Exposure Assessment Approaches For Chemicals Used As Soil Fumigants

Consideration Of The Soil Fumigant Exposure Assessment System (SOFEA) - A Case Study With 1,3-Dichloropropene

Presented To The FIFRA Science Advisory Panel By:

U.S. EPA Office Of Pesticide Programs
Health Effects Division

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1 INTRODUCTION

On August 24-25, August 26-27, and September 9-10, 2004, the FIFRA Scientific Advisory Panel (SAP) will hold three separate meetings to consider and review three fumigant bystander exposure models. At the August 24-25 meeting the SAP will review the Probabilistic Exposure And Risk Model For Fumigants (PERFUM) using iodomethane as a case study. On August 26-27, the SAP will review the Fumigant Exposure Modeling System (FEMS) using metam sodium as a case study. On September 9-10, the SAP will review The Soil Fumigant Exposure Assessment System (SOFEA) using 1,3-dichloropropene as a case study. In preparing for these meetings, preparation of this document, and development of questions for the Panel, the Agency has worked closely with scientists from the California Department of Pesticide Regulation who have significant experience with inhalation exposure modeling.

The purpose of this document is to provide general background information for the FIFRA Science Advisory Panel (SAP) meeting pertaining to the evaluation of the *Soil Fumigant Exposure Assessment System* (or SOFEA). SOFEA represents a potential evolution of the Agency's current methodology for calculating exposures to bystanders who can be exposed by being in proximity to fields treated with soil fumigants prior to planting crops such as strawberries or tomatoes. SOFEA is also capable of defining exposures from multiple sources within an airshed based on the California township system. SOFEA was developed by the registrants (i.e., manufacturers or licensees) of the soil fumigant 1,3-dichloropropene. At the upcoming SAP meeting, a detailed SOFEA case study will be presented based specifically on 1,3-dichloropropene data for illustrative purposes by its developers. More specific background materials pertaining to the theories and code included in SOFEA than there are in this document, are available in the following which has been provided by its developers for consideration (available at: http://www.epa.gov/oscpmont/sap/2004/#top).

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The Agency has a broad range of goals for this meeting in that it wishes to evaluate the methodologies inherent in SOFEA from a general perspective to (1) determine their scientific validity and (2) determine if there is any general applicability for evaluating risks associated with many or all soil fumigants. There are three key criteria that the Agency considers when considering the integration of a model into its risk assessment process and these include: (1) public availability; (2) peer review for scientific validity; and (3) adherence to Agency guidelines for model development. In order to have SOFEA considered by the Agency and by the SAP the developers of SOFEA have agreed to make it available for public use.

The Agency is currently involved in the development of a comparative risk assessment for 6 pesticides that are used for soil fumigation purposes. Some of these chemicals also have other allowed uses but, for clarity, the discussion within this document focuses only on soil fumigation since it is of key concern and it accounts for the majority of the annual usage for each chemical. The chemicals which are included in this assessment are: chloropicrin, dazomet, iodomethane (i.e., methyl iodide), methyl bromide, metam-sodium (or other salts), and 1,3-dichloropropene. Each of these chemicals (or their breakdown products, metam-sodium and dazomet both emit MITC or methyl isothiocyanate which is the volatile component) are

extremely volatile especially when compared to most common pesticides. Most common pesticides are considered semi-volatile organic chemicals (or SVOCs) while soil fumigants would be considered volatile organic chemicals (or VOCs). The volatility of each material is the key characteristic associated with their use and achieving a satisfactory measure of efficacy. This volatility, however, can lead to a potential for human exposures because it leads to transport away from targeted application areas to non-target receptors such as nearby human populations.

The Agency's goal for this risk assessment is to quantify emissions from treated fields and use them as a determinant of human risks. Emissions from treated fields can be categorized in two ways including:

(1) **Known Source:** include those directly associated with a single application (or series of associated applications) adjacent to a receptor where the source and emissions specific to the application(s) can be quantified. An example would be treating a field that borders a residential subdivision then defining the amount of off-target residue movement associated with that specific application. The concept of a buffer zone as a risk management tool is commonly associated with these situations.

(2) **Multiple Source (Ambient Air):** includes those associated with multiple applications or general use within a region where many non-quantifiable applications can possibly contribute to overall exposure levels. In general, ambient exposures within a region cannot be easily attributed to specific application events. An example of this type of emission might be those air concentrations measured at a school location when the school is located within a growing region where fumigants are extensively used. The concept of a localized use cap or exposure limit as a risk management tool is commonly associated with these types of exposures.

In order to quantify emissions from known sources (i.e., single application events), the Agency currently uses an approach that first considered the monitoring data available for each of the six soil fumigants along with a deterministic modeling approach. It was clear that given the breadth of the uses associated with soil fumigants (e.g., varied atmospheric conditions, application methods, and emission reduction technologies such as tarping or watering in) that use of monitoring data alone for risk assessment purposes was limited by the relatively small number of samples which can reasonably be generated for different times after treatment, distances from the application site, and use patterns. This conclusion led to the development of the Agency's current modeling approach and the possible evolution of that approach represented by SOFEA. The model-based approach considers temporal and spatial factors, extrapolating from available monitoring data, thus providing an estimate of the range of exposures which are possible at different times and locations when input parameters are varied.

The Agency is currently using a deterministic modeling approach for defining air concentration gradients downwind of known single applications for each chemical. In this approach, the Agency has based its analysis on a standardized set of meteorological conditions intended to represent a stable atmosphere and unidirectional wind patterns that is intended to provide high-end estimates of exposure. To this end, the Agency has developed a methodology based on the Office of Air model ISC3 (Industrial Source Complex Model) that is routinely used for regulatory purposes. ISC3 is a steady-state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources. ISC3 is a publically available

system and can be downloaded from the Agency (http://www.epa.gov/scram001/tt22.htm#isc).

Stakeholders have commented to the Agency a belief that these standardized meteorological conditions used for known source assessments are not representative of actual atmospheric conditions where soil fumigants are used and therefore solely provide screening level results which are inadequate for risk mitigation decision making purposes. To this end, the 1,3-dichloropropene registrant has submitted to the Agency the SOFEA model for consideration. SOFEA integrates actual meteorological data into ISC3 which then provides for the calculation of multi-directional air concentration gradients based on these data. As with the Agency's approach, these resulting concentration gradients would ultimately be used as a determinant of human health risks. Additionally, it should also be noted that the SOFEA model uses a probability based approach for integrating emission data which are unique to this system.

In order to quantify emissions from multiple sources (i.e., ambient air levels), the Agency currently uses an approach based solely on available monitoring data. To date, a modeling approach that can be used to predict ambient air levels has not been defined by the Agency. The Agency believes that the use of monitoring data alone can provide useful information to risk managers about levels in the environment which might be a source of exposure in the general population. The Agency believes that ambient air levels are related to the amounts of material applied within airsheds, the distances of receptors to use sites, meteorological conditions within a region, and how chemicals are applied. SOFEA can calculate exposure levels from multiple sources within an airshed so it can potentially be used to predict ambient air levels. This could prove useful to the Agency in refining its assessment of these types of exposures but it is limited because extensive use data are needed to operate the model which is generally only available in California.

This document describes the Agency's current approach for model use in *Section 2: Summary Of Current Modeling Approach*. *Section 3: Overview of Soil Fumigant Exposure Assessment System (SOFEA)* provides a brief summary of the approaches that have been incorporated into the system. *Section 4: Charge To Panel* details the specific questions pertaining to the use of SOFEA which the Agency would like the SAP panel to address in its deliberations.

2 SUMMARY OF CURRENT MODELING APPROACH

The goals of the Agency in its fumigant assessment are to estimate risks for populations in proximity to fields that have been treated with soil fumigants as well as to explain and reduce, whenever possible, the uncertainties associated with these analyses. In order to achieve these goals the Agency considered monitoring data specific to each chemical but, due to the limitations of those data and the flexibility that modeling represents, have since focused on model results as the key predictor of exposures. [Note: As discussed above, SOFEA can be used to predict exposures from both single and multiple sources as well as varying durations. The Agency is only currently using modeling to evaluate exposures from single events so that is the focus of discussion in this section.]

The Agency's current exposure assessment approach is based on a deterministic use of the Agency's Industrial Source Complex Model (ISC) which is routinely used by the Office of Air for regulatory decision making purposes. It is available from the following website at the *Technology Transfer Network Support Center for Regulatory Air Models (or SCRAM)* (http://www.epa.gov/scram001/tt22.htm#isc). ISC is a steady-state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources associated with an industrial complex or from other types of sources such as an agricultural field in this case. This model can account for the following: settling and dry deposition of particles; downwash; point, area, line, and volume sources; plume rise as a function of downwind distance; separation of point sources; and limited terrain adjustment. ISC can operate in both long-term and short-term modes but has been used in the short-term mode for the purposes of this assessment.

The Agency's current approach is summarized herein. *Section 2.1 Input Variables And Settings Used For ISC Calculations* describes the current modeling approaches used by the Agency including a description of the specific inputs and ISC settings used for the calculations. *Section 2.2 Outputs Based on Current Modeling Approach* provides examples of the outputs from ISC that might be presented for consideration by risk managers. To ensure a level of consistency in the evaluation of the SOFEA model, the examples presented below to describe the current Agency methodology are also based on a case study using 1,3-dichloropropene.

2.1 Input Variables And Settings Used For ISC Calculations

In order to define concentration gradients associated with the use of soil fumigants, which are ultimately determinants of exposure, the Agency utilized ISC by equating treated agricultural fields to an area source coupled with inputs that reflected a range of potential atmospheric conditions and application equipment/techniques used for the different fumigant chemicals. In order to do this, the Agency considered various combinations of four categories of input variables including:

- Field Size;
- Atmospheric Conditions;
- Application Equipment and Control Technologies; and
- Field Emissions Associated With Application Equipment and Control Technology.

[Note: As a convention, the Agency has used similar input variables for all of the 6 soil fumigant chemicals wherever possible. This allows for an easier determination of the relative risks amongst the 6 soil fumigants. Some input factors such as emission data, however, are by nature chemical-specific and have been treated as such in analyses completed by the Agency. This is the rationale behind providing a separate section which details how the emission data were analyzed for 1,3-dichloropropene.]

Field Size: The Agency generically is using a range of field sizes for single application events from 1 acre up through 40 acres. Specifically, the Agency based its calculations on field sizes of 1, 5, 10, 20, and 40 acres. It is believed that most distinct soil fumigation application events will be within this range of areas treated. It is also acknowledged larger fields could be treated on a single day. Results could easily be scaled to those larger acreages if needed. Field geometry can also impact the results of ISC modeling. For ease, the Agency has by convention completed all of its analyses based on the use of square fields.

Atmospheric Conditions: ISC calculates downwind air concentrations using hourly meteorological conditions, that include wind speed and atmospheric stability (for a more detailed discussion of stability see http://www.epa.gov/scram001/userg/relat/pcramtd.pdf). The higher the letter associated with a stability class the more stable the atmosphere becomes. The lower the wind speed and the more stable the environment, the higher the air concentrations are going to be close to a treated area (or source). Conversely, if wind speed increases or the atmosphere is less stable, then air concentrations are lowered in proximity to the treated area thereby lowering the potential for exposure. Atmospheric stability is essentially a measure of how turbulent the atmosphere is at any given time. Stability is affected by solar radiation, wind speed, cloud cover, and temperature among other factors. Instability in the atmosphere increases the movement of airborne residues because they are more readily pushed up into the atmosphere and moved away from the source thereby lowering concentrations in proximity to the source (e.g., treated field).

In order to simplify modeling the transport of soil fumigant vapors from a treated field, a single wind direction, wind speed, and stability category are used for a given duration of concern (i.e., 24 hours). The Agency has decided to present a series of results based on a range of possible, and plausible, meteorological conditions to allow for a better characterization of risks compared to just completing the analyses based on a single set of meteorological conditions. The different conditions considered by the Agency are presented in Table 1.

For comparative purposes, the California Department of Pesticide Regulation, in its determination of buffer zones for methyl bromide, based its decisions upon a windspeed of 1.4 m/s and a class C atmospheric stability value for a 24-hour period. During the daytime hours, these conditions represent a stable atmosphere which is relatively calm but this stability is not considered overly calm for nighttime conditions. We believe these values provide higher-end air concentrations. [Note: This is supported by an analysis methyl bromide buffer zones by DPR available at: www.cdpr.ca.gov/docs/dprdocs/methbrom/mebrmenu.htm.]

Table 1: Meteorological Combinations Used in ISC Calculations		
Wind Speed (mph)	**Wind Speed (meters/second)**	**Stability Category#**
2.25	1.0	D
3.1*	1.4*	C*
4	1.8	C
5	2.2	C
6	2.7	C
7	3.1	C
8	3.6	C
9	4.0	C
10	4.5	C
10	4.5	B

= The lower the assigned "letter" the less stable the atmosphere. Categories A to D are generally seen in daylight conditions. Nighttime conditions are generally even more stable than even the most stable daylight conditions.
* = Conditions used in DPR assessment and risk management decisions for methyl bromide.

Application Equipment and Control Technologies: Application equipment and control technologies are varied and depend on many factors including the environmental fate characteristics of the chemical, terrain where the chemical is being used, economic considerations, and other agricultural practices. Application equipment can take many forms but applications typically involve the use of some sort of probe that is used to inject material beneath the surface of the soil, a broadcast application of a liquid solution or solid material across the surface of a treated area, or the delivery of chemicals through some sort of plumbed system throughout the treated area (e.g., some chemicals are delivered via irrigation water).

Along with the various application methods there are a number of control technologies that are intended to minimize the emissions from treated fields. These can take many forms but essentially involve one of three basic techniques that include: (1) change in injection depth and probe design; (2) use of tarping or bedding techniques; and (3) watering-in.

Ultimately, the goal of the Agency is to categorize different combinations of application methods and control technologies in order to have these serve as a systematic basis for risk assessments. The ability to do this, however, varies depending upon the data available for each chemical. In some cases, such as methyl bromide, there is a preponderance of data that allows for characterization based on a large number of possibilities as described by the California Department of Pesticide Regulations in its permit conditions which are presented on their website (http://www.cdpr.ca.gov/docs/legbills/mebrbuffer.pdf).

The situation with 1,3-dichloropropene is similar in that DPR has instituted regulations at this time to control exposures. These include buffer zones, soil sealing requirements, depth of placement, and required field conditions at the time of application. DPR is also evaluating the use of township caps to limit ambient exposures from multiple sources or applications. Based on the available data, the Agency has developed categories of application methods associated with 1,3-dichloropropene use (Table 2). These include 4 basic categories of application equipment with different potential exposure reduction technologies associated with each. This list is by no means inclusive of the ways that 1,3-dichloropropene might possibly be applied in agriculture but data are not available to adequately quantify other types of application methods or emission reduction technologies. Hence, all analyses that were completed were based on these categories.

Table 2: Summary Of Application Methods For 1,3-Dichloropropene

Application Method	Potential Emission Reduction Technology	Combination #
Shallow shank, broadcast flat fume	Soil roller	1
Shallow shank, row application in beds	None	2
Drip irrigation, raised bed	Tarped	3
Buried drip irrigation, 5 inch deep beds	None	4

Field Emissions Associated With Application Equipment and Control Technology: Emissions from treated fields are generally characterized as the amount of residues that are offgassing from a unit area per unit time. Emissions quantified in this manner are referred to as flux ($\mu g/m^2$-s). Flux rates are specific to the conditions of the field experiment for which they were generated but can be used in a generic sense by normalizing the data to the maximum application rates of 362 pounds per acre for the shank injection methods and 164 pounds per acre for the drip irrigation methods. The rates vary based on label specifications for different application methods which were considered for the purposes of this example. Flux rates were calculated using the aerodynamic flux rate method based on direct measurements of flux in the field in the monitoring studies. The normalized flux rates which were determined for 1,3-dichloropropene are summarized below in Table 3.

Table 3: Summary Of Normalized Flux Rates For 1,3-Dichloropropene			
Application Method	**Potential Emission Reduction Technology**	**24 Hour Flux Rates ($\mu g/m^2$ - s)**	**Combination #**
Shallow shank, broadcast flat fume	Soil roller	91	1
Shallow shank, row application in beds	None	70	2
Drip irrigation, raised bed	Tarped	8	3
Buried drip irrigation, 5 inch deep beds	None	32	4
Note: These values are subject to change as the Agency was finalizing these calculations during the time this document was prepared. Additional information concerning these flux calculations will be presented by the Agency at the SAP meeting during introductory remarks.			

Other Settings/Parameters: Along with the input variables described above that have been considered by the Agency in this assessment there are other parameters (or settings) that must be defined in order to complete an ISC analysis. These parameters include (see Figure 1):

- Rural conditions are used;
- Mixing height 692 m for rural settings (based on DPR analysis);
- Receptor height at ground level (similar to DPR analysis);
- Source (i.e., the treated field) is treated as an area source;
- Source (i.e., the treated field) is square oriented in north/south direction;
- Grid origin is SW corner of field;
- Receptors are centerline of field to the south, buffers are from edge of field;
- Release height is 0 meters;
- Flux rates determined from monitoring data using aerodynamic flux rate method which was based a direct measurement of flux in treated fields;

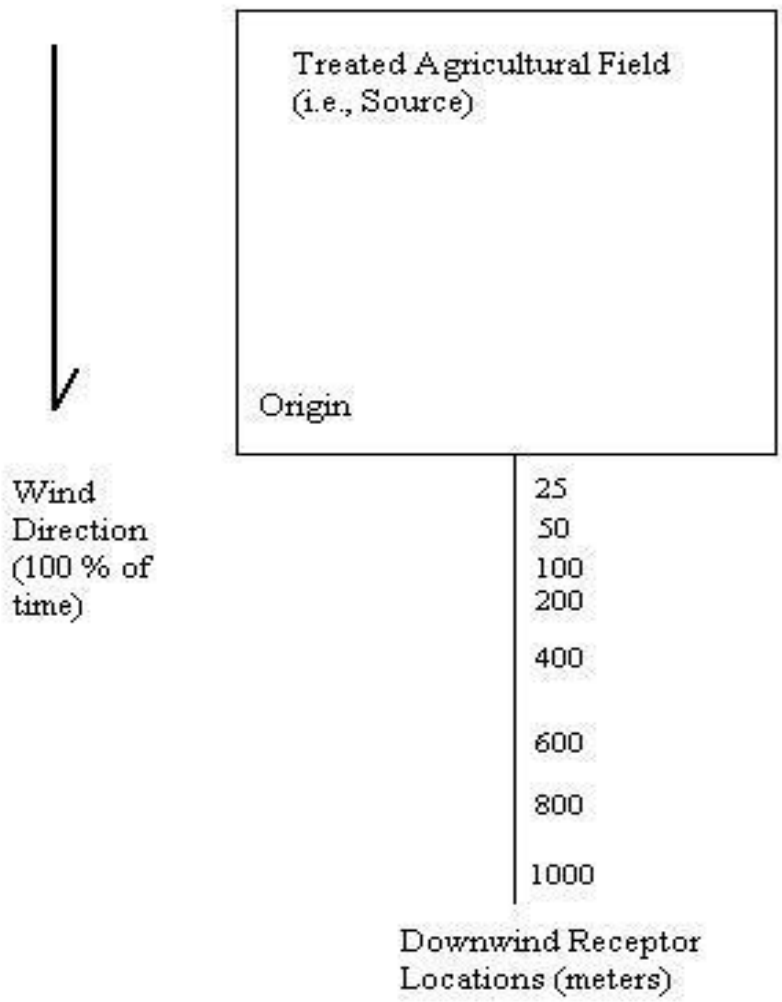
- Deposition is not accounted for and is expected to be minimal due to volatility of chemical; and

- Standard regulatory default options as defined in ISC User's Guide Volume 1 have been used.

2.2 Outputs Based on Current Modeling Approach

Examples of the kinds of outputs which can be generated by ISC based on inputs similar to those described above are presented in this section. For the purposes of this example, the outputs represent 24 hour average concentrations at selected downwind receptor points. The receptor points are illustrated in Figure 1 along with the unidirectional nature of the meteorological conditions (i.e., wind direction) upon which the assessment is based.

Figure 1: ISC Source & Receptor Grid - Std. Analysis



The results based on the Agency's deterministic method are presented below for the shallow shank broadcast flat fume with soil bed roller scenario (Combination 1). These results are only included for illustrative purposes and are solely intended to provide an example of the Agency's calculation method. These results include air concentrations (µg/m^3) at selected receptor points downwind for a variety of meteorological conditions (Table 4). The conditions considered in this analysis range from a stable atmosphere conducive to higher concentrations in proximity to treated areas to conditions that are much less stable which lead to lower concentrations in proximity to treated areas.

Table 4: ISC Calculated Air Concentrations At Selected Distances Downwind (µg/m^3) For Pre-Plant Agricultural Field Fumigations

ER	Fld Size (A)	DW Dist. (M)	Air Concentrations At Differing Meteorological Conditions									
			1 m/s 2.3 mph	1.4 m/s 3.1 mph	1.8 m/s 4 mph	2.2 m/s 5 mph	2.7 m/s 6 mph	3.1 m/s 7 mph	3.6 m/s 8 mph	4.0 m/s 9 mph	4.5 m/s 10 mph	4.5 m/s 10 mph
			Stab D	Stab C	Stab C	Stab C	Stab C	Stab C	Stab C	Stab C	Stab C	Stab B
0.19	1	25	1,799	830	646	528	430	375	323	291	258	182
		100	795	336	261	214	174	152	131	117	104	62
		500	144	41	32	26	21	18	16	14	13	5
	40	25	4,489	1,992	1,549	1,268	1,033	900	775	697	620	431
		100	2,818	1,206	938	767	625	545	469	422	375	255
		500	1,238	479	373	305	249	217	186	168	149	84

Note: ER = emission rate which defines flux in terms of the percentage of the amount applied. The emission rate of 19 percent or 0.19 for this application method was calculated by dividing the flux rate of 91 µg/meter squared -second by the application rate of 362 pounds/acre/day after conversion to similar units and adjustment of the flux rate to a 24 hour value. The flux data upon which this analysis is based is from study with MRID 450105-01.

The air concentrations presented in Table 4 would then be used to calculate a risk estimate for each condition. The Agency uses *Margins of Exposure* to represent non-cancer risks which are calculated using the following formula:

$$MOE = \frac{HEC\ (\mu g/m^3)}{Air\ Concentration\ (\mu g/m^3)}$$

Where:

MOE	=	Margin of exposure, value used to represent risk or how close a chemical exposure is to being a concern (unitless);
Air Concentration	=	The concentration in air to which an individual could be exposed (µg/m^3); and
HEC	=	Human equivalent concentration is the air concentration of a toxicant at a level at which an effect might occur (e.g., NOAEL or LOAEL) after it has been adjusted to pharmacokinetic differences between the test animal species and humans.

The Agency wishes to focus discussion at the SAP meeting on the methodologies contained in SOFEA that could potentially lead to an evolution in the manner in which the Agency calculates exposure concentrations such as in Table 4 and not on other risk assessment related issues specific to the 1,3-dichloropropene case study example. As such, the Agency has not included any risk estimates in this document for the case study.

3 OVERVIEW OF SOIL FUMIGANT EXPOSURE ASSESSMENT SYSTEM (SOFEA)

The *Soil Fumigant Exposure Assessment System (SOFEA)* is a modeling tool that could potentially represent an evolution in the manner in which the Agency calculates exposures from soil fumigants. It is the methodologies included in SOFEA that the Agency wishes the SAP panel to consider in its deliberations. This section contains a very brief overview of the SOFEA system and how the outputs might differ from those generated using the current Agency approach for calculating exposures. Definitive discussions of SOFEA can be found in the following (http://www.epa.gov/oscpmont/sap/2004/#top).

SOFEA © (Soil Fumigant Exposure Assessment System) (User's and Programmer's Guide), van Wesenbeeck and Cryer, Copyright 2004

In addition, 3 different case studies were completed using SOFEA (or its direct precursors) by its developers. [Note: None of the case studies referenced below corresponds directly with the calculations described above for the Agency's approach. However, an evaluation of the potential refinements offered by SOFEA compared to Agency's current approach can still be completed based on the available information.] These are included in the following documents which should be considered in conjunction with the User's and Programmer's Guides referenced above:

Predicted 1,3-Dichloropropene Air Concentrations Resulting From Tree and Vine Applications In California; S.A. Cryer and I.J. van Wesenbeeck; J. Environ. Qual. 30: 1887-1895 (2001).

Predicting Regional Emissions and Near-Field Air Concentrations Of Soil Fumigants Using Modest Numerical Algorithms: A Case Study Using 1,3-Dichloropropene; S.A. Cryer and I.J. van Wesenbeeck and A.J. Knuteson; J. Agric. Food Chem.. 51: 3401-3409 (2003).

Predicting Soil Fumigant Acute, Sub-Chronic, and Chronic Air Concentrations Under Diverse Agronomic Practices; S.A. Cryer, Dow AgroSciences, Inc. Document (included in SAP background materials); (2004).

The purpose of this discussion is to provide readers with an overview of the approaches included in SOFEA. Much of the discussion in this section and the graphics included herein are excerpted directly from the above documents. It should also be noted that the SOFEA developers used data specific to the soil fumigant, 1,3-dichloropropene, as the basis for the these documents. The Agency believes that the methods applied in this analysis have generic applicability to all fumigants and wishes that SOFEA be considered in this manner yet keeping in mind that some of the inputs used for this analysis have to be specific to 1,3-dichloropropene in order to complete the case study analysis.

SOFEA (Soil Fumigant Exposure Assessment System) is a stochastic modeling tool that can be used to evaluate human exposure potential. SOFEA can calculate fumigant concentrations in air arising from volatility losses from treated fields for entire agricultural regions using multiple transient source terms (treated fields), GIS information, agronomic specific variables, and user defined thresholds. A modified version of the USEPA Industrial Source Complex Short-Term model (ISCST3) is used for air dispersion calculations. SOFEA uses field observed or numerically generated fumigant flux profiles from soil as transient source terms for both shank injection and drip irrigation applications. Reference flux observations are scaled based upon depth of incorporation and the time of year to model the complete flux response surface from field/numerical observations. Weather information, field size, application date, application rate, application type, depth, pesticide degradation rates in air, tarp presence, ag-capable land, field retreatment, buffer setbacks, and other sensitive parameters are varied stochastically using Monte Carlo techniques to mimic region and crop specific agronomic practices. Agricultural regions up to 19,000 square miles can be simulated for temporal periods ranging from 1 day to 70 years for the purpose of assessing all different durations of exposure (i.e., acute through chronic durations). Multi-year simulations can also be conducted using random field placement in all agricultural capable areas as well by selectively placing fields in historical or prospective use areas. Regional land cover, elevation, and population information can be used to refine source placement (treated fields), dispersion calculations, and exposure assessments. SOFEA also allows for simulating exposures based on current as well as anticipated/forecasted fumigant use over time.

Specifically, in the case studies developed based on 1,3-dichloropropene, the following options/inputs were considered:

- Basic simulations include 9 township grids with 1 centrally located township grid (6 by 6 miles) and up to 19000 square miles can be considered per simulation.;
- There are 100,489 receptor points within each township;
- Receptors are at 1.5 m breathing zones;
- Dispersion parameters were fixed at the ISCST3 regulatory default values;
- A modified version of the Pesticide Root Zone Model (PRZM3) can be used to model flux rates;
- Cryer *et al*, 2001 focused on vine/trellis crops;
- Cryer *et al*, 2003 focused on soil fumigation and used scenarios in Georgia, North Carolina, Washington, Florida, and California which were selected based on use data;
- Flux data were predominantly based on direct in-field monitoring and were defined based on the aerodynamic flux method; and
- Meteorological data were processed using PCRAMMET.

The following several figures describe some of the input parameters and outputs of SOFEA. Figure 2 provides a description of the township approach which is used in the SOFEA analysis.

Figure 2: Townships & Land Cover Near Santa Cruz, California

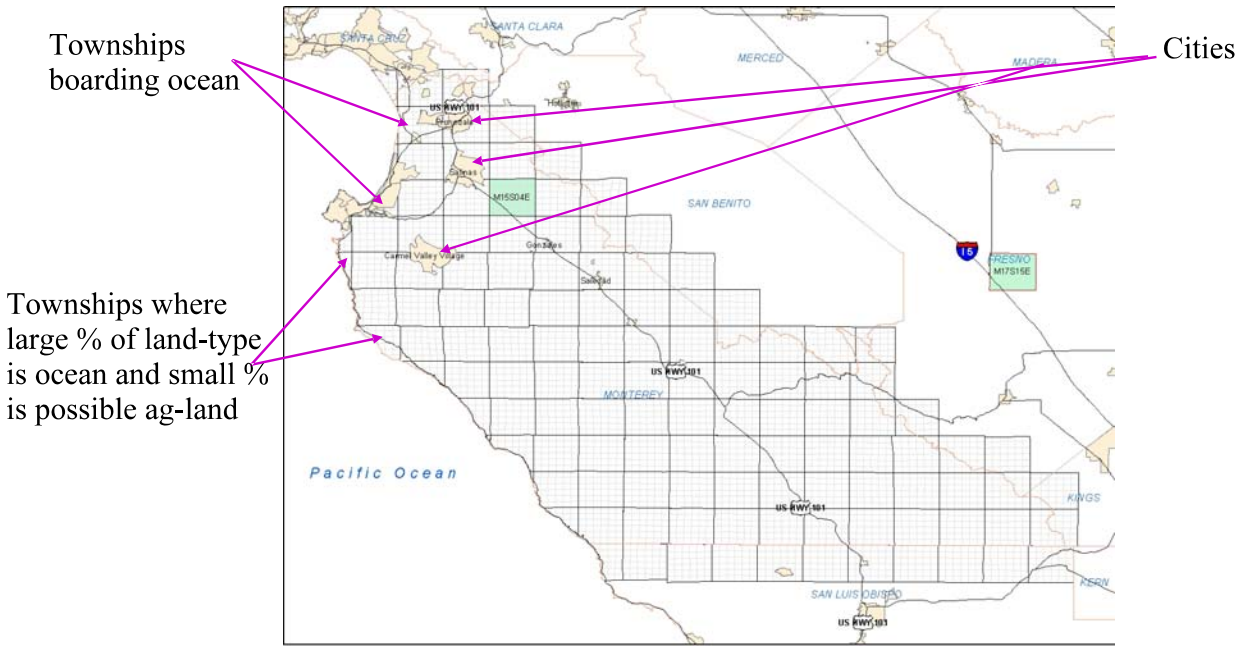


Figure 3 provides and example of the types of flux/emission data that was available for 1,3-dichloropropene.

Figure 3: 1,3-Dichloropropene Flux Rates vs. Time For Shank Injection At 122 lb/acre

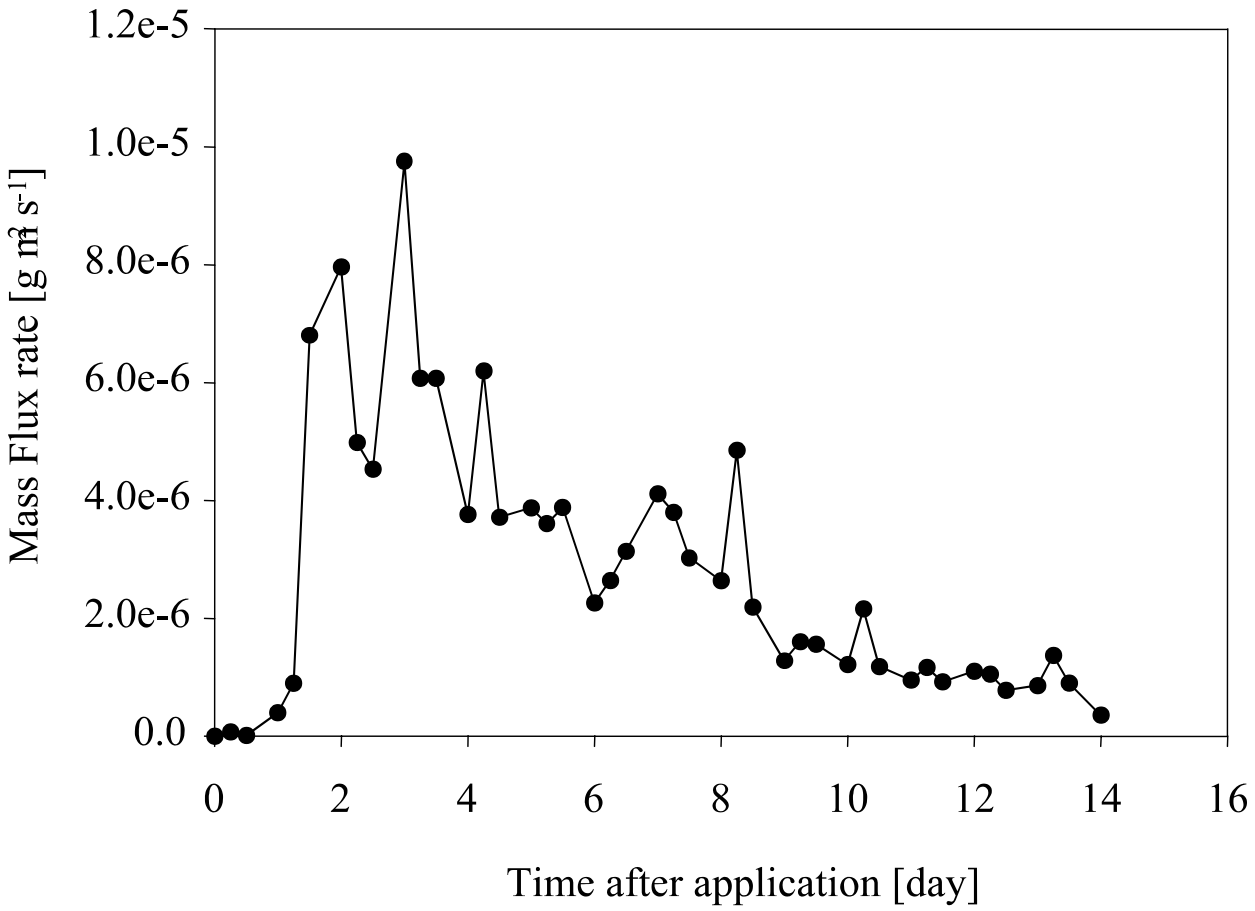


Figure 4 illustrates SOFEA field placement results for both random and section weighting for a 3x3 township simulation domain. In this example, it is near Ventura California. Each small square represents a source term for different crop types. The total mass of fumigant applied within a township is a user specified input.

Figure 4: Example Random & Section Weighted Field Placement For Various Crops

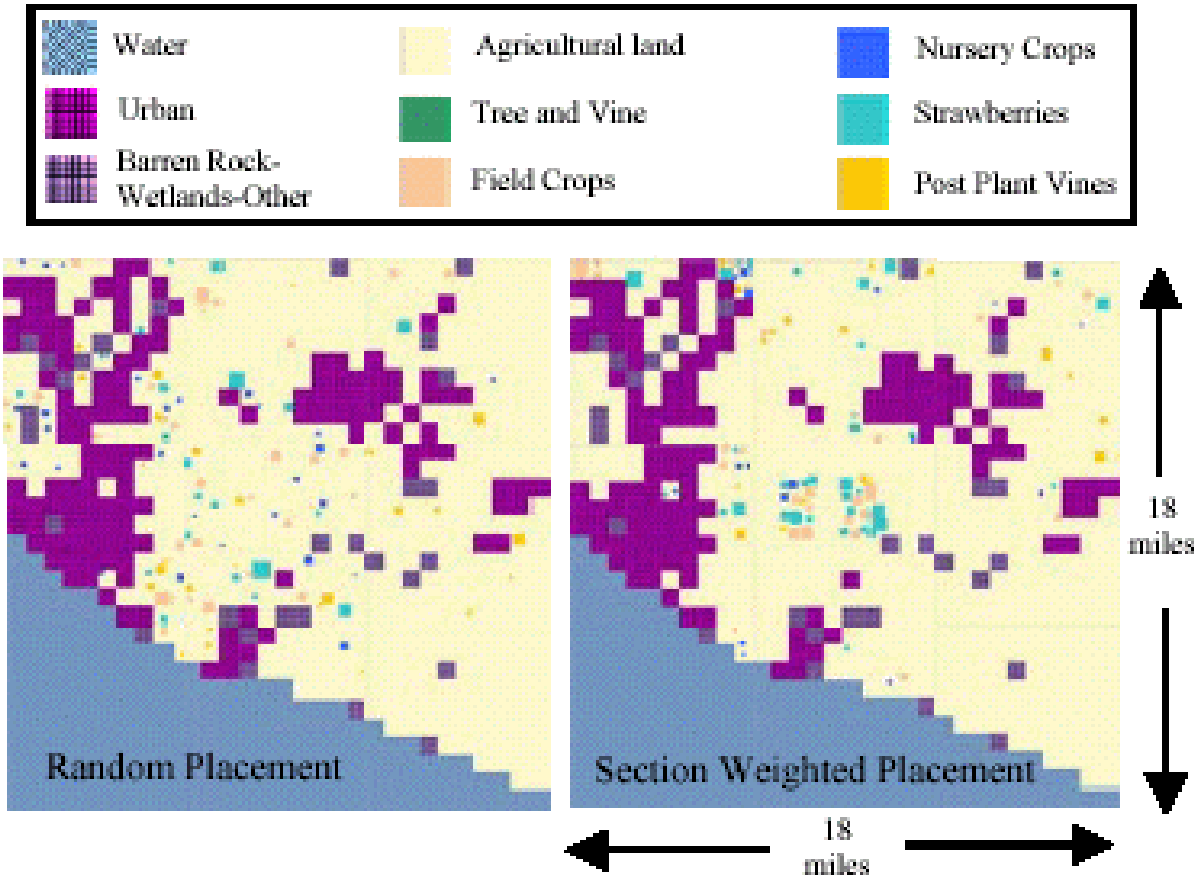
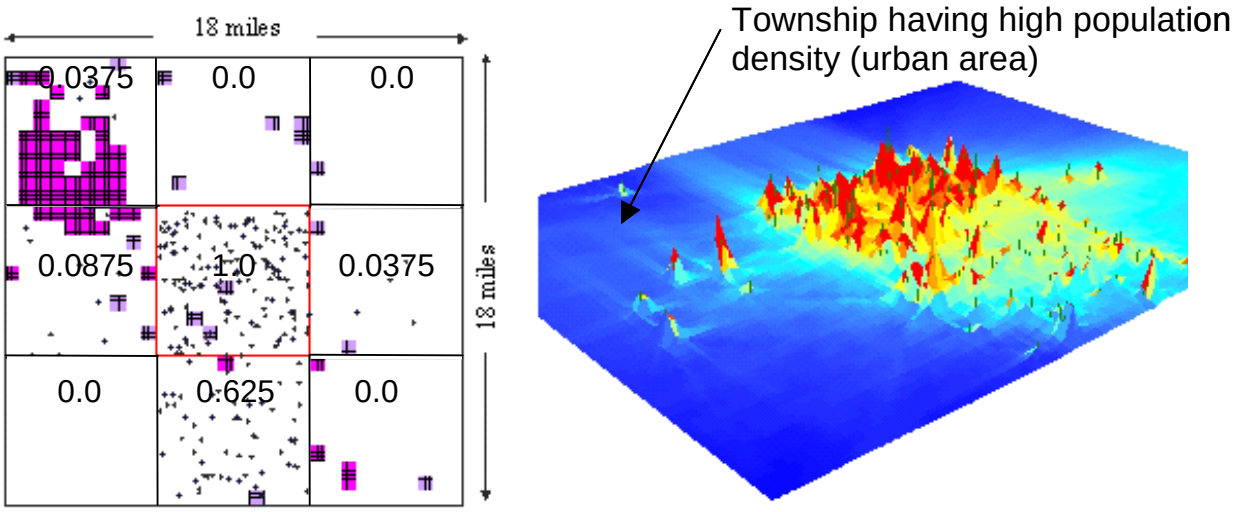


Figure 5 illustrates how geo-referenced population data can be superimposed on the air concentration data generated by SOFEA to address risks for a population within a selected airshed. Each receptor of the uniform grid within a township is assigned a population density. This example provides results for Monterey County, California where it is evident that the lowest air concentrations occur near the area with the highest population density and conversely, the areas with the highest air concentrations are near the more agricultural land.

Figure 5: Example Results Based On Monterey County California Based On A 3x3 Township Domain



4 CHARGE TO PANEL

This section presents the charge questions the Agency wishes the panel to consider in its deliberations pertaining to SOFEA. The nature of these questions are varied and range from issues pertaining to the documentation, design, and operation of SOFEA to the manner in which results are presented. For simplicity, the Agency has grouped the questions by subject matter that reflect critical elements pertaining to the use of SOFEA and results generated by SOFEA. The key subject matter areas include: (1) documentation; (2) system design/inputs; and (3) how results are presented.

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. Please comment on the detail and clarity of these documents. Are the descriptions of the specific model components accurate? Do the algorithms in the annotated code perform the functions as defined in this document? Please discuss any difficulties encountered with respect to loading the software and evaluating the system including the presented case study?

Critical Element 2: System Design/Inputs

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. Please comment on these proposed processes, the nature of the components included in SOFEA and the data needed to generate an analysis using SOFEA? Are there any other potential critical sources of data or methodologies that should be considered?

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. 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? 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. 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? Please comment on SOFEA's capability to adequately consider multiple, linked application events on an airshed basis as well as single source scenarios. Does SOFEA appropriately address situations where data are missing?

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. Can the panel comment on the value of adding this information for conducting spatially realistic simulations? 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? 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. Data quality and uncertainty associated with these data vary with the source. Does the panel agree with the approaches used to characterize these factors? 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? Does SOFEA treat meteorological stability class inputs appropriately? Does SOFEA appropriately calculate bounding air concentration estimates?

Question 5: The Agency model, ISCST3 is 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. Please recommend any parameters that should be altered to optimize the manner that they are used in SOFEA? 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?

<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. 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?

Question 7: Please comment on whether SOFEA adequately identifies and quantifies airborne concentrations of soil fumigants that have migrated from treated fields to sensitive receptors? 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? Please comment on SOFEA's approach for calculating and presenting probability distributions of moving average concentrations for differing durations of exposure. 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.

Question 8: What types of sensitivity/uncertainty analyses of SOFEA are recommended by the panel to be the most useful in making scientifically sound, regulatory decisions? 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? Does the panel recommend any further steps to evaluate SOFEA and if so, what? 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?