UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES, AND
TOXIC SUBSTANCES

November 12, 2004

MEMORANDUM

SUBJECT: Transmittal of Meeting Minutes of the FIFRA Scientific Advisory Panel Meeting Held September 9 - 10, 2004

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

FROM: Joseph E. Bailey, Designated Federal Official /s/
FIFRA Scientific Advisory Panel
Office of Science Coordination and Policy

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

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

Attached, please find the meeting minutes of the FIFRA Scientific Advisory Panel open meeting held in Arlington, Virginia on September 9 - 10, 2004. This report addresses a set of scientific issues being considered by the Environmental Protection Agency pertaining to the SOil Fumigant Exposure Assessment System (SOFEA) using Telone as a case study.

Attachment

cc:

Susan Hazen
Margaret Schneider
Anne Lindsay
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Debbie Edwards
Steven Bradbury
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Tina Levine
Lois Rossi
Frank Sanders
Randolph Perfetti
George Herndon
William Jordan
Douglas Parsons
Enesta Jones
Vanessa Vu (SAB)
Jeffrey Dawson
Michael Metzger
OPP Docket
Bruce Houtman, Dow AgroSciences

FIFRA Scientific Advisory Panel Members

Stephen M. Roberts, Ph.D. (FIFRA SAP Chair)
Steven G. Heeringa, Ph.D. (FIFRA SAP Session Chair)
Stuart Handwerger, M.D.

FQPA Science Review Board Members

S. Pal Arya, Ph.D.
Paul W. Bartlett, M.A.
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SAP Report No. 2004-08

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

Fumigant Bystander Exposure Model Review: SOil Fumigant Exposure Assessment System (SOFEA©) Using Telone as a Case Study

September 9 – 10, 2004
FIFRA Scientific Advisory Panel Meeting
held at the Holiday Inn National Airport
Arlington, Virginia

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 of 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 a 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 parties are invited to contact Joseph E. Bailey, Designated Federal Official, via e-mail at bailey.joseph@epa.gov.

In preparing these meeting minutes, the Panel carefully considered all information provided and presented by the Agency and Dow AgroSciences, LLC, 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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Arlington, VA

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

Fumigant Bystander Exposure Model Review: SOil Fumigant Exposure Assessment System (SOFEA©) Using Telone as a Case Study

Mr. Joseph E. Bailey
Designated Federal Official
FIFRA Scientific Advisory Panel
Date:

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

Federal Insecticide, Fungicide and Rodenticide Act
Scientific Advisory Panel Meeting
September 9 – 10, 2004

Fumigant Bystander Exposure Model Review: SOil Fumigant Exposure Assessment System (SOFEA©) Using Telone as a Case Study

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INTRODUCTION

On August 24-25, 2004, August 26-27, 2004 and September 9-10, 2004, the Federal Insecticide, Fungicide and Rodenticide Act Scientific Advisory Panel (FIFRA SAP) held three separate meetings to consider and review three fumigant bystander exposure models. These meeting minutes focus on the FIFRA SAP meeting held September 9-10, 2004 to review the SOil Fumigant Exposure Assessment System (SOFEA©) using Telone as a case study. The FIFRA SAP also 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 August 26-27, 2004 to review the Fumigant Exposure Modeling System (FEMS) using metam sodium as a case study. Minutes from each of these 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 September 9-10, 2004 meeting was published in the *Federal Register* on July 23, 2004. The review was conducted in an open Panel meeting held in Arlington, Virginia and was chaired by Steven G. Heeringa, Ph.D. Mr. Joseph E. Bailey served as the Designated Federal Official. Mr. Joseph J. Merenda, Jr. (Director, Office of Science Coordination and Policy) and Randolph Perfetti, Ph.D. (Associate Director, Health Effects Division, Office of Pesticide Programs) offered opening remarks at the meeting. Mr. Jeffrey Dawson (Health Effects Division, Office of Pesticide Programs) provided an introduction and highlighted the goals and objectives of the meeting. Bruce Johnson, Ph.D. (California Department of Pesticide Regulation) participated with the EPA in this meeting. Steven A. Cryer, Ph.D. (Dow AgroSciences, LLC) provided a detailed description of SOFEA© with additional clarifying comments being provided by Ian van Wesenbeeck, Ph.D. and Bruce A. Houtman, CIH, also with Dow AgroSciences, LLC.

EPA's Office of Pesticide Programs is engaged in pesticide tolerance reassessment activities as mandated by the Food Quality Protection Act (1996). As part of that process, the Agency is currently involved in the development of a comparative risk assessment for six soil fumigant pesticides that include chloropicrin, dazomet, iodomethane, methyl bromide, metam-sodium, and telone. Each of these chemicals has a degree of volatility associated with it which is a key characteristic needed to achieve a satisfactory measure of efficacy. This volatility, however, can contribute to human exposures because these chemicals can travel to non-target receptors, such as nearby human populations. Commonly referred to as bystander exposure, it is considered by the Agency to be the primary pathway through which human exposure to fumigants may occur.

In order to address bystander exposures, the Agency developed a method based on a deterministic use of the Office of Air model entitled Industrial Source Complex Short-Term Model (ISCST3) that is routinely used for regulatory decisions. ISCST3 is publicly available from the following Agency website:

http://www.epa.gov/scram001/tt22.htm#isc. In this approach, the Agency uses chemical-specific measures of volatility to quantify field emission rates for modeling purposes. Additionally, the Agency uses standardized meteorological conditions which represent a stable atmosphere and unidirectional wind patterns that provide conservative estimates of exposure.

Stakeholders expressed concern that the conditions represented by the current approach provide results that are not sufficiently refined for regulatory actions such as risk mitigation. In response, Dow AgroSciences, LLC, the registrant for Telone (Note: Telone, or 1,3-dichloropropene, will be referred to as 1,3-D throughout this report), has submitted the SOFEA© model for consideration as a possible refinement to the Agency's approach. The Agency believes that this model also may have the potential to be used generically to calculate exposures for the six soil fumigants being evaluated in the current risk assessment. The key differences between SOFEA© and the current Agency approach are that it calculates fumigant concentrations in air arising from volatility losses from treated fields for entire agricultural regions using multiple transient source terms (e.g., different treated fields), GIS information, agronomic specific variables, user specified buffer zones and field re-entry intervals. A modified version of the ISCST3 is used for air dispersion calculations.

The purpose of this FIFRA SAP meeting was to evaluate the approaches contained in SOFEA© for integrating these different factors into an analysis that considers exposures on a regional level. Additionally, the Agency sought a specific evaluation of the methods used pertaining to field emission rates, statistical approaches for data analysis, receptor locations, modifications to ISCST3, and defining the exposed populations. Finally, the Agency sought a determination as to the scientific validity of the overall approach included in SOFEA©.

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 at the meeting, especially the Panel's response to the Agency charge.

PUBLIC COMMENTERS

No oral statements were made during the meeting.

Written statements were received from:

California Rural Legal Assistance Foundation and Farmworker Justice Fund.

SUMMARY OF PANEL DISCUSSION AND RECOMMENDATIONS

The SOFEA© bystander exposure model uses Excel for the user interface and requires installation of a proprietary Excel-based software package, Crystal Ball, to operate correctly and conduct the Monte Carlo analysis. The model also incorporates the U.S. EPA air dispersion model the Industrial Source Complex Short-Term Model (ISCST3). The Panel indicated that since tables of data are produced using macros in the Excel framework, graphical output would also be helpful. Although the Panel thought that the SOFEA© User's and Installation Guides are generally clear and unambiguous and the Programmer's Guide helpful to modify SOFEA©, they agreed that the documents would benefit from careful editing, some reorganization, and a more comprehensive review of the literature. A flow diagram and execution schematic that shows linkages and branching, and that identifies key computational procedures would be helpful.

Regarding specific model components, the Panel identified the following issues: 1) Excel spreadsheet cells that the user should not alter should be locked; 2) no information is given on ISCST3 or Crystal Ball; 3) the fumigant flux is modeled crudely with scaling factors, some of which may be difficult to obtain; 4) tarps and other control technologies are important for limiting emissions especially for surface applications and their effects should be considered; and 5) a more physically meaningful method of accounting for temporal differences is needed.

With regard to the algorithms, the Panel indicated that SOFEA© appears to generally perform the functions in an appropriate manner; however, an itemized list of modifications to ISCST3 was recommended. The Panel also indicated that potential performance issues include the fact that Crystal Ball is not supported on Windows 95 or Excel 95 and that there may be incompatibility problems using SOFEA© for future editions of Windows, Excel, Visual Basic, or Crystal Ball.

Panel members were generally able to successfully install and run SOFEA©, but noted that Crystal Ball is an expensive program required to successfully use SOFEA©. Although the program ran successfully for most Panel members, some had difficulties due to unexplained error messages. Overall, initial evaluation of SOFEA© by some Panel members was found to be more difficult due to the use of Excel as the user interface. After some experience with SOFEA©, the Panel concluded that the advantages of Excel seemed to outweigh the disadvantages.

Panel members concurred that the choice of ISCST3 as the dispersion model in SOFEA© posed some problems related to the weakness of ISCST3 to provide accurate estimates of chronic and acute exposures in comparison with other dispersion models. The Panel noted that SOFEA©'s methodology seems unable to relate townships to airsheds, two distinctly different simulation domains. Furthermore, the airshed for some chemicals may be larger than the largest region considered by SOFEA©. The use of the term airshed implies that all significant source areas have been included and this is not necessarily the case with SOFEA©.

The Panel reported that the receptor grids used for acute exposures seem to be adequate. However, for chronic exposures the uniform grid assumed to be used in SOFEA© is likely to underpredict exposures because of characteristics of the ISCST3 model. In the development of receptor grids for chronic exposure estimates, additional receptors close to treated fields should also be considered. The Panel noted that no sensitivity study of the grid density seems to have been made.

The aerodynamic gradient approach was the field method chosen to estimate the volatilization flux of 1,3-dichloropropene (1,3-D) and the Panel believed that it is probably one of the best methods for determining volatilization fluxes of pesticides from treated fields. However, the Panel identified a few limitations and drawbacks. Since meteorological input to SOFEA© is provided on an hourly basis, the Panel recommended that emission flux should also be based on hourly sampled concentrations. Several Panel members expressed concerns about the low fluxes determined during periods of stable meteorology at night. The Panel noted that the aerodynamic approach for flux calculations would benefit from the use of improved, as well as additional instrumentation. Several Panel members reiterated the importance of making concentration measurements with faster response instruments in flux studies and in comparisons between modeled and predicted concentrations, allowing for a more accurate representation of bystander exposure.

Regarding the probabilistic scaling of fluxes, SOFEA© treats the rate of application of 1,3-D as a stochastic variable. The Panel indicated this to be an unreasonable choice because the rate of application is a quantity about which there is the most certainty. Also, the Panel concurred that the probabilistic varied flux rate for each application based on variability in field flux measurements is useful and should be retained in the model; however, a joint probability distribution is needed for period flux rates and meteorological conditions. The depth-of-injection scale factor needs to include soil degradation of the applied fumigant. One Panel member noted that how soil structure (physics) influences diffusive and/or advective flux is the main factor which influences surface flux relative to injection depth. The capability to include probabilistic flux inputs is valuable in assessing the overall sensitivity of the model to the various parameters. Since field measurements are difficult and expensive, this capability would allow the investigation of various scenarios of field uncertainty, thus giving a more realistic range of the flux and emission estimates.

The Panel agreed that using a flux/emission factor based on a single monitoring study or a few studies is questionable. One Panel member emphasized the importance of considering whether a single flux profile is appropriately conservative or not. The emission flux behavior should be investigated for different soils and soil moisture conditions that might exist in different regions. In addition, considering the variability of emission fluxes, a stability index or parameter would be a more appropriate parameter to use than air temperature. Volatilization fluxes depend on wind speed and turbulence whose effects may be parameterized through a stability index. The use of scaling factors may be reasonable when cumulative fluxes are being considered, but they are not appropriate when acute, period fluxes and associated hourly downwind air concentrations must be estimated. The use of appropriate scaling factors seems to be based on the user’s judgment, but it would be more appropriate if a mechanistic approach was used to develop them for the various field conditions expected to be encountered. As in most measurements and modeling applications, the question of how representative the data are of the proposed application is critical to whether the results are valid.

The Panel commended the developers of the SOFEA© model for attempting to consider multiple, linked application events in the model's design. However, its reliance on the ISCST3 model for description of atmospheric dispersion limits the accuracy of the multiple-source simulation. The capability of considering multiple sources is very important, particularly when predicting chronic exposures. More detailed land use data may also improve the model's capabilities.

The Panel noted that SOFEA©'s documentation does not discuss the model's ability to address missing data. It is implicit that all the inputs are required; otherwise, the model will not run. In that sense, it forces the user to ascertain whether the input is complete. The Panel recommended that future documentation address how SOFEA© deals with missing data, particularly the use of PCRAMMET.

The Panel concurred that the addition of hourly-averaged meteorological information and GIS data seems to be a useful part of the methodology implemented in SOFEA©. Such information seems to be a step forward from the present assumption of worst case meteorological conditions over the duration of the release. For acute exposures, using meteorological conditions from a distant meteorological station may not accurately reflect local conditions, especially effects such as drainage flows. For chronic exposures, dispersion modeling must be done over much larger distances. The use of hourly meteorological information from a single monitoring station should not be replicated over large areas (airsheds) because simple replication of the same meteorological data for all sources will ignore terrain features which importantly effect conditions. To increase the reliability of meteorological input to a dispersion model, the Panel suggested incorporating the Atmospheric Data and Parametrization Tool (ADPT) or the Naval Research Laboratory's Coupled Ocean/Atmospheric Mesoscale Prediction Systems (COAMPS).

The Panel recommended the use of quality-assured meteorological data selected from the closest representative site, whether it is a National Weather Service location, state air quality or climatological site, or an industrial monitoring site. At least five years of continuous data were also recommended, but longer periods of data might be necessary when evaluating long-term chronic exposures. If on-site data for a short period are used, it should be compared with the nearest available long term NWS data. The maximum domain extent recommended for use in SOFEA© should be influenced by the dispersion model it incorporates. The ISCST3 assumption of constant hourly-averaged meteorology and flat terrain over the entire ISCST3 domain is questionable for larger model domains such as might be required for modeling an airshed. Approaches to characterize the quality and uncertainty of meteorological data were described by the developers of SOFEA© (e.g., filling in missing data and appropriate data record length for long term exposure assessments), but it was not clear to the Panel that these factors had been fully addressed. The Panel agreed that the use of wind observations at anemometer heights used in some data sources, other than the standard height of 10 m used by ISCST3, should be considered. For SOFEA©'s current use of ISCST3, the Panel believed that stability class inputs were treated appropriately. For a number of reasons, including the coarse receptor grid, the overflow algorithm and treatment of calm conditions, the Panel concurred that SOFEA©, as currently configured, may not yield the highest upper-bound concentration estimates.

The Panel raised questions about the accuracy of the use of the PRZM3 model in SOFEA© to describe 1,3-D flux from soil and thought the CHAIN-2D to be more realistic. They noted an inherent limitation of PRZM3 to be the fact that it produces results based on daily (24-hour) time steps. In general, the Panel thought the methodology for emissions flux estimation in SOFEA© is too simplistic. Meteorological influences on emissions fluxes should be considered, as should soil type and soil moisture and emission flux estimates should be based on more highly resolved temporal measurements (e.g., hourly). In addition, the time of application should be considered as a factor. Flux estimates might be substantially off if the time of application is much different from that of the field test used to estimate fluxes.

In the ISCST3 model, estimated downwind concentrations are inversely proportional to the windspeed. When the windspeed goes to "zero", the model cannot be used. In addition, its use with low – but non-zero – winds is not recommended. The Panel expressed concern about the use of the SOFEA© model to predict dispersion estimates under calm conditions. Several approaches were offered to deal with SOFEA©'s shortcomings associated with "calm" scenarios and wind reversal patterns. They are: 1) examine existing field measurement data to determine if measurements were made during calm, low-wind, or recirculating conditions; 2) consider abandoning the use of the ISCST3 model as the "engine" driving the dispersion estimates in SOFEA©. (In its place, a more realistic model that does not have as severe limitations under calm, low-wind, and recirculation conditions could be considered such as CALPUFF or other Lagrangian puff models.); and 3) allow the emissions flux during calm hours to build up, so that the emissions in the first hour after a calm period would include that hour's emissions plus all the emissions during the preceding calm period. This would not address the low-wind or recirculation problem and would only partially address the calms problem, but it seems to be better than the present approach.

While there do not appear to be major methodological problems with the successful application of SOFEA© in settings other than California, SOFEA© developers reported on a case study of 1,3-D use in central California in which order-of-magnitude agreement was found between predicted and measured concentrations. The Panel agreed that successful applications of SOFEA© to other areas are hindered by data needed to run the model such as product use data, flux estimate data, and weather and topographical data. One Panel member noted that the development of "scenarios" that use site specific data that are more representative of other regions of the country may be helpful.

The Panel concurred that, in many respects, the SOFEA© model does not adequately identify and quantify airborne concentrations of soil fumigants that have migrated from treated fields to sensitive receptors, particularly estimates of worst case, near field exposures. The Panel recommended the consideration of using the CALPUFF/CALMET models in SOFEA©. Because of the use of ISCST3 in SOFEA©, the Panel stated that acute and chronic exposures may be underestimated. Migration of soil fumigants from treated fields at large distances from sensitive receptors will be necessarily limited to about 50 km. Beyond this distance ISCST3's dispersion coefficients should not be used. Other more appropriate wind flow and dispersion models might be used if long-term exposures from distant fields are of interest.

According to the Panel's assessment, SOFEA© model results were clearly presented; however, concentrations in the upper ends of the distribution may be underestimated for chronic exposures at long distances, under calm and low windspeed conditions, and with multiple source scenarios. The ability of SOFEA© to predict worst-case concentrations is likely to be progressively worse for longer distances and exposure durations. Continuous meteorological data over the longest period of exposure may be necessary to get concentrations in the upper ends of the distribution. No information was found in the SOFEA© documentation about the methodology used to calculate probability distributions using moving average concentrations for differing durations of exposure. This descriptive documentation should be included.

Ideally, atmospheric dispersion models, such as SOFEA© with ISCST3, should be evaluated by comparing model predictions for a particular time period at specific locations with measurements made at the same locations during the same time periods. In carrying out such an evaluation, it would be important to utilize the meteorological and emissions data for the same period. The Panel recommended that this type of model evaluation be carried out for SOFEA©. At higher percentiles, SOFEA© underpredicts monitoring measurements. These results show that further refinement of the model is necessary to correct the upper end of air concentration distribution estimates and to determine why this underprediction is occurring.

The Panel suggested several specific factors to include in the sensitivity analysis of SOFEA©: background (ambient air) concentrations, terrain, location (inland versus costal), and crop type. Model inputs that affect fumigant dispersion and degradation need to be included in the analysis such as soil temperature, weather stability, and soil degradation of the applied fumigant. Atmospheric degradation factors should also be considered as they affect the maximum volatilization and maximum losses through emission into the atmosphere.

Because SOFEA© will potentially be used for both acute and chronic exposure assessment, the Panel recommended an evaluation of the uncertainty in both periodic and cumulative emissions. Some Panelists believed that uncertainty would be higher for periodic emissions than for cumulative. There was strong agreement for the requirement of meteorological record longer than the five-year CIMIS record to ensure that some "worst case" scenarios would figure in the sensitivity analysis.

There was general agreement among the Panel members that the inputs required should include the fumigant applied, application rate, type of application, application depth, tarp use or none, field size (or numbers of fumigated fields for regional analysis), soil conditions that will affect fumigant dispersion in the soil and subsequently into the atmosphere, and weather parameters that affect stability. The outputs should include flux rates, fumigant concentrations at buffer perimeters relative to toxicity concentrations, exceedance frequency, distance from the source at which exceedances occur, maximum daily emission, and losses over time through emission into the atmosphere.

The Panel noted that SOFEA©, like any other model at this stage of development, will need a line-by-line code audit by an independent programmer to ensure that the code does what it is supposed to do. Documentation and testing of the random number generator in Crystal Ball is needed, and if it proves to be deficient, a better random number generator must be used.

The Panel was concerned that "calms" could be very important and had not been adequately incorporated into the model. Perhaps the ISCST3 model is not conservative enough in this regard. It is a limitation of ISCST3 that no stability categories are applicable for nighttime calm and near calm conditions.

The Panel recommends running a series of simulations to determine whether the shape of fumigant flux profiles impact acute or chronic exposure estimates generated by the model. Profiles can be developed from published or unpublished studies or they could be simulated. Simulations should be run under a variety of worst-case conditions to determine the extent to which "extreme" conditions (high or low temperature, wind, stability etc.) may influence results.

Because of the wide range of expertise on the Panel, there were many suggestions for enhancing the model, and some of these may make a significant difference in model output under some scenarios. In summary, the Panel recommended incorporating those proposed enhancements that look most promising and doing more validations (or pseudo-validations) in comparison to field data, looking particularly for agreement in upper percentiles and under both typical and extreme scenarios.

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.

Agency Charge

Critical Element 1: Documentation

Question 1: The background information presented to the SAP Panel by the* SOFEA© *developers provides both user guidance, a technical overview of the system, and a series of case studies.

(1A) Please comment on the detail and clarity of these documents.

Panel Response

SOFEA© uses Excel for the user interface. The spreadsheet contains 17 worksheets for input and output. A proprietary Excel-based software package, Crystal Ball, is used to conduct the Monte Carlo analysis. This program must be installed before SOFEA© will operate correctly. The model also incorporates the U.S. EPA air dispersion model the Industrial Source Complex Short-Term Model (ISCST3). One worksheet is used to define the input probability density functions (PDFs) and other model parameters, several worksheets are used to include spatial and temporal information, and four worksheets provide the primary output. Optional Geographical Information System (GIS) input of crop cover, elevation, and population is available in SOFEA©. None of the output is presented graphically. Since tables of data are produced using macros in the Excel framework, graphical output should be able to be automatically generated and would be helpful for interpretation and quality assessment of the model predictions.

Regarding the documentation, the SOFEA© User's and Installation Guides were generally clear and unambiguous. A Programmer's Guide was included that would help a user modify SOFEA© (even though such changes might complicate model standardization). The documents would benefit from careful editing, some reorganization, and a more comprehensive review of the literature. The oral presentation to the Panel provided additional explanation that would be useful to include in the written documentation.

In the SOFEA© User's Guide, it can be difficult to identify information on certain topics (e.g. PDFs that describe agronomic practices). There were also many incorrect citations (e.g., all appendices) and in some cases failure to properly support statements such as “Research has shown”. A flow diagram and execution schematic that shows linkages and branching, and that identifies key computational procedures would be very helpful.

Stylistically, the User’s Guide is a blend of a “user’s manual” and a “case study”. Users who are not familiar with California regulatory programs could be confused by references to terms such as the “maximum total mass that can be applied to a township”, which is unique to California. “Side-bar” discussions on this and other topics (e.g. buffers) could help avoid confusion. A number of other issues identified by the Panel are as follows:

- There is no information in the User’s Guide for the ‘Forecast Worksheet’. Space appears to be available for text, so maybe this was a printing error. Also, #REF was found in the spreadsheet indicating an addressing error.
- Comment fields are used to help describe the cellular data, for example a PDF cell. It is not clear if Crystal Ball or the authors of SOFEA© generated the comment statements in the spreadsheet.
- For the Town_Mass_Wt worksheet, it seems that more than the township mass could be entered without the user knowing this happened. It is possible to enter data in two locations causing the data to be incorrectly added. Warning messages are given in comment statements, but there should be some form of error checking to make sure this is not allowed.
- There is substantial documentation in the Excel spreadsheet, but since all data are available to the user in the spreadsheet format, it is easy to be overwhelmed while learning SOFEA©. It can be difficult to know where to make changes in the file. Although this may not be a problem for an experienced user, it might be helpful to summarize input and critical output on a single worksheet.
- The section that describes how fields are handled during overflow conditions is somewhat confusing. Rewriting this section would be helpful.
- A brief description should be provided on how Crystal Ball is used in Excel (i.e., the basic manipulations required to incorporate Crystal Ball into Excel). This should include some information about how to create a PDF cell, how to change the Monte Carlo parameters, and guidance on assigning probability distribution parameters.

One Panel member found that the Programmer’s Guide contained much useful information that was not necessarily related to programming. For example, the flow diagram in Figure 5 (page 15) helped explain the flux calculations. It is recommended that much of the information contained in the first section of the Programmer’s Guide be included in the User’s Guide. Also regarding the Programmer’s Guide, Figure 11 on page 22 of the guide is confusing because it is not clear how the three tables denoted by a), b) and c) that contain numerical figures relate to the three graphs below the tables.

(1B) Are the descriptions of the specific model components accurate?

Panel Response

With regard to the descriptions of the specific model components, the following data integrity issues were identified:

- Most (if not all) data cells can presently be changed in the Excel spreadsheet. It might be a good idea to lock all the spreadsheet cells that the user should not alter. For experienced users, a button could be added to unlock selected cells. If input data are deleted or altered without the user's intention, the output could be in error without the user's knowledge. In some worksheets, rudimentary error checking is performed (i.e., calculating sums that should theoretically equal 100%, etc). Further error checking would improve SOFEA©.
- SOFEA© utilizes ISCST3 but no information is given on ISCST3 (which can be obtained from the EPA web site).
- No information or source of information is provided for Crystal Ball. Some Panel members found it easy to change the PDF parameters, but it was not so clear how to use Crystal Ball's more sophisticated features.
- The fumigant flux is modeled crudely with scaling factors reflecting the type and depth of application as well as seasonal effects based on temperature, and scale factors are applied to measured fumigant flux from a particular field study with known application rate. This scale factor would be location and application specific and could be difficult to obtain. The method does not account for the effect of soil degradation of the applied fumigant, which can be important for surface applications using a tarp (especially with virtually impermeable films).
- Tarps are an important control measure for limiting emissions especially for surface applications, but their efficacy is highly dependent on temperature and fumigant used. Using PRZM3, the presence of a tarp was predicted to reduce emissions to 64% of those in the absence of a tarp. For high density polyethylene (HDPE), 1,3-D is highly permeable and for a soil with low degradation (i.e., 0.06 d^{-1}), cumulative emission would be approximately 91% of the applied 1,3-D. Increasing the degradation rate by a factor of 10 (i.e., 0.6 d^{-1}) gives a cumulative emission of 76%.
- Temporal scaling is based on a personal communication with California Department of Pesticide Regulation (CDPR) and utilizes a ratio of summer to winter flux of 1.6. Although one would expect a summer flux to be greater than in the winter, a simple ratio is not likely to be generally correct. A more physically meaningful method of accounting for temporal differences is needed.
- A detailed list of subroutines was provided and would be very helpful if someone wished to modify the program. This list would also be helpful for error checking or debugging.

(1C) Do the algorithms in the annotated code perform the functions as defined in this document?

Panel Response

With regard to the algorithms, SOFEA© appears to generally perform the functions in an appropriate manner. Error messages seen during model execution caused concern about how well the algorithms perform and about potential effects on the results of an assessment (discussed below). An itemized list of modifications to ISCST3 is needed. Also, some demonstration should be provided showing that the core ISCST3 algorithm has not been affected by the modifications. Some potential performance issues include the following:

- Crystal Ball is not supported on Windows 95 or Excel 95, but this should not be a serious problem since this operating system and program are not likely to be used in the future.
- There may be incompatibility problems using SOFEA© for future editions of Windows, Excel, Visual Basic, and Crystal Ball. Any significant change in these programs may cause the system to fail to run successfully.

(1D) Please discuss any difficulties encountered with respect to loading the software and evaluating the system including the presented case study.

Panel Response

Panel members were generally able to successfully install and run SOFEA©. Crystal Ball is an expensive program ($2500 for Professional version) that is required to use SOFEA©. A trial version of Crystal Ball was obtained to test SOFEA©. Many of the buttons in the Excel spreadsheet do not function properly unless Crystal Ball has been installed. Some of these buttons do not appear to have any direct relationship with the Monte Carlo analysis, so the reason for their lack of operation is puzzling. However, the documentation is clear about the required use of Crystal Ball. Problems reported by Panelists included the following:

- During a demonstration simulation of SOFEA©, the "Run Township Simulation" button on the "PDF parameters" page was pressed prior to installation of Crystal Ball. The simulation started and completed in 15 minutes. It is difficult to know what the results represent since the User's Guide states that Crystal Ball is a mandatory requirement for SOFEA©. If this is the case, then SOFEA© should generate an error message and/or not allow execution of the program if Crystal Ball is not actively running.
- One Panel member experienced problems running the program, possibly due to using an older computer. Once installed, Crystal Ball returned three error messages during each loop: "Unable to Complete the Operation Due to an Unexpected Error". The cause of these error messages was never determined. After Crystal Ball was installed, SOFEA© reached 50% completion before total

failure. It seems that the ISCST3 weather file for the current (failed) loop was for 1999, but the input file listed 1996. Trying to run ISCST3 in stand-alone mode produced an error. Editing ISCST3.INP and changing the dates to match would allow ISCST3 to run. However, the error in SOFEA© occurs at a point where restart is not possible (a panel member was not able to change ISCST3.INP, run ISCST3, then get SOFEA© to restart). The problem may be related to the poor performance characteristics of the test computer (i.e., Dell Inspiron 8000, 800 MHz, 256MB). SOFEA© was run to completion by restricting the PDF for YEAR to 1996-1997 (i.e., only allow 1996). This forced all the ISCST3 output files to have the correct information. However, three Crystal Ball error messages were again received and the cause was never determined.

- The program ran correctly for other Panel members.

Initial evaluation of SOFEA© by some Panel members was found to be more difficult due to the use of Excel as the user interface. This is a somewhat unusual approach to create a user interface. While this has many advantages (ease in creating "what if" scenarios, near universal availability, no or low cost (for Excel), everything in one place, programming flexibility, etc.) some are offset by the high cost of Crystal Ball, potential for SOFEA© to be incompatible with Excel, potential to change something inadvertently, and the potential to get "lost" in the pages and pages of numbers. The importance of this latter point could be reduced if the columnar output was captured in some figures. After some experience with SOFEA©, the Excel interface advantages seemed to outweigh the disadvantages. One Panel member did feel that the Excel interface made the program user friendly and facilitated its installation and use, but recommended that a "standalone" version that does not use Crystal Ball be developed. The Panel member indicated that given the limited use of stochastic sampling, a version of SOFEA© that operates on set scenarios may be equally or more effective in developing potential exposure profiles.

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

Question 2: In the background documents, a series of detailed individual processes and components included in* SOFEA© *are presented. The key processes include (1) incorporation of ISCST3 into* SOFEA©*, (2) probabilistic scaling of flux rates; (3) defining source placement within an airshed; (4) development of receptor grids within airsheds; and (5) generation of probability distribution functions based on use patterns and application parameters.

***(2A) Please comment on these proposed processes, the nature of the components included in* SOFEA© *and the data needed to generate an analysis using* SOFEA©.**

<u>Panel Response</u>

The choice of ISCST3 as the dispersion model incorporated in SOFEA© poses some problems as follows:

- For 1,3-D, chronic exposures must be estimated over long distances. Consequently, dispersion estimates must be made over distances that are much greater than are considered appropriate when using ISCST3. There was concern expressed that the original intent of estimating the acute exposure to a bystander is fundamentally a different task from estimating chronic exposure to the public (because of the very different time and length scales for these two problems). Furthermore, the inherent weaknesses of the ISCST3 model when applied to estimating chronic exposures over long distances severely limits the applicability of SOFEA© to the long term health issues surrounding the use of 1,3-D.
- For acute exposure, concentrations must be estimated over near field distances (less than 100 m). Over such short distances, there is some indication that ISCST3 may underpredict concentrations in comparison with other dispersion models. Isakov et al. (2004) report that ISCST3 may substantially underestimate pollutant concentrations in the vicinity of the source. Coulter and Eckhoff (1998) report that ISCST3 consistently predicts concentrations that are lower than CALPUFF when variable meteorological conditions are used.

The model, in the form that was presented, computes flux estimates using a single flux profile developed during a registrant study in California. In SOFEA©, the proposed flux profile is adjusted by stochastically sampling PDFs representing agronomic factors such as depth of application, application rate, and timing. The variation in flux associated with differences in soil properties, moisture content, temperature, and other factors is not presently taken into account with a PDF.

Regarding the probabilistic scaling of fluxes, SOFEA© treats the rate of application of 1,3-D as a stochastic variable. This seems to be an unreasonable choice because the rate of application is a quantity about which there is the most certainty (farmers are going to choose how much to apply and carefully make that application, especially in California where strict reporting is required). Since the total amount of 1,3-D applied in a township is limited by regulation (California is the only state where township caps apply) and most townships use the maximum amount allowed, stochastic variation will mean that the model will be making predictions as if some townships (arbitrarily) use less and some use more -- a modeling technique which will incorrectly predict the tails of the distribution. Other parameters associated with the flux estimates would seem to be more appropriately modeled as stochastic variables. For flux estimates based on field experiments, variability arises from factors such as meteorological conditions that reflect the differences between field measurements and modeled application days. In contrast, deterministic models for flux can be used with stochastically varied meteorological conditions to predict the variability in a given application.

Regarding source placement within an airshed, SOFEA© uses the definition of a township as the basic simulation domain because the maximum amount of 1,3-D that can be applied is specified by township. For the purpose of this response, an airshed will be defined by the source, transport, and fate of the chemical in question, but airshed boundaries have no relationship with townships, and SOFEA©'s methodology seems unable to relate the two. Furthermore, the airshed for some chemicals (such as 1,3-D for which chronic exposure is important) may be larger than the largest region considered by SOFEA© (23 by 23 township region or 222 km by 222 km). As discussed above, ISCST3 model predictions should not be used at such long distances.

SOFEA© places treated fields randomly in a township. In practice, treated fields may be clustered and even juxtaposed, although treatments may not occur at the same time. The average concentrations downwind from such a cluster might be larger than if the fields were distributed randomly.

For townships with high application rates, source placement can be dictated by the overflow algorithm, which is invoked when the random placement of fields restricts the placement of additional fields in the same township section. Consequently, the overflow algorithm spreads sources over a larger geographic area than happens in practice. Since the same amount of 1,3-D is modeled by the overflow algorithm as a release over a larger area, the modeled exposure will be less than would be predicted if the 1,3-D application were modeled over the correct area. Consequently, the overflow algorithm reduces the predicted exposure in areas where 1,3-D application is the highest.

The receptor grids used for acute exposures seem to be adequate. However, the receptor grid for chronic exposures is assumed to be uniform, and such a uniform grid is likely to underpredict exposures unless it is fairly dense, particularly because of the characteristics of the ISCST3 model used in SOFEA©; ISCST3 predicts a plume trajectory to follow the wind trajectory from a source to downwind distances of greater than 50 km based on the hourly wind direction. Put simply, the trajectory of the maximum concentrations for a plume may miss all grid receptors if the grid is sparse, and while the Gaussian plume models maximum concentrations at a given downwind distance reasonably well, it does a notoriously poor job of predicting the locations of such maxima. No sensitivity study of the grid density seems to have been made. In the development of receptor grids for chronic exposure estimates, additional receptors close to the treated fields should also be considered. Spatial averages of these near-field receptors should be given, in addition to those for the uniformly-spaced receptors. Near-field receptors are likely to be exposed to much higher concentrations on both short term and long term bases. However, computer resource requirements can increase to impractical levels for dense grids. This problem only appears to be discussed very briefly in the documentation, and clearer warnings and more specific guidance should be provided. Also, it would be helpful if a warning message would be generated if the user selects a grid size too large to provide meaningful answers to the questions under consideration.

(2B) Are there any other potential critical sources of data or methodologies that should be considered?

Panel Response

The preliminary efforts at including GIS information and land use data, such as the Pesticide Use Records (PUR), look as though such efforts may be effective at providing realistic exposure estimates. However, there were some concerns expressed as to the reliability of PUR especially as it relates to missing data. A member of CDPR admitted that this was a concern and that work was being done to address this issue.

Question 3: The determination of appropriate flux/emission rates is critical to the proper use of the* SOFEA© *model as these values define the source of fumigants in the air that can lead to exposures. 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. In* SOFEA©*, measured flux rates specific to the conditions at the time of the monitoring studies used are adjusted based upon incorporation depth and seasonal differences to account for varying application conditions. Emissions of 1,3-dichloropropene are sensitive to soil temperature and incorporation depth. Incorporation depth is addressed using the EPA model PRZM3 and also the USDA model CHAIN-2D. Scaling factors were used to address temperature differences.

(3A) What, if any, refinements are needed for this process including the manner in which flux values were directly monitored and calculated using the aerodynamic flux approach?

Panel Response

The aerodynamic gradient approach was the field method chosen to estimate the volatilization flux of 1,3-D. This method has been widely used and is well documented in the literature. It is probably one of the best methods for determining volatilization fluxes of pesticides from treated fields, although it does have a few limitations and drawbacks that will be discussed below. The primary usage regions for 1,3-D were reported to be Washington, California, North Carolina, Georgia, and Florida. To date, field studies have only been conducted in Florida (single study) and California (four studies) using a variety of application methods.

The single study conducted in Salinas, California was selected as the "worst case" or most representative of shank application conditions because it resulted in the highest mass loss and, therefore, the most conservative example. The resulting 14-day flux profile was used as the representative source emission input to the model in all test cases. For acute exposure assessment, however, use of this high mass-loss flux profile does not guarantee the "worst-case" because factors such as application timing and meteorological conditions were not considered. Long sampling periods used in the field study (two 6 hour samples followed by a 12 hour sample overnight) cannot reflect the variability in the emission fluxes. The environmental conditions that affect volatilization are continuously changing, and very dramatic and important changes can occur over much shorter time periods. The empirical flux-gradient relations, called stability correction factors by the presenters, are generally based on 30 to 60 minute-averaged data and may not be appropriate for 6-12 hour averaging or sampling times over which stability conditions, turbulent eddy diffusivities, and fluxes can vary considerably. Using flux estimates averaged over several hours to estimate hourly exposure concentrations will underpredict the actual downwind air concentrations at some times and overpredict the concentrations at others. Since meteorological input to SOFEA© is provided on an hourly basis, the

Panel recommended that emission flux should also be based on hourly sampled concentrations. The Panel recognized that this will add considerable expense to field studies to collect hourly gradient samples. It is possible to automate hourly air concentration sampling using multiple cartridges and a solenoid switching system at each height, similar to the one used in the chamber studies described in the presentation (slide 39).

As described in the oral presentation, concentration, wind speed, and air temperature measurements were made at 33, 50, 90, and 150 cm heights above ground level; concentration was also measured at 15 cm. By convention from some previous work, only the data collected at two heights (33 and 90 cm) were used to estimate the flux densities with the aerodynamic gradient approach. It would be more appropriate to use data from all height levels and reduce the error in the calculated flux by averaging the estimated values at several heights based on gradient estimates between adjacent heights. For gradient estimates, the logarithmic finite-difference approximation is considered superior to the linear finite-difference approximation and is often used in micrometeorology (Arya, 2001). The same approach should be used for the estimation of the gradient Richardson number. The logarithmic approximation can be used between adjacent heights even when the whole profile may not be logarithmic, as the log law is strictly valid only under neutral stability conditions.

Several Panel members expressed concerns about the low fluxes determined during periods of stable meteorology at night. The measured values at or near zero do not seem real. This is likely due to the relatively high threshold levels for the wind speed sensors utilized in the study. The following suggestions about the use of improved and additional instrumentation, would benefit the aerodynamic approach for flux calculations:

- A potential inaccuracy in the measurement of the near-surface temperature arises from the use of naturally aspirated temperature-sensor housings. These housings were used appropriately in the presented field study and are well accepted for similar studies. There is a problem, however, with using these sensor housings because the housing may artificially cool the sensor at night when the wind is less than 2 m/s and the sky is clear. A 1996 study compared measured air temperatures from naturally ventilated and forced ventilated temperature housings (NUMUG, 1996). Although the cited study used less efficient housings than the Dow field study, a similar effect would be present. It is conceivable that such temperature measurement errors could lead to lower flux estimates. Furthermore, the Richardson number is dependent on the average air temperature. This may help explain the differences between emission rates calculated by the aerodynamic gradient approach and back-calculation flux methods made at night.
- The incorporation of completely correlated wind and chemical measurements would be of value in reducing the flux measurement uncertainty. Hourly wind averages along with hourly air temperature and concentration measurements would allow a better understanding of the dynamics over time.
- Meteorological sensors using sonic anemometry could be used to collect very low threshold values. Vaisala, Inc. (www.vaisala.com) has a 2-D sonic sensor with a

"virtually zero starting threshold." Other companies have 3-D research grade instruments that allow the measurement of vertical components (www.apptech.com) as well as a higher frequency for gathering information on turbulence. A fast 3-D anemometer/thermocouple would make direct measurements of momentum and heat flux. The use of sonic anemometers will also lower the wind speed measurement threshold thereby enabling fluxes to be estimated during very stable/low wind conditions. With new technologies on the market, such sensors are now inexpensive and appropriate for use in field studies.

- Another sensor that may be useful is an IR thermocouple to measure soil surface temperature. This parameter would be helpful when comparing results from different times of the day, and even different field studies. An IR thermocouple is inexpensive, easy to incorporate into existing field loggers, and is very stable and accurate.
- Although it is understood that open-path FTIR was used with poor results in one of the field trials, another possible open-path technology is tunable diode laser (www.boreal-laser.com, www.unisearch.com). This technology is potentially more sensitive than FTIR due to beam-throughput issues and is well-suited for a single species measurement scenario.
- Conventional air monitoring equipment can easily meet the need for short-term air samples with high sensitivity. Using EPA Method TO-15 (www.epa.gov/ttn/amtic/airtox.html), one can collect samples for periods as short as approximately one minute and up to 24 hours or more (www.entechinst.com). There are at least 20 commercial analytical laboratories that provide detection limits as low as 0.1 part per billion by volume (ppbv) on a routine basis (e.g., www.airtoxics.com, www.easlab.com).
- Another instrument that may be useful is a fast-response closed-path IR spectrometer. Although it may not be fast enough for direct measurement of chemical flux, this instrument may be appropriate for measurement of chemical concentrations with averaging times between several seconds and a few minutes.
- A commercially available portable gas chromatograph/mass spectrometer with an on-board pre-concentrator module can provide for sub-ppbv measurements with 10 minutes of sample collection followed by a 10 minute or less analysis time, providing MS-quality data consistent with laboratory measurements (www.hapsite.com). This instrument has been evaluated by EPA's Environmental Technology Verification Program (www.epa.gov/etv/verifications/verification-index.html). Other field-portable instruments such as gas chromatographs are available (e.g., www.photovac.com), although it's not certain all would meet the main requirement of ppbv sensitivity.
- One panel member noted that a gas chromatograph with an electron capture detector and a pre-concentrator module would be the best choice for field portable instrumentation because it would likely be more stable in the field than a GC-MS instrument and provide enhanced sensitivity for 1,3-D over gas chromatography with photoionization detection instrumentation.

Commercially available technology exists for collecting emissions data using the relaxed eddy accumulation method, a gradient method similar to the aerodynamic method (www.apptech.com, www.hamptontechnologies.com).

Several Panel members reiterated the importance of making concentration measurements with faster response instruments in flux studies and in comparisons between modeled and predicted concentrations. Faster response concentration measurements will allow for a more accurate representation of bystander exposure.

(3B)* SOFEA© *can easily be modified to probabilistically vary flux rate for each application based on variability in field flux measurements (e.g., application method or temperature) or model generated flux. Please comment on this potential modification.

Panel Response

The probabilistically varied flux rate for each application based on variability in field flux measurements is useful and should be retained in the model. To obtain the probabilistic flux values, however, a joint probability distribution is needed for period flux rates and meteorological conditions. The emission fluxes are dependent on temperature, atmospheric stability, and precipitation. The stochastic selection of a flux value should also depend on these processes.

The depth-of-injection scale factor needs to include soil degradation of the applied fumigant. In the absence of soil degradation, cumulative emissions will be 100%. Soil degradation is the controlling process affecting cumulative emissions. Depth of injection affects emissions by changing the soil residence time (i.e., the amount of time over which soil degradation occurs). The depth-of-injection scale factor is valid only for soils with the "calibrated" degradation rate from the reference field study.

The capability to include probabilistic flux inputs is valuable in assessing the overall sensitivity of the model to the various parameters. Since field measurements are difficult and expensive, this capability would allow the investigation of various scenarios of field uncertainty, thus giving a more realistic range of the flux and emission estimates.

1,3-D, as commercially marketed, consists of two isomers, *cis*- and *trans*-. The two isomers have different physicochemical, biological, and toxicological properties. These should be considered as two different chemicals. The degradation rates of *cis*- and *trans*-1,3-D in Florida sandy soils have been found to be essentially the same as that in sterile soils with both isomers having the same degradation rate. Soils with a history of repeated application of 1,3-D were found to exhibit more rapid degradation in live soil than in sterile soil, and the degradation of *trans*-1,3-D was more rapid than *cis*-1,3-D (Chung et al., 1999; Ou et al., 1995). This phenomenon has been termed differential enhanced degradation. The *cis*- and *trans*-1,3-D isomers in non-enhanced soils were principally degraded by chemical hydrolysis to the corresponding *cis*-3-chloroallyl alcohol (IUPAC name: 3-chloropropene-1-ol) and *trans*-3-chloroallyl alcohol. Since the hydrolysis rates of the two isomers in water are the same, the degradation rates for the two isomers in non-enhanced soil should be the same. The two chloroallyl alcohols were then degraded microbially to corresponding *cis*- and *trans*-3-chloroacrylic acid, and eventually to CO_2 and H_2O (Ou, 1998). A bacterial degrader has been isolated from the enhanced soil that also exhibited differential enhanced degradation between *cis*- and *trans*-1,3-D.

Since *cis*- and *trans*-1,3-D are first degraded in soil to *cis*- and *trans*-3-chloroallyl alcohol by chemical hydrolysis (non-enhanced soil) or chemical and biological hydrolysis (enhanced soil), chemical hydrolysis rates of the two isomers depend on soil or water temperature. For example, hydrolysis half-lives of *cis*- and *trans*-1,3-D in water at 20 and 30°C are 11.3 and 3.1 days, respectively (McCall, 1987). The average half-life values for both *cis*- and *trans*-1,3-D in non-enhanced soils and sterile soils at 24-25°C are about 8 days. Beside biodegradation rates of *cis*- and *trans*-3-chloroallyl alcohol, no information on the physicochemical and toxicological properties of these two alcohols has been found in the literature. Depending on the test duration and the body temperature of the laboratory animal, the toxicity of *cis*- and *trans*-1,3-D may actually come from the two alcohols, or a combination of 1,3-D and the alcohols because *cis*- and *trans*-1,3-D may completely or partially hydrolyze to corresponding *cis*- and *trans*-3-chloroallyl alcohol. The *cis*-1,3-D isomer is more toxic to soil nematodes than the *trans*- isomer (McKenry and Thomason, 1974; Shoemaker and Been, 1999).

Cis-1,3-D has a higher vapor pressure than *trans*-1,3-D, 34.3 and 23 mm Hg (Hornsby et al., 1995), respectively. After application of a commercial product of 1,3-D to field plots, *cis*-1,3-D was always found to be the first chemical to volatilize from a field plot surface in Florida sandy soil, usually 1 to 5 hours after application and followed by *trans*-1,3-D 1 to 3 hours later, depending on soil temperature. It was also found that during the first 48 hours after application, the flux rate for *cis*-1,3-D was about 1.5 to >3 times greater than *trans*-1,3-D. The ratio between the two isomers gradually declined. Since large amounts of *cis*- and *trans*-chloroallyl alcohol may form in soil, the two alcohols may volatilize into the atmosphere. A similar chemical, 2-chloropropene-1-ol, has a boiling point of about 133°C. Therefore, the two alcohols could be less volatile than *cis*- and *trans*-1,3-D.

Because of toxicity difference and higher volatility of *cis*-1,3-D, one possible approach would be to take into account the individual toxicity and emission flux for the two isomers for the establishment of buffer zones and threshold concentrations.

(3C) 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

Using a flux/emission factor based on a single monitoring study or a few studies is questionable. One Panel member emphasized the importance of considering whether a single flux profile is appropriately conservative or not. The emission flux behavior should be investigated for different soils, soil moisture conditions and environmental factors that might exist in different regions. In addition, considering the variability of emission fluxes, a stability index or parameter, such as the bulk Richardson number, would be a more appropriate parameter to use than air temperature. Volatilization fluxes depend on wind speed and turbulence whose effects may be parameterized through a stability index, such as Pasquill's. Both published and unpublished studies describing volatilization losses of 1,3-D and other fumigants should be carefully reviewed. At a minimum, the model developers should use data from all of their own flux field studies (described during their presentation) to develop a PDF describing volatilization losses of 1,3-D. The work of Gan et al. (1998), Kim et al. (2003), Thomas et al. (2004) and Schneider et al. (1995) should be consulted.

The plot of the field study summary (slide 49 in the presentation) shows the cumulative volatilization losses as a percent of the applied material. The results from the four studies show very different cumulative volatilization behavior. Both the Georgia (drip) and Florida (shank-bed) studies show very steep (high) initial losses for about four or five days followed by a leveling off of the emissions. The cumulative loss profiles for the two California studies (both shank) are not only different from the GA and FL studies, but they also show a very different cumulative loss pattern. The presenters stated that the Imperial, CA data were discounted because the study only lasted eight days. Unless there was some technical reason that the Imperial data cannot be used (none was stated), then it is reasonable to compare the results for the two studies. The loss pattern from the Salinas study shows almost a 2-day delay before the onset of significant losses, while the Imperial study shows a very gradual loss pattern with time. These are very different results. The slope of the curve is significantly different, with the values on day 2 (according to the flux profile plot) being the highest. But the difference between Imperial and Salinas shows 1% vs. 15% of the applied fumigant volatilized. It is hard to see how a scaling factor based on the Salinas data could be accurately applied to the Imperial data. The data presented in slide 49 is probably the best example of why the results of only one study should not be used as the basis of all source emission data input for the model.

The use of scaling factors may be reasonable when cumulative fluxes are being considered, but they are not appropriate when acute, period fluxes and associated hourly downwind air concentrations must be estimated.

Although the use of the scaling factors may be reasonable for accounting for some application factors, there is concern that some scale factors may not be realistic. For example, the factor of 1.6 between summer and winter temperatures appears too simplistic. In the summertime alone there is a probable temperature differential of close to that between the hot inland valleys such as around Kern County, California and the cooler, coastal areas around Santa Cruz and Monterey Counties, California.

The use of appropriate scaling factors seems to be based on the user's judgment, but it would be more appropriate if a mechanistic approach was used to develop them for the various field conditions expected to be encountered. That is, what are the most influential factors or processes that are driving the observed fluxes and how can these be input to the process. The model documentation should include a table of appropriate scaling factors recommended by the authors.

The use of local meteorological data is also suggested because weather patterns are significantly different between different regions such as the coastal areas and the valley areas of California. Other inputs into ISCST3 such as mixing height are regionally dependent.

(3D) Please comment on* SOFEA©*'s capability to adequately consider multiple, linked application events on an airshed basis as well as single source scenarios.

Panel Response

The model developers can be commended for attempting to consider multiple, linked application events. The regulatory agencies are urged to consider the effects of multiple, linked application events of a particular compound, and indeed, of other compounds. In the real world, such events are happening and people are exposed to fumigant emissions and other types of emissions in combination. However, as discussed in relation to other questions, SOFEA©'s reliance on the ISCST3 model for description of atmospheric dispersion limits the accuracy of the multiple-source simulation. Field locations cannot presently be specified as source area inputs to the model, but certain areas in the quadrant can be assigned a higher weighting factor. This was viewed by some Panelists to be an acceptable compromise, but other Panelists pointed out that fields can be abutted in practice (which would increase impact over that predicted by the model), and the overflow algorithm effectively spreads application of the fumigant over a larger area (which would decrease predicted impact). The capability of considering multiple sources is very important, particularly when predicting chronic exposures. More detailed land use data may improve the model's capabilities.

(3E) Does* SOFEA© *appropriately address situations where data are missing?

Panel Response

The ability of SOFEA© to address missing data was absent from the presentation and the provided documentation. It is implicit that all the inputs are required; otherwise, the model will not run. In that sense, it forces the user to ascertain whether the input is complete, which can be a beneficial process. The documentation does not address how it deals with missing data, however, and this aspect should be included in the future, particularly the use of PCRAMMET.

Question 4: The integration of meteorological data into ISCST3 is one of the key components that separates the* SOFEA© *methodology from that being employed by the Agency in its current assessment. This information, coupled with GIS (Geographical Information Systems) data such as the amount of ag-capable land cover, elevation, and population densities are optional inputs for* SOFEA©*.

(4A) Can the Panel comment on the value of adding this information for conducting spatially realistic simulations?

<u>**Panel Response**</u>

The addition of hourly-averaged meteorological information and GIS data seems to be a useful part of the methodology implemented in SOFEA©. Such information seems to be a step forward from the present assumption of worst case meteorological conditions over the duration of the release. As discussed previously, the case study for SOFEA© was based on 1,3-D for which acute and chronic exposures must be considered.

For acute exposures, using meteorological conditions from a distant meteorological station may not accurately reflect local conditions, especially effects such as drainage flows.

For chronic exposures, dispersion modeling must be done over much larger distances. The use of hourly meteorological information from a single monitoring station should not be replicated over large areas (airsheds) because simple replication of the same meteorological data for all sources will ignore terrain features which importantly effect conditions. (Although SOFEA© provides for gridded inputs of elevation and land cover, it does not utilize them to determine wind vectors or surface roughness.) A mass-consistent wind flow model, such as the National Atmospheric Release Advisory Center's (NARAC) Atmospheric Data and Parametrization Tool (ADPT) or the Naval Research Laboratory's Coupled Ocean/Atmospheric Mesoscale Prediction Systems (COAMPS), could be incorporated into SOFEA©. Such a flow model takes a few observations of wind and temperature from surface stations and profilers, and creates a grid of surface wind vectors. This increase in sophistication of wind flow comes at a heavy cost but would substantially increase the reliability of meteorological input to a dispersion model. Alternatively, mesoscale models such as the National Center for Atmospheric Research (NCAR) Mesoscale Model version 5 (MM5), or the Colorado State Regional Atmospheric Modeling System (RAMS), can be employed to yield terrain-influenced wind vectors.

Using a constant value of mixing height may be adequate. SOFEA©'s suggested value of 320 m appears to be on the conservative side, but local air regulators should be consulted. In reality, daytime mixing heights have a wide range and show strong diurnal and seasonal variations. They also depend on the land use and proximity to coastline. Changes to the mixing height will only affect predicted concentrations several kilometers from the source.

(4B) There are several potential sources of meteorological and GIS data (e.g., National Weather Service and California Irrigation Management Information System or CIMIS). Please comment on the methods used to select these data including locations for meteorological stations.

<u>Panel Response</u>

Major sources of meteorological data are the NWS, CIMIS for California, and other local and state climate, agricultural, and industrial meteorological stations. Measurement height for surface data may vary from 2 to 10 m. Quality-assured data should be selected from the closest representative site, whether it is a NWS location, state air quality or climatological site, or an industrial monitoring site. At least five years of continuous data are recommended, but longer periods of data might be necessary when evaluating long-term chronic exposures. If on-site data for a short period are used, it should be compared with the nearest available long term NWS data. The local air quality regulators should be consulted for the selection and use of appropriate meteorological data.

(4C) What criteria should be used to identify airsheds for analysis and how should data be selected to address each airshed? Please comment on the manner in which these data are processed.

<u>Panel Response</u>

An airshed is not defined by the particular domain of the SOFEA© model, i.e., 23 X 23 townships or smaller, but rather, by the relevant meteorology and transport of the chemical of interest. For some chemicals, the significant airshed (i.e., source areas over which a given receptor may experience significant exposure levels) may be larger than the largest domain allowed in the current version of SOFEA©. The use of the term airshed implies that all significant source areas have been included. This is not necessarily the case with SOFEA©.

The maximum domain extent recommended for use in SOFEA© should be influenced by the dispersion model it incorporates. With the choice of ISCST3, the domain should be limited such that the largest distance between any source and receptor of interest is less than about 50 km. Over larger distances, Gaussian dispersion parameters cannot be specified because the Pasquill-Gifford dispersion coefficients used in ISCST3 were originally based on experimental data taken within about 30 km from the source. (ISCST3 seems to arbitrarily limit the extent of a plume to 80 km.) The ISCST3 assumption of constant hourly-averaged meteorology and flat terrain over the entire ISCST3 domain is questionable for larger model domains such as might be required for modeling an airshed.

(4D) Data quality and uncertainty associated with these data vary with the source. Does the Panel agree with the approaches used to characterize these factors?

Panel Response

Approaches to characterize the quality and uncertainty of meteorological data were described by the developers of SOFEA©, but it is not clear that these factors have been fully addressed. A procedure for filling in missing data was discussed. The SOFEA© model applies meteorological data from a previous or future year for the date and hour(s) of the missing data. A better alternative would be to use the meteorological data from the previous valid hour or valid hour after the missing period, thereby using the consistency method.

A critical factor to consider is the length of the meteorological record used in the model. In the case study reported, the CIMIS meteorological data of 5 consecutive years was used in a much longer-term exposure analysis. These data were sampled stochastically during a simulation assuming a uniform distribution with each weather year assigned an equal probability. The 5-year length of weather record in this case study appears inappropriately short for the treatment of long (>20 years) term exposures. Criteria should be developed for the appropriate data record length for long term exposure assessments that will ensure that extreme events which most likely contribute the highest exposures will be taken into account. This is the standard practice when conducting exposure assessments to estimate the magnitude of human and ecological risks associated with pesticide use.

(4E) Anemometer sampling height has been identified as a concern by the Agency in preparation for this meeting. What are the potential impacts of using data collected with different anemometer heights in an analysis of this nature?

Panel Response

In SOFEA©, the ISCST3 model uses the mean wind speed and wind direction at a standard height of 10 m to estimate the mean transport wind conditions in the Gaussian plume formulas for surface sources. Some data sources have wind measurements at a lower elevation (e.g., 2 m in CIMIS). The exact details of how the ISCST3 model uses windspeed and elevation data for area sources as used in SOFEA© needs to be considered.

The use of wind observations at 2 m elevation may be appropriate for evaluating short term, acute exposures because the lower measurement level may be more reflective of conditions relevant to near-field 1.5 m high receptors. The difference between the wind measured at 2 m and 10 m is, in general, subject to the stability conditions of the atmosphere and the type of terrain. (It should be noted that the Panel reviewing the Fumigant Exposure Modeling System (FEMS) using metam sodium as a case study, stated it is preferable to have vertically resolved air concentrations and to have meteorological data for 1.5-2 m and 10 m during the testing period. See SAP Report No. 2004-07 dated November 9, 2004.)

(4F) Does* SOFEA© *treat meteorological stability class inputs appropriately?

Panel Response

SOFEA© treats stability class inputs appropriately for its current use of ISCST3. Dispersion coefficients are specified as a function of the Pasquill stability classes (which are a discrete measure of stability). Other dispersion models, such as AERMOD, can treat stability as a continuous variable.

(4G) Does SOFEA© appropriately calculate bounding air concentration estimates?

Panel Response

The current approach used in SOFEA© may not yield the highest upper-bound concentrations.

- The coarse receptor grid used for chronic exposures may be a serious limitation. For determining highest upper-bound concentrations, additional receptors should be considered at short distances (just outside the buffer zones) from the treated fields.
- As pointed out in the response to Question 2, multiple treated fields can be abutted in practice (which would increase impact over that predicted by the model), and the overflow algorithm effectively spreads application of the fumigant over a larger area (which would decrease predicted impact).
- The emission flux based on the single field test and treated in a stochastic manner may not yield the highest concentration, especially when considering the tails of the exposure distribution and the potentially high degradation rates in the selected field test.
- The highest concentrations from surface sources, such as treated fields, are likely to occur during very stable, low-wind or calm conditions. A Gaussian dispersion model, such as ISCST3 used in SOFEA©, is not particularly applicable under such conditions. For such conditions, more sophisticated models, such as CALPUFF, should be considered. Drainage flows would likely impact acute exposures, but these are not considered in ISCST3.
- A recent study has shown that ISCST3 may significantly overestimate vertical dispersion, i.e., "sigma z" (Minnick et al, 2002). Such an overestimation of vertical dispersion will result in an underestimation of concentration. Such underestimates may greatly influence the peak concentrations observed in the near field.

Question 5: The Agency model, ISCST3 is a critical component of the* SOFEA© *approach. This model has been peer reviewed and is commonly used for regulatory

purposes by the Agency.* SOFEA© *also uses other Agency systems such as PCRAMMET and PRZM3 as well as the USDA model CHAIN-2D.

(5A) Please recommend any parameters that should be altered to optimize the manner that they are used in* SOFEA©*.

Panel Response

Questions were raised about the accuracy of the PRZM3 model. CHAIN-2D was considered to be more realistic than PRZM3. However, it was recognized that the computational resources needed to run the CHAIN-2D model were much greater than that needed for PRZM3.

SOFEA© developers used PRZM3 simulations to describe 1,3-D flux from soil. Order of magnitude agreement between measured 1,3-D losses and simulated results (cumulative loss) were reported (Cryer et al., 2003). These results suggest that PRZM3 may provide realistic flux estimates; however, considerably more data are needed before a meaningful (i.e., statistically valid) conclusion can be reached. An inherent limitation of PRZM3 is that it produces results based on daily (24-hour) time steps. This presents a problem in linkage of model outputs to ISCST3, which simulates dispersion based on hourly time steps. Since meteorology can vary greatly from hour to hour, the use of emissions flux estimates averaged over much longer time periods may introduce significant errors into the estimates. Cryer et al. (2003) addressed this (in their application of PRZM3) by converting the PRZM3 daily flux to weighted hourly flux estimates. A number of assumptions were required, and it is unknown to what extent such assumptions affected estimates because sensitivity analyses were not reported. No flux data were collected on hourly time scales in any of the field studies described so that data are not available to evaluate the validity of the assumptions.

In general, the methodology for emissions flux estimation in SOFEA© is thought to be too simplistic. Meteorological influences on emissions fluxes should be considered, as should soil type and soil moisture. Emission flux estimates should be based on more highly resolved temporal measurements (e.g., hourly). In addition, the time of application should be considered as a factor. If the time of application is much different from that of the field test used to estimate fluxes, then the estimates might be substantially off.

The algorithms used in the PRZM3 model are believed to be very similar to those used in the PEARL and PELMO models, described in Wolters et al., 2003. In this paper, the latter two models were evaluated by comparing their predictions with experimental measurements. It was found that "…model predictions deviated markedly from measured volatilization rates and showed limitations of current volatilization models…." The deviations were particularly pronounced in the initial emissions stages, and sometimes the measured flux was significantly higher than the simulated flux.

(5B) ISCST3, as integrated into* SOFEA©*, was run in regulatory mode which includes the use of the "calms" processing routine. Does the Panel concur with this approach? If not, please suggest a suitable alternative?

Panel Response

In the ISCST3 model, estimated downwind concentrations are inversely proportional to the windspeed. When the windspeed goes to "zero", the model cannot be used. In addition, its use with low – but non-zero – winds is not recommended. Thus, methodologies have been developed for the use of ISCST3 model in these conditions.

There is some uncertainty as to exactly what methodologies were followed in these conditions within the SOFEA© modeling system. The model developers present at the meeting were not able to describe the methodologies used. And, unfortunately, there seems to be some ambiguity in various documents purporting to describe these methodologies (e.g., ISCST3 source code and User's Guide; EPA web site material; 40 CFR Ch I.; PCRAMMET source code and user's guide).

In the following, a particular set of methodologies is assumed to have been followed. The Panel assumed that in the regulatory-mode application of the ISCST3 model, if the meteorological data specifies "calm" or a wind speed of 0 m/sec, all downwind concentrations are set to zero. A slight correction is made by not counting that particular hour in estimating the average concentration. That is, if one is averaging over 24 hours, and 2 of the hours are "calm", then one takes the average concentration just for the 22 hours that were non-calm. However, even this slight correction only goes so far. For example, in regulatory mode, if there are less than 18 non-calm hours in a 24-hour period, then the 24-hour average is estimated by dividing the sum of the non-calm concentrations by 18. This has the effect of reducing the estimated average concentration.

If the meteorological data specifies a wind speed greater than zero but less than 1 m/sec, then the wind speed is arbitrarily increased to 1 m/sec in the use of ISCST3 in regulatory mode. This procedure also has the effect of reducing the estimated concentrations.

The methodologies are described in 40 CFR Ch. I. Unfortunately these methodologies have the potential to allow the highest actual concentrations to be underestimated or even set to zero. This is perhaps the most critical of all the ways in which the SOFEA© model may underestimate concentrations in high exposure situations.

Not all models or methodologies have the limitations that the ISCST3 model has at zero and low wind speeds. In one study (Coulter and Eckhoff, 1998), the CALPUFF model was compared with ISCST3, and because of the method of handling calms, low-wind-speed situations, and wind reversals in ISCST3, the ISCST3 model tended to underestimate concentrations relative to the CALPUFF model.

The "recirculation" problem deserves special mention here. Consider the following set of circumstances. In the first hour, the wind is blowing in a particular direction at a fairly low speed. As a result, there are relatively high concentrations in the near field downwind of the source. In the next hour, imagine that the wind "reverses" direction but still remains relatively low. In reality, the pollutant dispersed the previous hour will be blown back to the same near-field receptors "hit" in that previous hour, increasing their exposure. Since these are the conditions of highest exposure (i.e., low wind speed), the "extra" exposure due to this wind reversal may be significant. In the ISCST3 model, when the wind reverses that second hour, all upwind concentrations are set to zero, and the "extra" exposure due to recirculation is not counted. In estimating average exposure averaged over all wind directions for long periods, the effect of this unrealistic ISCST3 methodology may not be overwhelmingly significant. However, in the estimation of peak concentrations and exposure, the effect of this problem may be very significant. This is another example of the way in which the current version of the SOFEA© model is vulnerable to underestimating peak exposures.

There are several approaches that might be investigated to attempt to deal with the various shortcomings discussed above.

- Existing field measurement data should be examined to determine if measurements were made during calm, low-wind, or recirculating conditions. If such data exist, they can be used to (a) characterize the degree of "error" in the ISCST3 simulation and (b) serve as a basis for developing an empirical correction to model predictions. If insufficient data are available from existing studies, current and future field studies could be modified to introduce measurements under calm, low-wind, and/or recirculation conditions.
- Consider abandoning the use of the ISCST3 model as the "engine" driving the dispersion estimates in SOFEA©. In its place, a more realistic model that does not have as severe limitations under calm, low-wind, and recirculation conditions could be considered such as CALPUFF or other Lagrangian puff models.
- A simple approach that might offer some improvement would be to allow the emissions flux during calm hours to build up, so that the emissions in the first hour after a calm period would include that hour's emissions plus all the emissions during the preceding calm period. This would not address the low-wind or recirculation problem and would only partially address the calms problem, but it seems to be better than the present approach. Other *ad hoc* approaches may be possible, but all such approaches should be carefully considered.

<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.

(6A) Please comment on to what extent the methodologies in* SOFEA© *can be applied generically in order to assess a wide variety of fumigant uses? What considerations with regard to data needs and model inputs should be considered for such an effort?

Panel Response

The oral presentation at the meeting described a case study of 1,3-D use in central California (CA) and found order-of-magnitude agreement between predicted and measured concentrations. However, results indicated that SOFEA© may under-predict both chronic and peak exposures at the high-end of exposure distributions (>90%). It is unknown whether this is a characteristic of the model. Additional study may provide insight. Several recommendations were made by SAP Panel members, which may help to guide future efforts.

While there do not appear to be major methodological problems with the successful application of SOFEA© in settings other than the CA Central Valley, successful applications are hindered by data needed to run the model. There are four principal areas of concern: product use, flux estimates, weather and topography. One Panel member noted that the development of "scenarios" that use site specific data that are more representative of other regions of the country may be helpful.

Product Use

For the CA 1,3-D case study, the registrant hired a contractor to "mine" use data from the CA Pesticide Use Records (PUR) database to obtain critical information needed to run SOFEA©. PUR includes information on application locations (Township, Range, and Section), application date, rate, depth, field size, crop type, and total pounds of fumigant used. One SAP Panel member expressed misgivings about the quality of data available in the PUR database. The California Department of Pesticide Regulation (CDPR) representative present at the meeting acknowledged this and indicated that there were some efforts to "correct" extreme and or missing values. While uncertainties remain, PUR currently represents the best available data and is the only data gathering effort of this type in the country. In the absence of data of this type, pesticide use data at a watershed and/or airshed scales are estimated using "census of agriculture" data, farm-gate reports (# acres in production by county) or other estimates of land use and USDA-National Agricultural Statistics Service pesticide use profiles for various crops. The general approach is described by Thelin and Gianessi (2000). The result provides a "best-guess" estimate of pesticide use by active ingredient type and amount. Uncertainty bounds on estimates are unknown and are likely large in some cases. Agricultural census data are collected and reported nationally on 5 year cycles. Where population pressures result in rapid conversion of land to non-agricultural uses, the census may not be representative of current conditions. This is also the case with cropping patterns where changes in crop distributions may be quite rapid due to factors such as pest pressure or economics.

As pointed out by SOFEA© developers, obtaining land-use data that delineates whether land is agriculturally capable is relatively straightforward. LANDSAT imagery and other data sources are readily available and can be used for this purpose. The problems are in identifying how much land is associated with a given crop and its pesticide treatment history for a given year. In the absence of these data, the "actual use" approach described for the 1,3-D case study does not appear feasible in many locations.

An alternative is to create crop use scenarios. This approach is well-established in FQPA drinking water risk assessments. Scenarios for a variety of crops have been developed for the PRZM3 model to examine the potential for pesticide runoff impacts on surface water quality. In these scenarios, pesticide applications are assumed to be at the maximum label rate with adjustments for the percent crop area in a watershed (USEPA, 1999). This is in keeping with the need to assess potential versus actual exposures. This approach could be extended to fumigant exposure risks where product use data are not available.

Flux Estimates

Issues surrounding use of a single flux profile developed in a CA study to compute flux estimates are described under Question 3 in this report. There was agreement among the Panel that this approach has significant limitations even for use within the region where measurements were made. This is not to say that the approach is without merit for regulatory purposes, provided there is agreement on what constitutes an appropriately conservative flux profile.

In a generic sense, to use the model in other settings or for other fumigants, region and fumigant specific profiles need to be determined experimentally. This should take into account factors such soil type and properties such as bulk density and organic matter levels, water content, the potential for enhanced biodegradation, local weather, and other conditions which likely influence flux rates. It is important to obtain data for new and improved fumigation practices, especially those that include emission reduction methods. An example is the use of tarps described in the presented 1,3-D case study. Use of traditional films (i.e., high-density polyethylene) may not be very effective in controlling 1,3-D or other fumigant emissions. Surface water sealing may be useful as a cost-effective emission-reduction strategy. Virtually impermeable films have been shown to significantly reduce emission in small-scale studies. More information is needed at agronomic scales. If emissions can be reduced, lower application levels should provide equivalent control.

When studies are conducted to obtain flux estimates, the Panel agreed that the aerodynamic method is the best approach (see responses to Question 3). Some studies using 1,3-D were described at the meeting, and several Panel members noted that there is a large body of soil flux data for fumigants such as methyl bromide. Compilation and comparison of results across regions may prove useful in the identification of generic profiles that are suitable for use as a SOFEA© input. The same approach may prove useful in identifying ways to scale flux loss by the time of year in which the fumigant is applied. The case study approach used a single value to represent summer and winter conditions. Other metrics such as soil temperature on application date may be a more effective method of seasonal adjustment in other regions. In the humid southeast, where rainfall is 120 to 150 cm per year, some consideration should be given to conduct of experiments that quantify impacts of rain and or irrigation on fumigant flux. Data reported by Gan et al. (1998) indicated that water sealing (which may occur after a treated field receives rain or is irrigated) may suppress cumulative emissions by as much as two-fold. Not taking this into account, will tend to make flux estimates (and the modeled concentrations) more conservative.

In the absence of measured data, it was suggested that models may be used to simulate flux profiles. Use of the USEPA model PRZM3 for this purpose was reported in one published study (Cryer et al., 2003). Order-of-magnitude agreement between measured and simulated flux profiles was reported in two cases. However, the utility of PRZM3 to predict fumigant flux in other settings is unknown. Given this and other concerns discussed in Question 5, it appears that other models need to be identified and evaluated. Cryer et al. (2003) showed that simulated results obtained with the USDA model, CHAIN-2D, provided a reasonable fit for measured values. While potentially useful, it appears that data requirements may limit CHAIN-2D applications in some cases.

Weather and Topography

Proximal weather data in sufficient detail and quality (observations and length of record) may not be available to conduct SOFEA© simulations. Thus the best available data from other stations (in close proximity) are used. There are inherent uncertainties in this approach that are difficult to quantify. Meteorological situations including urban, complex terrain, fields in densely wooded areas that may need special treatment should be identified. Mesoscale models such as the National Center for Atmospheric Research (NCAR), Mesoscale Model version 5 (MM5), and the Colorado State Regional Atmospheric Modeling System (RAMS) can be used to generate more sophisticated gridded micrometeorological wind vector data for these situations. In addition, when used for regional or statewide assessments, emission data should accurately characterize the average behavior across the region for each time period. For accuracy, this information needs to be appropriate for a given locale, time of year, and fumigation type. This could be aided by development of a series of cropping and "worst-case" weather scenarios that would serve to provide a template for SOFEA© applications.

Question 7A: Please comment on whether* SOFEA© *adequately identifies and quantifies airborne concentrations of soil fumigants that have migrated from treated fields to sensitive receptors.

Panel Response

In many respects, the SOFEA© model does not adequately identify and quantify airborne concentrations of soil fumigants that have migrated from treated fields to sensitive receptors. In particular, estimates of worst case, near field exposures do not appear to be adequately identified or quantified by the SOFEA© model. Some of the reasons for this deficiency are:

- Poor or nonexistent treatment of calms and weak winds (<2 m/s) with highly variable wind direction (see Question 5);
- Cutoff of emission events at 14 days, when significant emissions might occur after that period;
- Inadequate consideration of worst-case conditions of application location, receptor location, emissions, meteorology, etc., that might result in extreme exposures; and
- Actual times and conditions of application are different from those of the field measurements used to derive emission flux profile (see Question 5).

SOFEA© assumes a receptor height of 1.5 meters, to simulate an adult's inhalation exposure. Children are also potentially exposed, and lower receptor heights should be considered especially for near-field locations where the concentrations are highest. Because children are more vulnerable to exposure (due to their lower body weight and potential interferences with developmental processes), any underestimate of their exposure should be avoided.

The CALPUFF model follows the trajectory of previously emitted air pollutants when calculating hourly concentrations which ISCST3 cannot do. The use of CALPUFF/CALMET models in SOFEA© should be considered. Acute and chronic exposures may be underestimated because of the use of ISCST3 in SOFEA©

Migration of soil fumigants from treated fields at large distances from sensitive receptors will be necessarily limited to about 50 km beyond which ISCST3's dispersion coefficients should not be used. Other more appropriate wind flow and dispersion models might be used if long-term exposures from far fields are of interest.

(7B) 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

SOFEA© model results seem clearly presented. However, concentrations in the upper ends of the distribution may be underestimated for several reasons previously discussed: chronic exposures at long distances (see Question 4G), calm and low windspeed conditions (see Question 5), and multiple sources (see Question 3). Empirical evidence for the inability of the model to estimate exposures at the upper ends of the distribution was provided by slides 93 and 112 of the oral presentation at the SAP review meeting.

The ability of SOFEA© to predict worst-case concentrations is likely to be progressively worse for longer distances and exposure durations. Continuous meteorological data over the longest period of exposure may be necessary to get concentrations in the upper ends of the distribution. SOFEA© predicts receptor exposure with ISCST3, which assumes steady-state plume existence in the wind direction for each hour of meteorological data. ISCST3 seems to arbitrarily limit the extent of a plume to 80 km (see responses to Questions 2A and 4C). Put another way, SOFEA© could predict no exposure beyond ISCST3's artificial limit even for very long periods of time.

There was considerable discussion by the Panel about the placement of near-field receptors for chronic exposures. A comparative study of peak concentrations and spatial distribution of peak-to-mean ratios might be useful. It is possible that the highest calculated concentrations at uniformly spaced grid locations may be multiplied by a defensible factor to estimate the potentially higher concentrations in the gaps between modeled receptor locations. Two sets of receptors may be used: (1) a uniform grid for far-field exposures; and (2) receptors in close proximity (minimum distance allowable in the model) to treated fields. Although it would increase the computation time, the uniform grid spacing should be tested by reducing it to one-half of that used in the current application and comparing the results.

(7C) Please comment on* SOFEA©*'s approach for calculating and presenting probability distributions of moving average concentrations for differing durations of exposure.

Panel Response

No information is found in the documentation about the methodology used to calculate probability distributions using moving averages. It should be described in greater detail as applied to the SOFEA© model results.

Hourly observations of winds should be sufficient to characterize dispersion in every case except when sub-hour exposure is important to risk assessment. To estimate short-term acute exposure, a temporal peak-to-mean ratio could be employed.

(7D) Please comment on the types of monitoring data that would be required to define the accuracy of simulations made with* SOFEA© *for differing durations of exposure.

Panel Response

Ideally, atmospheric dispersion models, such as SOFEA© with ISCST3, should be evaluated by comparing model predictions for a particular time period at specific locations with measurements made at the same locations during the same time periods. In carrying out such an evaluation, it would be important to utilize the meteorological and emissions data for the same period. This type of model evaluation could be carried out for SOFEA© and is needed, but does not appear to have been done. Data sets with fast response measurements could be time averaged with different time scales to compare with model predictions of the same.

Data were presented for a comparison of simulated and measured concentrations for selected field experiments (slide 33 of the oral presentation). While the initial visual comparison of the simulated and measured concentrations looks reasonable, on closer inspection one finds significant under-predictions of concentrations during certain periods of high concentrations. Also, the results of only two out of eight sampler locations were presented for one field experiment. It is unknown whether this comparison is representative of the other experiments and measurements. In the pseudo-evaluation shown on slide 93, the results for 2001 were presented, but what were the results for the year 2000? Such comparisons should be reported completely.

The best way to evaluate a model is through comparison with actual field monitoring. This was done in the Kern County exercise when the model concentration estimates at selected downwind receptor points were compared to California Air Resources Board (CARB) ambient monitoring results for 1,3-D. The 10-year simulated concentrations versus exceedance percentiles (slide 93 of the oral presentation) seem to have good agreement with the CARB ambient air monitoring data up to about the 90th percentile. At higher percentiles, SOFEA© underpredicts monitoring measurements. These results show that further refinement of the model is necessary to correct the upper end of air concentration distribution estimates and to determine why this underprediction is occurring. Depending on how much 1,3-D-targeted monitoring information is available from the CARB, or if 1,3-D is included in the toxics air monitoring network, all available ambient air concentration data should be used to evaluate the model output, including the concurrent environmental conditions, such as meteorology, field characteristics (soil type, moisture, etc.), etc., to determine the most influential processes affecting the results at either end of the concentration distribution. These may be different than the original set of factors used.

SOFEA© results are strongly dependent upon the quality of the source emission flux. Using the "worst-case" field data and the appropriate scaling factors may be a rational approach for estimating the flux. The coarse concentration averaging periods (6, 6, and 12 hr sampling durations) influenced the estimated flux values. The accuracy of exposure estimates can be assessed by taking field data at sufficient detail to capture the effects of important parameters (such as meteorological conditions). Such data can then be averaged over different time scales, and SOFEA© simulations can be compared for various durations of exposure.

Question 8A: What types of sensitivity/uncertainty analyses of* SOFEA© *are recommended by the Panel to be the most useful in making scientifically sound, regulatory decisions?

<u>Panel Response</u>

In the initial stages of model development, it is enough to run selected scenarios and interpret the results one scenario at a time. *SOFEA©* is now ready for more than that. There are good discussions of experimental design for sensitivity analysis in SAP Minutes 2004-01 "Refined (Level II) Terrestrial and Aquatic Models Probabilistic Ecological Assessments for Pesticides: Level II Aquatic Model Session" (see the response to charge 3d) and 2004-03 "Refined (Level II) Terrestrial and Aquatic Models

Probabilistic Ecological Assessments for Pesticides: Terrestrial" (in the General Comments). In the Level II Aquatic Model Session (2004-01), the work of Kleijnen (2004) was cited. This approach uses principles of experimental design, fractional factorials in particular, and response surface methodology, to determine which assumptions in the model are critical and which factors drive the simulation. The Panel again advocates that the Agency try these methods.

Panelists had a number of specific suggestions for factors to include in the sensitivity analysis: background (ambient air) concentrations, terrain, location (inland versus coastal), and crop type. Inputs into the model that affect fumigant dispersion and degradation need to be included in the analysis: soil temperature, weather stability, and soil degradation of the applied fumigant. Atmospheric degradation factors should be considered as they affect the maximum volatilization and maximum losses through emission into the atmosphere.

The horizontal (Sigma-Y) and vertical (Sigma-Z) dispersion coefficients in the ISCST3 model could be examined probabilistically by selecting a random multiplier to Sigma-Y and Sigma-X in the ISCST3 model code. The distribution of the random multiplier would be based on the cumulative distribution function observed in field experiments.

Because *SOFEA*© will be used for both acute and chronic exposure assessment, there is a need to evaluate the uncertainty in both periodic and cumulative emissions. Some Panelists believed that uncertainty would be higher for periodic emissions than for cumulative.

While the efforts taken to produce reliable emission inputs should reduce uncertainty of the experimental conditions, information about sources of error and uncertainty in the flux estimation should be provided.

Sensitivity analysis could be done on the individual components of the model, ISCST3, PRZM3 and CHAIN-2D. These results might already be available in the literature.

There was strong agreement that a meteorological record longer than five-year CIMIS record was required, to ensure that some "worst case" scenarios would figure in the sensitivity analysis.

(8B) What should be routinely reported as part of a* SOFEA© *assessment with respect to inputs and outputs? Are there certain tables and graphs that should be reported?

Panel Response

Since Excel is the user interface, all information concerning input (system parameters, probability distributions, spatial and temporal inputs) and basic numeric output are in an Excel workbook. Users should have no difficulty adding graphs and tables to a worksheet and these will be updated automatically each time SOFEA© is run. A strength of SOFEA© is the possibility of "what if" scenarios. The output figures and tables will be dependent on the problem being studied.

SOFEA© returns tables giving exposure at many locations at a sequence of times. In the first stages of testing, all sorts of plots will be needed to look for aberrant values and generally help decide if the results make sense. Time series plots, box and whisker plots, and scatter plots will be useful here for as many variables and combinations of variables as one can think of. Note that while box and whisker plots are very useful for exploratory data analysis, they are very clumsy to create in Excel. Further down the line, end-users will appreciate geographical contour plots for median and upper percentiles of acute and chronic exposure.

The results for upper percentiles will only be meaningful if the model captures all sources of variation and enough simulations are run under each scenario.

The plot of concentration versus exceedance percentile for the pseudo-validation shown in the Agency presentation (handout page 47) shows concentration on a log scale. Even though statisticians like log scales because the plots look neater, a linear scale would in this case de-emphasize the good agreement at low concentrations and exaggerate the poor agreement at high concentrations, giving a very different impression. If we accept that it is more important for models to be accurate at upper percentiles, diagnostic plots should be on linear scales.

Not all Panelists were able to try running SOFEA© because most did not have access to Crystal Ball, and hence only a few Panelists were able to make specific suggestions concerning routine reporting of inputs and outputs.

There was general agreement that the inputs required should include the fumigant applied, application rate, type of application, application depth, tarp use or none, field size (or numbers of fumigated fields for regional analysis), soil conditions that will affect fumigant dispersion in the soil and subsequently into the atmosphere and weather parameters that affect stability. The outputs should include flux rates, fumigant concentrations at buffer perimeters relative to toxicity concentrations, exceedance frequency, distance from the source at which exceedances occur, maximum daily emission, and losses over time through emission into the atmosphere.

Another recommendation is to add graphics showing the distribution of statistical parameters at a selected number of receptors, say, 100–200 receptors at various distances from the source. The graphics can show the median at each receptor based on the Monte

Carlo runs, as well as the coefficient of variation (standard deviation/mean), and variability/uncertainty range:

(2.5th percentile - mean)/mean; (97.5th percentile - mean)/mean.

8(C) Does the Panel recommend any further steps to evaluate* SOFEA© *and if so, what?

Panel Response

SOFEA©, like any other model at this stage of development, will need a line-by-line code audit by an independent programmer to ensure that the code does what it is supposed to do. The hardest programming errors to detect are those that deliver results that look correct but in fact are wrong. A code audit should pick up any errors of this kind. The FORTRAN code in particular needs to be audited because it is so detailed. SOFEA© relies on code within Crystal Ball and Excel. A number of the statistical functions in Excel are known to be deficient. Serious problems with the Excel random number generator were identified in SAP Minutes 2000-01 "Session III: Dietary Exposure Evaluation Model (DEEM)", citing McCullough and Wilson (1999). We need documentation and testing of the random number generator in Crystal Ball and if it too proves to be deficient, a better random number generator must be used.

The Panel was concerned that "calms" could be very important and had not been adequately incorporated into the model. Perhaps the ISCST3 model is not conservative enough in this regard. It is a limitation of ISCST3 that no stability categories are applicable for nighttime calm and near calm conditions.

The Panel recommends running a series of simulations to determine whether the shape of fumigant flux profiles impact acute or chronic exposure estimates generated by the model. Profiles can be developed from published or unpublished studies or they could be simulated. Cumulative losses would be held constant. A factorial experiment where cumulative losses are also varied may prove insightful and help guide decisions on the conduct of additional flux field experiments or in the selection of an "appropriately" conservative flux profile for use in exposure assessments. Another area that should be explored is the impact of weather. Simulations should be run under a variety of worst-case conditions to determine the extent to which "extreme" conditions (high or low temperature, wind, stability etc.) may influence results.

Further evaluation of SOFEA©'s ability to simulate acute and chronic exposure at receptor points would be helpful, but this will be difficult without the availability of extensive data sets. It may be possible to use available methyl bromide data, but evaluation of SOFEA© with this chemical may not be of interest to the developers. This may be an appropriate activity for EPA or CDPR. This might also be a good first step in promoting SOFEA© to the user community.

Despite these difficulties, SOFEA© should be evaluated with other fumigants under various conditions. There is a need to evaluate the model with at least two other different types of fumigants using real data from different areas where it could prove useful. Since a specific fumigant may be widely used in certain areas and use rates are frequently high, knowledge of chronic exposures could be a useful regulatory tool for risk assessment and management.

The broader question of determining whether the model is good enough is much more difficult to address. Because of the wide range of expertise on the Panel, there were many suggestions for enhancing the model, and some of these may make a significant difference in model output under some scenarios. Because we could go on forever improving the model, the question is not so much whether the model is completely realistic, but rather, is it complete enough for regulatory purposes? At this stage, the Panel recommends incorporating those proposed enhancements that look most promising and doing more validations (or pseudo-validations) in comparison to field data, looking particularly for agreement in upper percentiles and under both typical and extreme scenarios. It is encouraging that comparison with observed field data seems to be very feasible in these applications.

(8D)* SOFEA© *uses a Monte Carlo based approach based on varied random number streams for each simulation. Can the Panel comment on the appropriate statistical techniques that should be used to define differences between outputs for different scenarios?

Panel Response

This is the correct way to run simulations. In the exploratory stage of development, scenarios should be run several times with independent random number streams. It is important to run enough replications to see stability, allowing for variability in field sampling data.

If the results are presented as cumulative probability distributions, however, it will be difficult to analyze them, as statistical tests such as the Kolmogorov Smirnov test to compare distributions are too powerful and cannot easily be extended to compare the results of many different scenarios. The best approach would be to summarize each run by an upper quantile, making the response univariate. The variability in the results can then be displayed simply with box and whisker plots or superimposed time series.

When the developers proceed to a more formal sensitivity analysis using the methods advocated in (8A), the variability between simulations due to independent random number streams will be taken into account in the factorial analysis of variance.

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