a, b, c) observed methyl bromide cumulative fluxes from 25-75% at several locations in Southern California.

A sensitivity analysis should be conducted to determine what happens when low values (i.e. ~2.5%) or high values (i.e. ~97.5%) of the probability distribution are repeatedly sampled.

A sensitivity analysis of the weather data would be helpful to ensure that there are no systematic deviations causing a bias in the buffer zone calculation. There is a need to test whether the natural patterns and persistence in the measurements are retained for the perturbed data.

More graphs of measured and modeled concentration versus distance would be helpful. It would be especially helpful if measured and modeled results could be plotted on a single graph.

The Panel questioned why the <50 meters downwind data were not used. It would be helpful to show this data. Also, even though distances greater than 100 meters are generally used in Gaussian plume models (as a rule-of-thumb), shorter distances will probably yield reasonable results since the rule-of-thumb applies to point sources. The upwind edge of the field would generally be much greater than 100 meters.

Finally, it was not surprising that the results are most sensitive to the input emission rate. Without emission, there will be no buffer zone and no toxicological exposure.

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