Background Document

Fumigant Emissions Modeling System

David A. Sullivan, Certified Consulting Meteorologist
Dennis J. Hlinka, Certified Consulting Meteorologist
Mark T. Holdsworth, Environmental Engineer

Sullivan Environmental Consulting, Inc.
1900 Elkin Street, Suite 240
Alexandria, VA 22308

Sponsored By:

AMVAC Chemical Corporation, Taminco N.V., and Tessenderlo Kerley, Inc.

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EXECUTIVE SUMMARY

Agricultural fumigants represent a complex and intermittent source category that is not amenable to routine modeling methods commonly used to estimate downwind exposures to air emissions. The complexity is a function of the infrequent nature of fumigant applications, the variability in emissions, and the impact of the diurnal (day/night) changes in meteorological and soil conditions on emissions and exposures. Because no currently available model captures these and related factors, efforts were undertaken to develop a model that addresses the most relevant characteristics of fumigant applications, and improves the accuracy of the exposure estimates for this complex source category. The result of these efforts is the development of the Fumigant Exposure Modeling System (FEMS) model, which is being submitted to the U.S. Environmental Protection Agency (EPA) Federal Insecticide, Fungicide, and Rodenticide (FIFRA) Scientific Advisory Panel (SAP) for peer-review, with the ultimate objective of making this model publicly available for assessing airborne exposures from agricultural fumigants.

The FEMS model was developed with three critical design considerations in mind: (1) the intermittent nature of the release; (2) the wide variability in emissions during the daily cycle; and (3) the need to propagate uncertainty in the input parameters through the modeling analysis. FEMS is based on probabilistic modeling methods that are fully consistent with EPA guidelines. Based on this design, FEMS helps to convey to risk managers greater perspective to support more informed risk management decisions.

FEMS is a modeling system based on existing EPA models (ISCST3 (EPA, 1999) and TOXST (EPA, 1993)) without altering these models' calculations. A Monte Carlo-based interface is used to account for uncertainty in the emission rates and the measured meteorological inputs to the modeling. Measured air quality data are used to empirically estimate the best fit and distribution of emission rates typically as a function of 4-hour time blocks, starting at the time of fumigant application, and extending for 96 hours. FEMS evaluates distances from the edge of an applied field that are needed to reach user-defined concentration endpoints. The intermediate outputs from FEMS also can be processed in custom runs to display distributions of exposures as a function of distance from the edge of the field. FEMS, in short, provides a probabilistic interface to support data inputs and post-processing for two EPA models, ISCST3 and TOXST.

Through the development of design features that are specific to the source characteristics and needs of agricultural fumigants, FEMS is more compatible with the source characteristics of agricultural fumigants than routine application of models, such as the stand-alone use of ISCST3, because it contains the means to address factors unique to the application of agricultural fumigants. Most importantly, FEMS can be used to model these exposures without resorting to the use of implausible assumptions to simplify the problem to the point that routine modeling methods can be used. Thus, FEMS can serve as a foundation to address the differing needs of various fumigants, and specific EPA needs. In modeling for exposures to agricultural fumigants, FEMS can consider the frequency and duration of exposure, model different averaging times (less than or equal to 24 hours), consider multiple field scenarios on an independent or planned sequential basis (through custom runs), and consider the variability and uncertainty of this complex source through the use of empirical emissions distributions developed from field studies.

EPA will benefit by using FEMS because it provides risk managers with results that quantitatively consider the variability and uncertainty in the model input data. In addition, the FEMS modeling approach will be useful to EPA and agricultural users for several reasons.

- First, the FEMS approach relies, to the extent possible, on existing EPA modeling methods, using the EPA ISCST3 dispersion model as the basis for the dispersion modeling, and the EPA TOXST model to account for the intermittent application in the form of the batch treatment in TOXST. Thus, the modeling methodology used to evaluate exposures from industrial batch operations, which is not fundamentally different in terms of air quality modeling from an agricultural fumigants source, already exists. The sequential use of ISCST3 and TOXST was designed to meet the specific needs of evaluating acute exposures from batch operations with intermittent use, and predictable emissions sequences once the batch is initiated.

- Second, FEMS generates distributional inputs to the modeling analysis for emission rates and meteorological terms that are consistent with EPA guidance documents.[1]

- Third, FEMS can resolve endpoint distances at a resolution of 10 meters to promote stability in model output.

- Fourth, FEMS retains a reasonable degree of over-prediction in the emissions treatment, which produces some positive bias in the modeled concentrations. As shown in Attachment 6, measured concentrations of the example chemical, methyl isothiocyanate (MITC), generally are 10 to 100 times lower in cooler weather studies than studies conducted during hot, dry, summertime conditions that serve as the empirical basis for the emission treatments currently used in FEMS for metam-sodium.

- Finally, FEMS provides a sound basis to reduce the uncertainty in the assessment of this rather unique and complex source. In this manner, FEMS promotes more accurate and realistic risk assessments of agricultural fumigants, which in turn promotes risk management decisions being made with greater perspective and confidence. On this basis, FEMS can serve as a foundation to address the differing needs of various fumigants and the specific needs of EPA.

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[1] *See* EPA Guidance on Monte Carlo and Aggregate Risk Assessments (EPA, 1997, 2001), the EPA Guideline on Air Quality Models, EPA Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models (EPA, 2003a), and the EPA Guideline on Air Quality Models (EPA, 2003b).

The report that follows summarizes the technical issues involved in modeling airborne emissions from agricultural fumigants, and describes the development and features of FEMS that were developed to meet this need. The conceptual design of FEMS is explained and its usefulness is demonstrated through the presentation of a test case and other field results. The flow charts in Figures 2 through 4 of this document display in red the features in FEMS that constitute developments beyond existing EPA models and routine inputs to such models.

The Fumigant Exposure Modeling System (FEMS) was developed to provide realistic acute exposure assessments for all agricultural fumigants. The modeling system was sponsored by the Metam-Sodium Task Force and Amvac Chemical Corporation. On this basis, metam-sodium is used as the example fumigant throughout this document, however, FEMS is equally applicable to all other agricultural fumigants where assessments are required for acute exposures to airborne pollutants. The following information summarizes metam-sodium's use as an agricultural pre-plant fumigant, among other uses, which is being provided as background material for the technical description of FEMS that follows.

Metam-Sodium Use Profile

- **Non-selective soil fumigant or sterilant:** metam sodium (sodium Nmethyldithiocarbamate) is a dithiocarbamate salt with fungicidal, herbicidal, insecticidal, and nematicidal properties. It quickly breaks down in the environment to the primary toxic degradate methyl isothiocyanate, or MITC. MITC is highly volatile and is responsible for the fumigant properties of metam sodium. In agriculture, metam sodium is typically used to sterilize the soil prior to planting, but it can also be used to fumigate the soil post-harvest. Metam sodium is also registered as an antimicrobial agent.

- **Use sites:** Metam sodium is registered as an agricultural soil fumigant for use on all food, feed, and fiber crops, including turf and ornamentals. Major agricultural use sites for metam sodium include potatoes, tomatoes, cotton, and carrots. Metam sodium is also registered for use on golf course turf, and for application to small areas of turf and soil. In addition, metam sodium is used as a root-control agent in drains and sewers, for vegetation control along drained ponds and lakes in California (through a Special Local Need registration), and as an antimicrobial agent for the following use sites: cane and beet sugar processing mills, wood poles and pilings, hides and skins (leather manufacturing), and sewage/organic sludge and animal waste.

- **Use classification:** Most metam sodium products are registered for general use. Only the metam sodium products registered specifically for use on golf courses, for use on small areas of turf and soil, and for antimicrobial uses including sewer root control, are registered as "restricted use". No metam sodium products are intended for use by homeowners.

- **Formulations:** Soluble concentrate, and ready-to-use aqueous solution.

- **Methods of application:** In agricultural settings, metam sodium is applied through chemigation or with tractor-drawn equipment. Chemigation methods include sprinkler irrigation (which accounts for 90% of irrigation applications), flood, furrow, and drip/trickle irrigation. Tractor-drawn applications are carried out with various types of shank soil injection and rotary tiller injection equipment. Applications to smaller areas can be made with handheld equipment, including sprinkler cans, hose proportioners (hose-end sprayers), power sprayers (handgun sprayers), or foam injectors. Metam sodium applications to potting soil may be made by adding the chemical to soil in a cement mixer, or by spraying it onto a soil stream as soil is ejected from a shredder. The antimicrobial uses of metam sodium have their own associated application methods, including use of a hand-held, pressurized pump or injector for making applications to wood poles and pilings, open pouring or applying through a metering pump for treating hides/skins in leather manufacture, and applying through a metering pump in sugar processing mills or for the treatment of sewage sludge.

- **Use rates:** The maximum application rate listed on most product labels for application to ornamentals, turf, food, feed, and fiber crops is 320 pounds of active ingredient per acre (lbs ai/A). Tobacco plant beds have a maximum application rate of 387 lbs ai/A on most product labels, but at least one product lists a rate as high as 412 lbs ai/A. For small areas of ornamentals, food and fiber crops, seed beds, plant beds, and lawns, the maximum application rate is 12 lbs ai/1000 square feet. For sewers and drains, the maximum application rate is 0.212 lbs ai/gallon of solution.

- **Annual pounds used in the United States:** Based on pounds of active ingredient used, metam sodium is the third most widely used agricultural pesticide in the United States. In 2002, 51-55 million pounds of metam sodium were used in U.S. agriculture. Since metam sodium is considered to be a potential methyl bromide (MeBr) replacement, its use is expected to increase as use of MeBr decreases.

- **Regional use:** Of the total U.S. agricultural use of metam sodium, use in the Pacific Northwest (ID, OR, WA) accounts for 50%, followed by CA at 36%, and the Midwest (mainly MI, WI) at 9%; FL accounts for just over 1% of use.

- **Tolerances:** There are no tolerances currently established for metam sodium on agricultural food or feed crops, or on livestock commodities. No residues in plants or livestock are expected from the use of metam sodium as a soil fumigant or antimicrobial agent.

- **Technical registrants (metam sodium):** Amvac Chemical Corporation, Buckman Laboratories International, Inc., Loveland Products, Inc., (formerly Platte Chemical Company), Taminco N.V., and Tessenderlo Kerley, Inc.

GLOSSARY OF KEY TERMS

AERMOD – AERMOD is a dispersion model under development by the U.S. EPA as the replacement for ISCST3.

Application -- In the context of this report, application refers to the application of a pre-plant fumigant to an agricultural field to control weeds, disease, and/or nematodes. Applications are generally applied once per year, sometimes less frequently, and in relatively rare instances more than once per year.

Atmospheric stability -- Used to describe the mixing capabilities of the lower atmosphere, often categorized into 6 discrete classes ranging from A (very unstable, vigorous mixing) to F (very stable, suppressed mixing).

Chemigation -- Fumigants can be applied by injecting the pesticide in liquid form into the irrigation lines for a field, either in line sets or through a center pivot irrigation system. Typically, the application of the fumigant is made over a six hour period (approximately).

Cubic function -- A function of the form $Y = A + Bx + Cx^2 + Dx^3$.

Cumulative distribution function (CDF) -- Obtained by integrating the probability density function (PDF). The CDF provides a quantitative relationship between the value of a quantity and the cumulative probability (percentile) of that quantity. CDF is used in FEMS to describe the distribution of mean emission rates computed per least squares analysis.

FEMS -- The Fumigant Emissions Modeling System developed to evaluate acute exposures to bystanders associated with the application of fumigants.

Fumigant -- A class of pesticides that are used on a pre-plant basis to prepare the soil for planting. Either alone or in combination, fumigants can control weeds, disease, and nematodes, providing a soil medium that promotes crop quality and quantity.

Intermittent water sealing -- A term that refers to a sealing method developed through research undertaken by the Metam-Sodium Task Force. An application of water directly after the pesticide has been applied, to seal the surface, followed by application of additional water (in one or two sessions) before late evening on the day of application..

ISCST3 -- Industrial Source Complex Model Short-Term, which is widely used for dispersion modeling applications in the United States. It can be used for industrial applications, agricultural applications, and at scales up to 50 km in size. ISCST3 currently is the EPA-recommended dispersion model for most applications, with the most notable exceptions being photochemical modeling, long-range transport, and the modeling of dense gas plumes.

Kurtosis -- A measure of the shape of a distribution based upon the fourth moment of the distribution. Kurtosis is an indication of the flatness or peakedness of a distribution.

Log-normal distribution -- Refers to a variable that approximates a normal curve after being transformed into natural logarithms.

Metam-sodium -- A pre-plant fumigant that is used to control weeds, disease, and nematodes.

Methyl isothiocyanate (MITC) -- MITC is the primary degradation product of metam-sodium. In a moist soil environment, metam sodium generally is transformed primarily into MITC typically within 30 to 60 minutes, longer with cooler temperatures. Metam-sodium is a non-volatile salt. MITC is a volatile chemical with vapor pressure and boiling point similar to water.

Normal distribution -- Referred to as a bell-shaped curve or as a Gaussian distribution. The normal function is fully defined parametrically by its first two moments, *i.e.*, the arithmetic mean and the standard deviation (or variance).

MITC -- An abbreviation for methyl isothiocyanate, a degradation product of metam-sodium.

Monte Carlo -- A numerical modeling procedure that makes use of random numbers to simulate processes that involve an element of chance. In Monte Carlo simulation, a particular experiment is repeated many times with different randomly determined data to allow statistical conclusions to be drawn.

Off-gassing -- Refers to the period when volatilization occurs during and subsequent to the application of a fumigant. The duration of the off-gassing period can vary from 1 to 5 days, or more, depending on the specific fumigant and the soil and atmospheric conditions.

PCRAMMET -- Software developed by the U.S. EPA to facilitate the preparation of meteorological data for dispersion modeling, primarily for ISCST3. PCRAMMET processes available National Weather Service or Federal Aviation Administration surface and upper-air meteorological data by computing atmospheric stability based on wind data and local sky conditions, computing estimates of hourly mixing heights based on twice per day soundings, converting wind direction to flow vectors, and making the necessary unit conversions.

Percent confidence of the mean -- A statistical term based on the standard error that estimates the percent confidence that the mean is within a specified range.

Percentile – Based on a division of a probability distribution into 100 equal areas; a percentile is a quantile equal to one one-hundredth of a total population.

Probabilistic analysis -- Analysis in which probability distributions are assigned to represent variability (or uncertainty) in quantities. The output of probabilistic analysis is likewise a distribution.

Probability -- The chance that a prescribed event might occur, represented as a number “p” in the range of $0 \leq 1$.

Probability Paper (Plot) -- Graph paper with the x-axis scaled in units of standard deviation or with other transformations. On this paper the cumulative distribution function for a normally distributed set of data will appear as a straight line.

Scatter plot -- A plot representing corresponding values of two variables "x" and "y" as points in Cartesian coordinates.

Shank injection -- An application method for fumigants where a tractor drawn device injects the fumigant directly into the soil below the surface.

Skewness -- A measure of the shape of a probability distribution based on the third moment of the distribution. A symmetric distribution has zero skewness. A distribution with a long tail to the left (toward large negative values) is negatively skewed. A distribution with a long tail to the right (toward large positive values) is positively skewed.

TOXST -- A post-processing routine (software) developed by the EPA Office of Air Quality, Planning, and Standards for use with the ISCST dispersion model. TOXST can be used to model batch operations at industrial facilities, or in this case, to more accurately simulate agricultural operations. TOXST also can be used to represent industrial facilities with broad ranges in emission rates at specific sources that can best be represented as stochastic treatments. (TOXST was developed by Sullivan Environmental, also the developers of FEMS).

Standard water sealing -- A single application of water directly after the pesticide has been applied, to seal the surface.

Stochastic -- A random process, a process not explainable by mechanistic theory but instead described in terms of probability.

Time series analysis -- A statistical analysis of data collected over time, which uses previous changes over time to forecast future changes.

Transformation -- In the context of this report, transformation refers to applying a consistent adjustment to every data point that defines a variable, such as by taking the natural logarithms of measured and modeled concentrations to improve the confidence in statistical analyses of emission fitting procedures.

Water sealing -- A terms that refers to applying irrigation water after a fumigant application to reduce the potential for volatile loss. Alternative methods of sealing include tarping, compaction, and soil covering.

Wind persistence -- Refers to how many hours in a row the wind flows from one sector (such as from one sector of a 16-point compass).

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1.0 MANAGEMENT OBJECTIVES

1.1 Scope of Problem

The application of agricultural fumigants at any given field presents a complex and highly variable source of airborne emissions that is not amenable to the use of standard modeling methods. Using dispersion modeling to estimate emissions from agricultural fumigation requires a realistic representation of the infrequent nature of fumigant applications, the variability in emissions, and the impact of the day/night cycle on emissions and dispersion in order to meet the objectives of exposure assessment, such as described in the National Research Council's "Science and Judgment in Risk Assessment". . . "*Exposure assessment involves specifying the population that might be exposed to the agent of concern, identifying the routes through which exposures can occur, and estimating the magnitude, duration, and timing of the doses that people might receive as a result of this exposure*" (National Research Council, 1994).

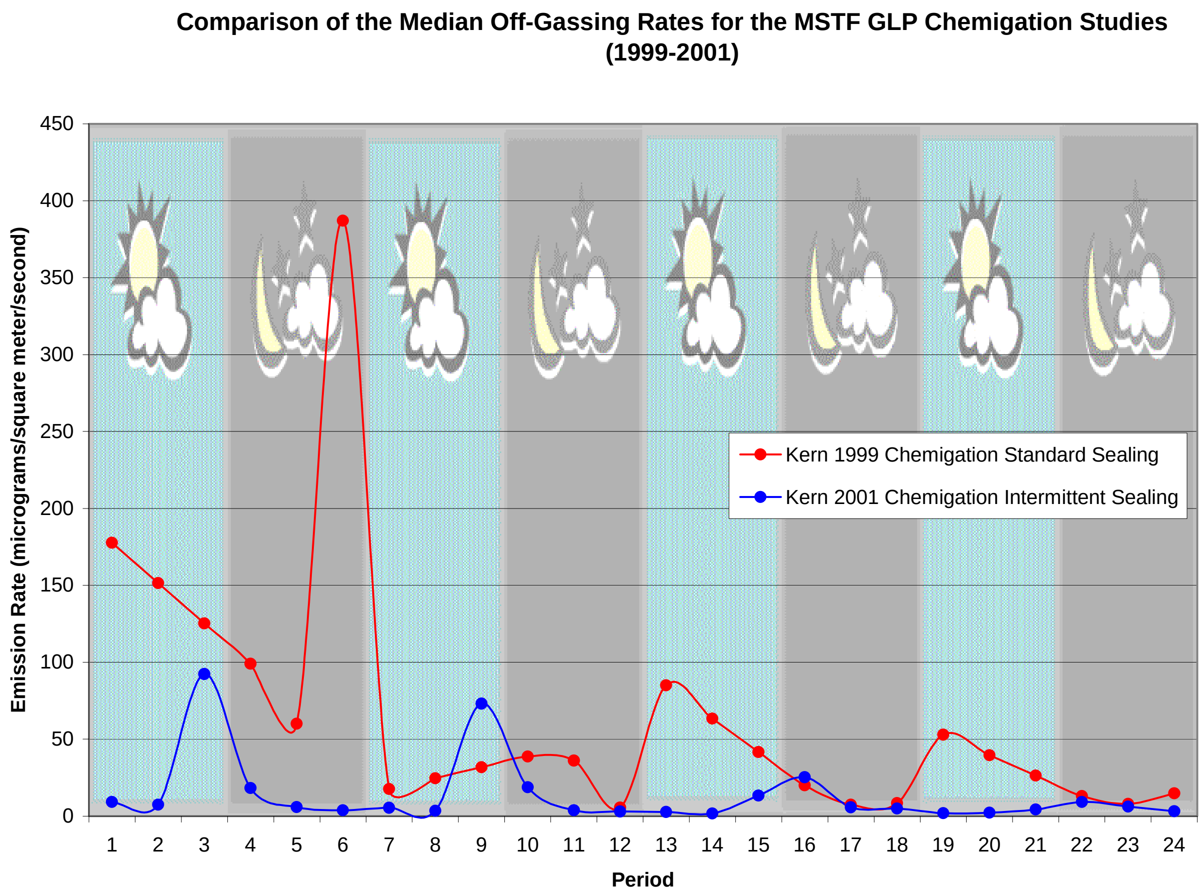
The exposures to be assessed through FEMS are those experienced by bystanders, those individuals potentially affected by downwind exposures associated with off-gassing of an applied field. Such individuals are not part of the application process, and generally would be exposed on adjacent or nearby properties, including their place of residence. FEMS is designed to evaluate acute exposures, which are defined in this context to be averaging times of 24 hours or less. For individuals residing or working near a field that is applied by agricultural fumigants, a typical frequency and duration of total potential exposure is once per year, generally with an off-gassing period of approximately 4 days, as is the case for the example chemical, metam-sodium. During those periods when there is wind flow from an applied field towards a downwind bystander, exposures might occur that are above background levels of the active ingredient. These are the exposures of interest in this report.

Empirically-computed emissions data show the complexity of modeling agricultural fumigants most directly. Figure 1 presents two examples of the diurnal (day/night) emissions patterns from applications of a soil fumigant, in this example metam-sodium was applied by irrigation systems, referred to as chemigation applications.[2] In all applications, metam-sodium primarily degrades in the soil to the active ingredient, methyl isothiocyanate (MITC), which can be released as a volatile substance. Both curves present an infrequent, "batch" source that is characterized by 3 to 4 days of fumigant emissions (off-gassing), which produces concentrations above general background concentrations. If the figure were extended to show the actual emissions patterns throughout the year, the emissions patterns would show roughly a 4-day period with emissions above background levels, followed by roughly 361 days of negligible to essentially no emissions. Realistic modeling treatments need to reproduce such a pattern when generating a distribution of exposures. Although the number of days with significant off-gassing rates are expected to differ from fumigant-to-fumigant, all fumigants are not found to differ in terms of needing to be modeled as "batch" operations, which are best addressed through the available EPA ISCST3 dispersion model and the TOXST post-processor,

[2] These examples, and others in this report, are based on studies of metam-sodium applications.

which itself was specifically designed to model "batch" sources, such as fumigant sources, with a Monte Carlo-based trigger to start the emissions sequence.[3]

Figure 1: Comparison of Chemigation Standard vs. Intermittent Sealing Field Studies MITC Emission Rates



Both emissions patterns shown in Figure 1 also exhibit large diurnal (day/night) variability in emissions and show a downward trend with time. Figure 1 also shows that once the

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3 TOXST only treats the start of an application as a Monte Carlo event based on probability computed from the assigned number of applications per year (defaulted to 1 application/year). Standard runs of TOXST do not consider the uncertainty in the emissions and meteorological data input to ISCST3 through Monte Carlo sampling. Uncertainty in these parameters is addressed in FEMS through tailored software used to pre-process the inputs to ISCST3, which then flow into TOXST. When the stochastic treatments for all input parameters are turned off in a model run, a standard TOXST model run is made. This is referred to as a benchmark run in this background document, which serves as the reference for comparison with existing modeling methods.

“batch” is triggered, there is a predictable and widely varying diurnal pattern that must be reproduced when generating a realistic distribution of exposures.

The suitability of the methods chosen for FEMS is greatly dependent on the goals of the modeling system. The primary goals of FEMS are to: (1) identify endpoint distances to user-defined thresholds (as a function of a percentile concentrations); and (2) serve the special need of displaying distributions of concentrations as a function of distance from an applied field. These outputs are distributional outputs. Importantly, the objective is to describe realistically distributions of concentration, not to set the standard of success dependent on the capability of a model to accurately represent each 4-hour period in sequence for 4 days after an application. More specifically, the goal is to describe realistically the emissions distributions on a daytime and nighttime basis because of the large differences in transport and dispersion conditions between daytime and nighttime. To meet these goals successfully, however, the estimation of emission rates (and ultimately concentrations) do not necessarily need to be accurate in sequence, although this is still the goal, but rather in distribution form on a daytime and nighttime basis

The distinction between estimating a distribution of emissions and concentrations, and the more constrained goal of matching emissions and concentrations on a sequential basis, is the difference between a realistic objective (in the former), and an unrealistic objective (in the latter). It is widely accepted by air quality modelers that the more a model is constrained to be accurate for specific times and space, the less reliable the model will be. For this application, estimating distributions as a function of distance is the output a risk manager needs to make an informed decision. For example, the direction of the maximum impacts may be off-set by a sector that is not an issue relative to the risk management decision. Success is realistically representing a distribution of concentrations as a function of distance from an applied field.

This distinction is especially important for emissions fitting. The least-squares analysis is based on solving the simple relationship:

$$Y = b\,X$$

Where:

Y = measured concentration $\mu g/m^3$

X = normalized concentrations $\mu g/m^3$

B = slope, which when multiplied times the normalized concentrations becomes the emission rate (the unknown in this case) $\mu g/m^2/sec$.

The measured concentrations are quite reliable in terms of the general uncertainties in the exposure assessment, often to within +/- 20 percent relative to known standards.

For modeling the most critical periods for bystander exposures (*i.e.*, for neutral through especially stable conditions), the Gaussian model is well-accepted as being reliable, with reasonably low bias, but produces considerable scatter on an hour-by-hour basis. Least squares analysis, including the evaluation of standard error, can be used to solve for best-fit emissions and then the distribution of the means, as described in Attachment 1, through the implicit assumptions that the measured data and the normalized model are both reliable, or accurate. These assumptions are much better met on a distribution basis without being constrained to expect the model to match one sequential period after another for the 24-periods of off-gassing. Some estimated concentrations may be low, and others high, but the distribution should be reasonably well-estimated. By setting the standard for success based on a distributional basis, the Gaussian fit can be considered reasonably unbiased with acceptable resolution in terms of the distributions of concentration as a function of distance.

Thus, effective modeling systems for agricultural fumigants must be able to account for the intermittent nature of fumigant releases, and reasonably represent the wide variability in emission rates (*e.g.*, 20- to 30-fold differences have been noted between the daytime and nighttime emission rates for agricultural fumigants), and create reliable distributions of concentrations that are used to support subsequent risk management decisions. Mismatches between the emissions and meteorological daily cycles, both of which can exhibit strong in-phase or out-of-phase diurnal cycles depending on application and sealing method, need to be avoided. Because no currently available model captures these and related factors, efforts were undertaken to develop a model that addresses the most relevant characteristics of fumigant applications and emissions, and reduces the degree of overestimation, while avoiding underestimating the magnitude of exposures. The result of these efforts has been the development of FEMS (Sullivan *et al.*, 2004a and Sullivan *et al.*, 2004b), which is being submitted to the U.S. Environmental Protection Agency (EPA) Federal Insecticide, Fungicide, and Rodenticide (FIFRA) Scientific Advisory Panel (SAP) for peer-review, with the ultimate objective of making this model publicly available for assessing exposures to agricultural fumigants.

1.2 Overview of FEMS

When modeling exposures associated with agricultural fumigation, FEMS provides flexibility to address specifically the following critical areas:

1. Frequency of exposure;

2. Monte Carlo to address uncertainty;

3. Maintaining mass balance;

4. Ability to address multiple field applications (through custom runs);

5. Ability to address averaging times of less than 24 hours;

6. Accurately accounting for distribution of emissions across the annual cycle; and

7. Providing useful output to risk managers.

Each of the preceding areas is discussed in the following sections.

- ***Frequency of Exposure*** -- The duration of exposure differs among fumigants, but the fumigants all share the common characteristics of off-gassing only a small fraction of the year. FEMS is a useful tool because it is designed to provide a realistic simulation of the frequency and diurnal pattern to emissions, thereby providing a refined option to support all fumigants without sacrificing accuracy.

  As stated in Cullen and Frey, 1999: "*Exposure models combine information about the frequency, intensity, and duration of human contact with environmental contaminants* . . . ." FEMS accurately considers the frequency of exposures and fluctuations within the emissions period when creating distributions in the output, including representing the empirically fit emissions sequences emissions appropriately matched on a diurnal basis to the application method of interest.

- ***Monte Carlo Application Addresses Uncertainty*** -- Monte Carlo sampling methods are used to propagate uncertainty through dispersion modeling analyses. Monte Carlo applications are useful in this context because the key inputs can align at the upper end of their uncertainty ranges to produce the relatively rare events that, under some review scenarios, may be important.

- ***Maintain Mass Balance*** -- In order for plausible assumptions to be employed, mass must be conserved when creating the distributions of exposure. FEMS promotes mass conservation by: (1) statistically initiating off-gassing to match the selected frequency of applications per year, using empirically estimated emissions data that simulate realistic off-gassing sequences as a function of time during the 4-day off-gassing period; and (2) by setting an upper bound on the emissions distributions for each period to avoid the situation where, for example, a 97.5 percent confidence of the mean would produce an emission rate that in one hour would exceed the potential active ingredient that could be available.

- ***Ability To Address Multiple Field Applications*** -- Standard FEMS model runs address exposures from a single hypothetical or actual field. As described in this background document, however, custom runs of FEMS (runs that do not include the automatic creation of files and results) can be conducted to address special situations, such as multiple field scenarios, seasonal analysis, and the consideration of distributions of subject weights and breathing rates, among others.

  In terms of multiple fields, the FEMS approach provides the important feature of setting seasonal probabilities, or annual if appropriate, with fields being simulated as either independent sources (such as with separate owners) or as a planned sequence (such as a grower applying a fumigant to a full quarter section (160 acres) in an 8-day application sequence). FEMS can simulate such realistic scenarios without having to rely on implausible assumptions, such as all fields off-gassing at maximum rates at the same time.

- ***Association To Indoor and Personal Exposures*** -- FEMS provides a connection between the ambient outputs of the system and an indoor modeling algorithm to support future estimation of indoor and personal exposures. On this basis, FEMS could produce output to generate distributions of exposures in mg chemical per kg body weight per day (mg/kg/day) as a function of ring distance from the edge of the field. Such information would provide a substantial increase in perspective relative to tools currently available to EPA at this time. Although this portion of the system has been coded, this aspect of FEMS is not specifically being requested for evaluation at this time. If this component is of interest to EPA, it could be developed to include distributions of subject weights and breathing rates to produce grouped distributions of these receptor inputs to more fully meet the probabilistic objectives of (EPA, 2001) in terms of showing distributions of mg/kg/day for bystanders as a function of distance from the applied field.

- ***Ability To Address Averaging Times Less Than 24 Hours*** -- Some fumigants are only regulated by 24-hour averages, while others could be regulated at averaging times as low as 1 hour. FEMS is capable of modeling from one to 24-hour averaging times, supporting all needs for acute exposure assessment,. FEMS accomplishes this by treating emission changes throughout the daily cycle, day-by-day, for the full off-gassing period and 1-hour meteorological data in the ISCST3 model.[4]

- ***Accurately Accounting for Distribution of Emissions Across the Annual Cycle*** -- There are basically two ways to approach the problem of modeling an intermittent source: (1) use the probability for the "batch" source to be in operation to represent the distribution of emissions; or (2) simplify the problem by conservatively assuming in the model that every day has the potential for an application at the worst case emission rate for the averaging time being evaluated. There is a large difference in terms of annual emissions from a source that operates continuously at maximum emission rate, compared to a representation of

[4] It is not routinely feasible to collect field data resolved to the hour-by-hour level of resolution to support direct estimation of hourly emission rates. One-hour averages at this time need to be based on the distribution of mean (integrated average) emission rates, typically of about four-hour duration, covering general changes in emission rates throughout the daily emissions cycle. Although it would not be generally expected that emission rates would rapidly change through throughout the day, it may be possible to improve the resolution of hourly emission rates in the future by using soil modeling methods to estimate relative changes expected within the integrated averages based on changes in the soil temperature and moisture characteristics, or possibly remote sensing for some fumigants.

the same source with the actual emission pattern represented over the four-day active off-gassing period, followed by zero emissions.

Risk managers are best served by having risk assessments that are based on realistic exposure distributions regardless if they focus their review on annual distributions of concentrations or distributions specific to the short-term off-gassing period. FEMS provides decision makers with results based on realistic distributions of concentrations to support the scale of temporal analysis and percentile of their choosing for all fumigants with acute exposure issues at 1 to 24-hour averaging periods.

- ***Providing Useful Output To Risk Managers*** -- Output from FEMS is designed to produce data to support risk managers in making informed decisions, without high levels of embedded (and potentially unrecognized) excessive uncertainty; already incorporated into the analysis. As structured, FEMS allows a risk manager to assess the likelihood of various concentration thresholds being reached. The degree of sensitivity to uncertainty in the various model input parameters will in turn depend on the endpoint and percentile of exposure evaluated, and can be displayed.

1.2.1. Additional Factors Specific to Modeling Agricultural Fumigants

The FEMS model is suitable for use in assessing exposures to agricultural fumigants because it contains the means to address factors unique to this source category. These factors include:

1. Modeling fumigants as simulated "batch" sources and providing capability to match application frequencies for the crop and region under review, as well as provide flexibility to account for:

    a. Application method;

    b. Sealing method;

    c. Application rate;

    d. Regional differences in conditions;

    e. Seasonal differences; and

    f. Adjacent field scenarios (1 - 80 acres per day with no limit on the number or size of contiguous field to be modeled in custom runs of FEMS).

2. Establishing emissions distributions for 4 to 6-hour time steps to represent specifically the large diurnal emissions variability in the context of selected fumigant application and sealing methods.

3. Modeling domain: 25 km radius from center of source/application.

4. Active emissions period: user specified (*e.g.* < 14 days, but typically ≤ 4 days). **This prototype version of FEMS needs to be run with a 4-day duration of the off-gassing period.**

5. Physical state of emission: applicable to gas-phase release.

6. Averaging times from 1 to 24 hours (FEMS can be used to model 1, 2, 3, 4, 6, 8, 12, and 24-hour averages).

1.2.2 Suitability of FEMS for EPA Use

The FEMS approach meets EPA's needs to have a modeling tool to support the evaluation of exposures from agricultural fumigants, particularly because of the following considerations:

- Relies to the extent possible on existing EPA modeling methods, using the ISCST3 dispersion model as the basis for the dispersion modeling, and the EPA TOXST model to account for the intermittent application in the form of the batch treatment in TOXST; and

- FEMS generates distributional inputs to the modeling analysis consistent with EPA guidance documents (EPA, 1997, 2001), including the EPA Guideline on Air Quality Models, EPA Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models (EPA, 2003a), and the EPA Guideline on Air Quality Models (EPA, 2003b).

2.0 CONCEPTUAL MODEL

This section presents an overview of FEMS, as a conceptual model. A summary of each item on the checklist contained in the Recommended Elements for Model Documentation in the OPP (EPA, 2001) is also provided.

2.1 Overview of Conceptual Model

- ***Modeling Objective*** -- The primary objective of FEMS is to identify the downwind distance where air concentrations for bystanders are below user-defined concentrations. The focus is on acute exposures. This objective will be met with appropriate consideration of the stochastic uncertainties in the key inputs to the exposure assessment.

- ***Agricultural Fumigants Are a Very Complex and Unique Source Category*** -- This source category is complex for three primary reasons: (1) intermittency; (2) variability (through daily cycle and with daily damped amplitudes of peak emissions); and (3) uncertainty, particularly in the emissions term. The development of FEMS started with the recognition that the EPA TOXST model, a post-processor to ISCST3, contains the core features to simulate batch operations, which are similar to agricultural fumigant emission periods. Once a Monte-Carlo based pre-processor of input data was established through FEMS the available features of two existing EPA models, ISCST3 and TOXST, could be used to quantitatively consider each of the three key factors: intermittency, variability, and uncertainty.

Empirical Treatment of Emissions Is Needed Within the Current State-of-the-Art -- Ideally, a soil model would exist that would develop emissions data to match the observed patterns such as those shown in Figure 1. Unfortunately, this is not the case at this time. Emissions rates are a function of numerous variables, including soil temperature, pH of the soil, soil moisture, organic carbon content, air temperature, surface wind speed, application rate, application method, and sealing method, among others. This matrix of conditions is too large to fill on a practical basis using an empirical approach. Therefore, the following course of action was taken, using metam-sodium as an example:

1. <u>Initially emphasize upper-end emissions potential</u>: Field studies were conducted to observe the upper-end off-gassing potential for each major application and sealing method. Generally such conditions are found in hot, dry climates, such as Kern County, California, where the metam-sodium field studies were conducted for shank injection and chemigation. High soil and air temperatures produce high vapor pressures and rapid drying of surface water, thereby promoting more rapid off-gassing rates than for typical conditions. The typical sandy soil conditions found in this setting also produces higher air porosity in the soil and contains low organic carbon, both of which are conducive to producing high off-gassing rates. Studies of this nature provide a reasonable upper limit for expected emission rates.

2. <u>Cover a wider range of conditions over time</u>: Subsequent to initial reliance on upper-end field studies, the data base for specific fumigants can be broadened as resources allow and needs dictate, to reduce the degree of uncertainty in this treatment by collecting additional field data in cooler climates and heavier soils. On this basis, variability can be more specifically represented in time, and regional and seasonal differences in off-gassing rates more accurately represented, as compared to using upper-end emissions data as proposed at this time. As more data are collected, it also is possible to reduce further the uncertainty in the results, which helps refine future analyses. This approach has the desirable feature of providing a mechanism to reduce uncertainty and enhance realism as knowledge improves of the relative differences in emission rates as a function of conditions.

Using metam-sodium as an example, very large differences have been noted between studies such as those conducted in summertime conditions in Kern County, California and cooler temperature scenarios that would be more representative of the majority of applications on a national basis. For example, for comparable application methods differences between applications near the upper limit of soil temperatures (90 ºF) and 50 ºF generally have shown 10 to 100-fold higher concentrations than for the cooler weather studies (*refer to* Attachment 6 for comparative data). On this basis, the ability to distinguish between upper-end and more typical application scenarios will provide the benefit in the future of tailoring regulatory requirements to meet the case-specific situation. For now, however, upper-end emissions data provide the starting point in this process.

- ***Model Development Is Consistent with EPA Guidance on the Use of Models, Including Addressing Uncertainty*** -- Consistent with EPA guidance,[5] the FEMS system includes a Monte Carlo sampling approach to account for uncertainty in the following model inputs:

1. The start of an application (based on assigned applications per year);

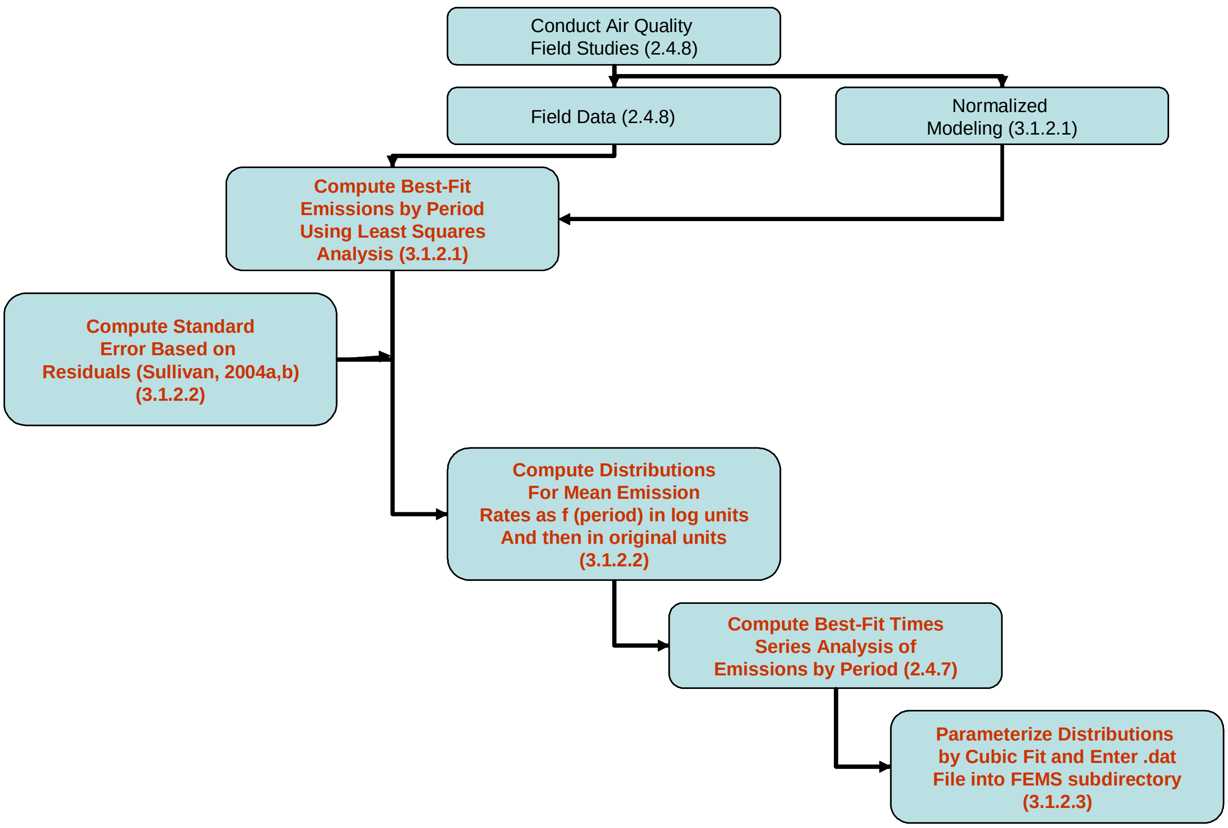
2. Emission rates representing the uncertainty in fitting the emission sequences in typically four-hour time steps; and

3. Meteorological data accounting for the uncertainty of the measured meteorological data to represent actual transport and dispersion conditions at a specific field in the region of interest, including wind speed, wind direction, and atmospheric stability.

Figures 2 through 4 present flow charts of the conceptual design of FEMS.

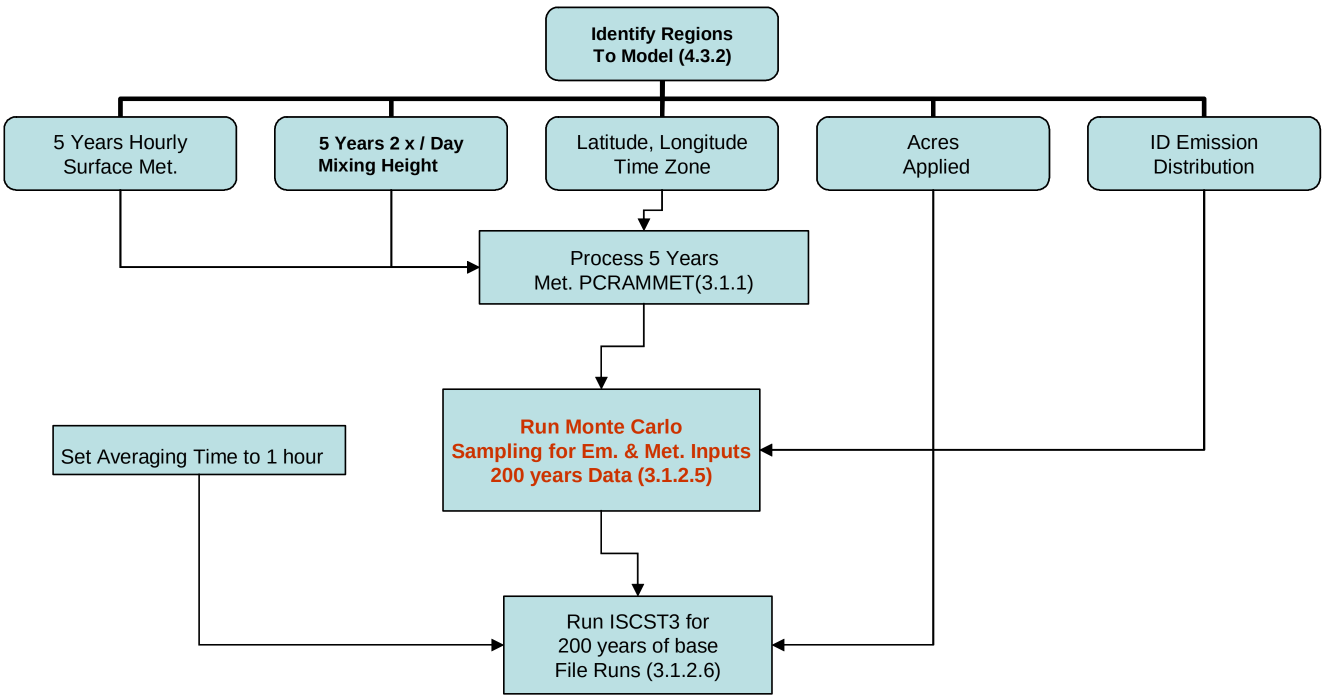
5 *See* EPA Office of Pesticide Programs Guidance on the use of Probabilistic Assessment (EPA, 2001) and the Guideline on Air Quality Models (EPA, 2003b).

Figure 2: Emissions Processing[6]



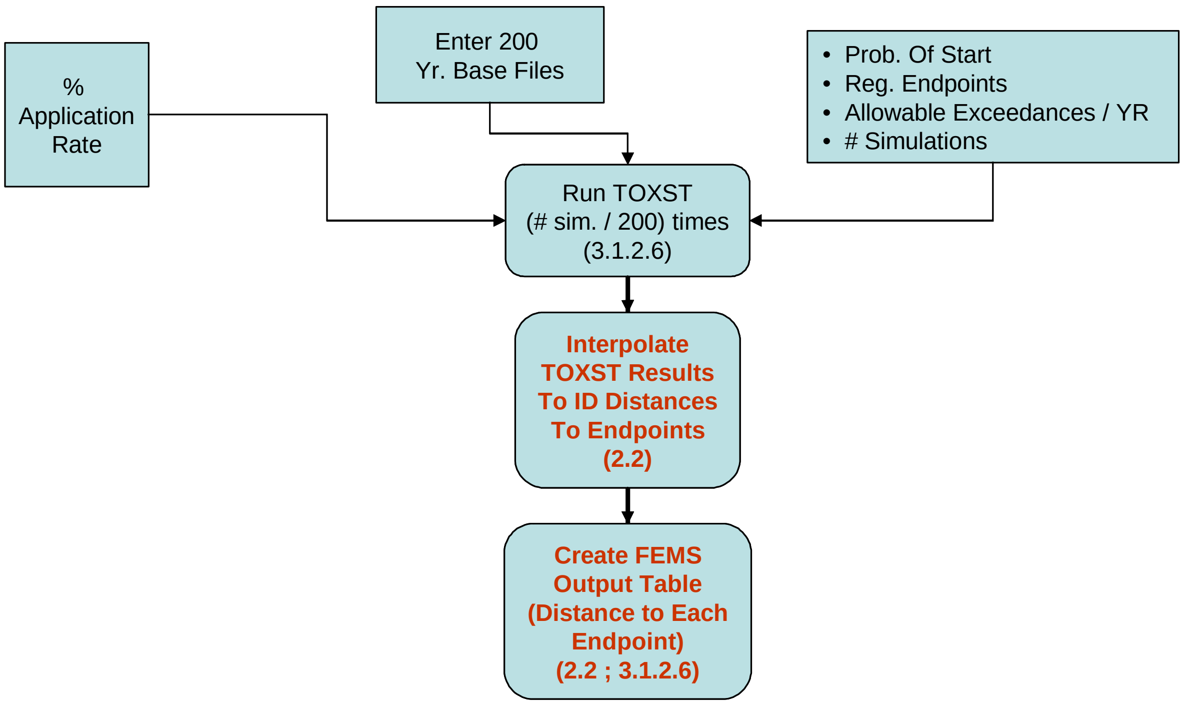
[6] Where applicable, section numbers of this report are shown in parentheses to provide a reference to the text.

Figure 3: Inputs to Model 200 Year Base Files that Are Used for Longer-Term Monte Carlo Sampling[7]



[7] Where applicable, section numbers of this report are shown in parentheses to provide a reference to the text.

Figure 4: TOXST Analysis[8]



8 Where applicable, section numbers of this report are shown in parentheses to provide a reference to the text.

2.2 Specific Technical Considerations With Regard to the Design of FEMS

- ***Random Number Generators*** -- The random number generator used to process model input data is drawn from two FORTRAN subroutines: RANDOM_SEED and RANDOM_NUMBER subroutines in FORTRAN. The RANDOM_SEED subroutine sets the pseudorandom number generator starting point (seed) used by the RANDOM_NUMBER subroutine. Running this subroutine each time the main program is run ensures that a different set of pseudorandom numbers will be generated in every FEMS analysis. This is done so that the same set of pseudorandom numbers is not repeatedly used, introducing correlations into the model outputs.

  The RANDOM_NUMBER subroutine uses a uniformly distributed pseudorandom number set in the range of $0 \leq x < 1$. The generator uses a multiplicative congruential algorithm with a period of approximately 2^{38} (Lahey, 2000). This sequence would repeat after approximately 275,000,000,000 hours, which is over 30,000,000 years. Section 5.3 shows the sensitivity testing of FEMS output to the number of simulations. This testing was done for a range of endpoint concentrations, including the 95th percentile concentrations during the active off-gassing periods, as well as upper-tail testing (in the form of 20-year recurrence intervals to further test the stability of the output). As shown, the simulations were stable at approximately 5,000 to 10,000 years for typical applications. Testing near the extreme of the upper tail, high recurrence events showed stable output at 100,000 years of simulation.

  TOXST contains a random number generator within a subroutine in the code. Figure 5 shows an example of the output from this function based on outputting 1,000 values in the range of 1 through 365. As shown, the output appears to be random based on visual observation. This function is only used to select the start of applications, and is not used for the more demanding task of accounting for uncertainty in serial data as is done with the FORTRAN random number generator to pre-process the model input terms. The specifications for this random number generator were not identified. It was noted, however, that a random seed is not used with this subroutine.[9] In order to ensure that the sequence of days selected in each execution of FEMS are random, and not in

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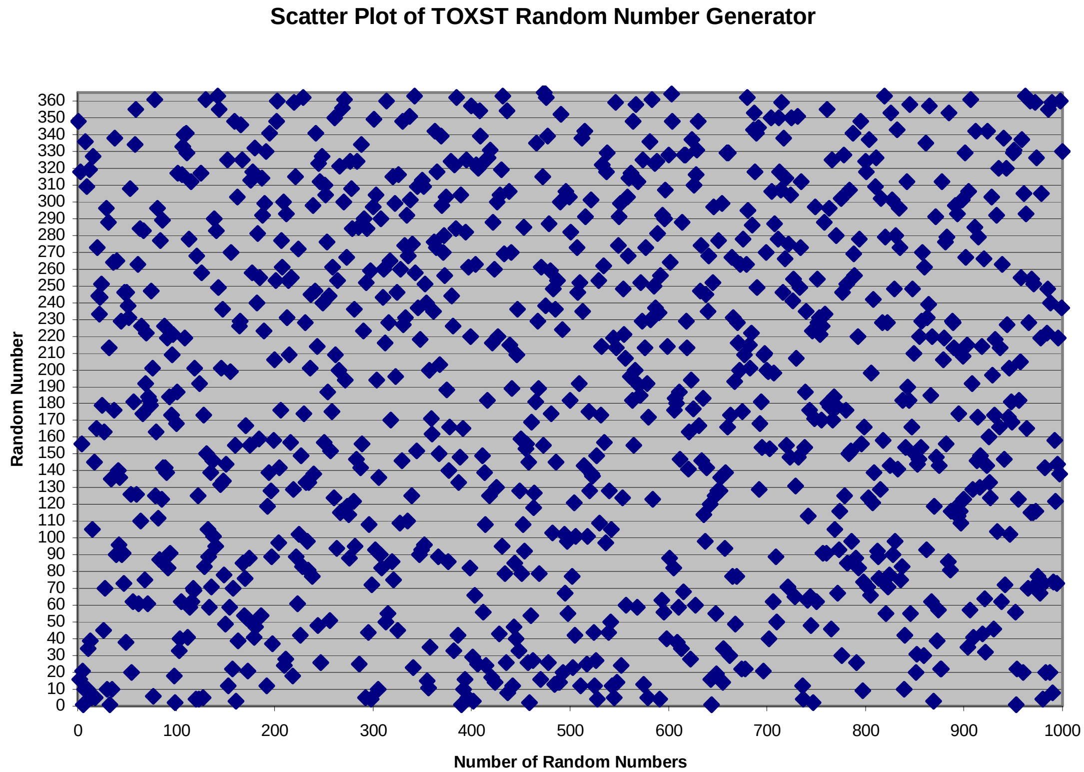
9 Standard applications of TOXST do not include Monte Carlo treatments for the meteorological data and do not include draws from distributions for emissions in batch operations. On this basis, and the more frequent batch operations at most industrial facilities, this limitation is much less an issue. With the more complete probabilistic treatment of the inputs and the low frequency of batches per year, such as 1 per year or less, the sensitivity to the random seed is more significant for use in FEMS. The random change in the starting point of each of the 40, 5-year data sets in FEMS compensates for this limitation in TOXST without requiring a code change within TOXST. Replacing the random number generator in TOXST would be another option if authorized by EPA.

fixed order, each of the 40, 5-year sequential meteorological data sets are processed through PCRAMMET and then cut on a random basis, similar to cutting a deck of cards. The sequential nature of the five-year data set is maintained, except for 1 discontinuity every 5 years, and the selection of application days is maintained as a random event.

Figure 5: Scatter plot of TOXST Random Number Generator (Based on 1,000 outputs in the range of 1 – 365)



- ***Emissions Processing Required to Create Emissions Distributions by Sequential Time Period Prior to Model Runs*** -- The user of FEMS selects an emission file for the application. The emissions distributions files, such as kern2001.dat shown in the test case, is created by the model user outside of FEMS and included in the FEMS subdirectory to be available for use during modeling analyses. For each fumigant, these emission sequence files need to be established based on empirical data and inserted into the FEMS subdirectory as a ".dat" file, in a comparable format to the other ".dat" files in FEMS, the distributions of which are typically based on measured air quality data of natural log-transformed measured and normalized modeled concentrations from networks established around fields. Least-squares analysis and evaluation of the standard error of the mean were used to compute parametrically-defined emissions distributions for each period of the emissions sequence to account for the uncertainty in calculating the mean (Berthouex and Brown, 1994; Sullivan *et al.* 2004a). Attachment 1 provides additional detail.

  Comparable emission distributions also could be established for flux chamber sampling or possibly for flux sampling based on the profile method, such as using three or more flux samplers. Uncertainty in this case would include the degree of non-homogeneity for the fetches at each sampler, and the uncertainty in the fitting procedure (assuming a homogenous surface). Rather than compute the uncertainty in the emission estimates based on the residuals of measured and modeled data, as is done with ambient monitoring networks, an alternative procedure using bootstrap sampling could be used to evaluate the variability and uncertainty of the emissions fit for flux monitoring networks. As with ambient sampling, uncertainty could be reduced with more monitoring locations.

  Monte Carlo sampling within the 95th percentile range around the mean is then used in FEMS to represent this uncertainty. Generally, FEMS is run for empirically-fitted emission cycles that are 4 days long, but there will be no constraint to the number of days of emissions (off-gassing) above background levels that can be input, as long the records in the emission distribution files match the selected number of days of off-gassing. The current FEMS prototype is restricted to 4-day off-gassing periods, which could be broadened to any off-gassing period subsequent to the prototype stage.

- ***Accounting for Uncertainty in the Meteorological Data*** -- Uncertainty in the representativeness of available measured meteorological data to account for transport and dispersion is quantitatively modeled by using the measured data in each hour of the 200-year meteorological data set that comprises the basis to account for variability and uncertainty in the meteorological data. The distributions used to represent uncertainty around the measured data are then sampled each hour from probability density functions, defined for common meteorological parameters used for modeling. These distributions were identified by expert elicitation (Hanna *et al.*, 1998, 2001, 2002) to create 200 base files (40 passes through the 5-year data sets), which include generated meteorological data and emissions data on an hour-by-hour basis. Again, the measured data are retained in proper sequence, with the uncertainty range (2 sigmas) used to represent the uncertainty in each input parameter. These 200 base files are then processed in simulations covering 200 to 100,000 simulated years of applications to a field.

- ***User Selection of Specific Model Inputs for Stochastic Treatment of Uncertainty*** -- Users of FEMS are provided the option to select on an individual basis which parameters to sample uncertainty on a stochastic basis, including emission rate, wind direction, wind speed, and atmospheric stability. Peak exposures would be expected when uncertainties in the various inputs coincide in a manner that produces maximum impacts. Monte Carlo sampling for all key emissions and meteorological input terms allows for this. The model user needs to make an independent decision whether or not to treat the uncertainty of any of the meteorological terms or emissions as a stochastic variable. In the extreme, the option of treating none of these terms with Monte Carlo sampling to represent uncertainty can be done, thereby making a standard TOXST model run, which is based strictly on standard TOXST and ISCST3 modeling. The only software review issue specific to FEMS for this benchmark treatment would be the interpolations done to compute the distance required to reach regulatory endpoints. If the TOXST results are processed and displayed in terms of an isopleth analysis of concentration, however, the distances to the endpoints can be directly computed without reliance on any of the computation features of FEMS. On this basis, there is an obvious checkpoint on the results. As shown during sensitivity testing (*refer to* Section 5 of this background document), the incorporation of the Monte Carlo sampling generally increases the endpoint distances in comparison to the benchmark treatment.

- ***All Emissions Variability is Handled in ISCST3, with TOXST Being Used Only to Trigger the Start of an Application and Process Distributions of Concentrations by Receptor*** -- All transport and dispersion modeling is done in the standard EPA regulatory model ISCST3. The diurnally varying emissions sequence that represents the user-specified off-gassing period for an application is continuously cycled through ISCST3 during the duration of off-gassing input for the model runs. From the start of a fumigant application through TOXST, based on the user-assigned probability, data are drawn from the looping ISCST3 output file until the full number of periods is processed to represent the complete off-gassing period as specified by the user. In time, when AERMOD (EPA, 1998) receives regulatory status, it could be inserted to the system to replace ISCST3.[10]

[10] As a neutrally buoyant, ground level source, however, the differences between ISCST3 and AERMOD generally are not expected to be substantial, especially during critical nocturnal conditions.

- ***Triggering an Application Sequence*** -- The random probability of the start of an application is treated via the EPA TOXST model. The FEMS set-up screen prompts the user to input the number of applications to be modeled (on average) per year. The system then computes the probability for the start of a sequence by considering the annual frequency and the duration. The standard FEMS runs are for annual probabilities. Custom runs can be made, however, using only data for a selected season to further refine consideration to match seasonal patterns by crop and by region. The computational methods are identical to the annual default treatment.

  The goal is to be realistic. It is important to acknowledge that in many cases, there will not be a uniform probability for applications because of the seasonal nature of planting and fumigation schedules. The objective when using seasonal analysis is to input meteorological data that are consistent with typical conditions expected for crops that are generally applied at that time. In some cases, tight planting windows may require adjustment to the probability for the start of an application to match regional requirements. Among the benefits of having the flexibility to do seasonal analysis is the ability to input season-specific emissions data for fumigants, when data are available, to support this level of analysis. The non-summer seasons would be expected to have much lower off-gassing rates, especially for the more northern climates.

  As examples, consider the following three special cases. These are real-world complications that can be addressed through FEMS:

  1. <u>Precipitation</u> -- Application of fumigants is not generally recommended during periods of precipitation. To maintain a tractable analysis, FEMS does not attempt to exclude days with precipitation. It is not expected that this factor is particular significant for most regions of the United States. As is true with all applied modeling, there is no substitute for applying user judgment to meet the case-specific needs of the analysis at hand.

  2. <u>Sequential Applications of Large Fields</u> -- If one grower were planning on fumigating a contiguous, 160-acre block, the fumigant application would be done over a series of consecutive days in most cases. Custom runs of FEMS can be made under this situation, extending the total application event duration to cover the multiple area sources that would be assumed to be applied on successive days. The incremental impacts from all segments would be considered, including the differences in daily attenuation within the off-gassing cycles of each field.

  3. <u>Multiple/Adjacent Fields Under Independent Control</u> -- Unlike the preceding scenario, fields under independent control would not be expected to be applied in a planned, consecutive sequence. Rather, each field would set up as an independent source in TOXST. Consideration would need to be given, however, to the reality that even within a season

there may not be a uniform probability for an application. Certain planting windows could compress the likely application periods (especially assuming common crops) to a smaller window, such as a one-month period for example. As necessary, probabilities for starting an fumigation application would need to be set accordingly for this special case scenario.

- ***Connection Between ISCST3 and TOXST*** -- ISCST3 produces output on an hour-by-hour basis, which serves as input information into TOXST. The TOXST model is an ISCST3 postprocessor designed to enhance the analysis of acute exposures for batch operations and also for continuous operations, but variable emission rates that are not amenable to hourly or parameter scaling in ISCST3. When processing many simulated years of applications at a field, the 200 years of ISCST3 model runs are used to represent the variability in the normalized modeling and emission treatments. The ISCST3 model output is constantly being cycled throughout the 24 sequential periods. When TOXST initiates the application starts according to the probability that is set, and TOXST then tracks the number of averaging periods needed to complete a full emissions cycle.

  For example, if 4-hour averaging and a 4-day emissions sequence are used (as required for the prototype version of FEMS), there will be 24 periods per application. If the start of an application is triggered in mid-cycle, for example in Period 5, then TOXST would process periods 5 through 24 emission rates from the current output from ISCST3 at that time, and then process periods 1 through 4 emission rates before terminating that particular application sequence. Because the analysis is based on distributions of concentrations at the averaging period of interest, and all periods are diurnally matched to the field data, the order of averaging periods is not relevant to the analysis**.** In the future, data from AERMOD could be output to support the TOXST input requirements, or alternatively, streamlined software could be developed along similar lines just to initiate the start of applications, track the number of periods, and then track the distributions and create the necessary outputs, rather than use TOXST.

- ***Computing Endpoint Distances*** -- The largest distance around the compass that is needed to reach the endpoint concentrations of concern is computed through FEMS by logarithmic interpolation of the TOXST output. This logarithmic curve is based on the expected drop in concentration with distance and matches well with modeling results. Once the approximate range is determined by assessing the rings with the closest number of occurrences to the threshold value, the two closest distance rings are used to target the proper distance by interpolation based on the equation of the curve that best simulates the decline in concentration with distance from the field without using complex mathematics. The equation for the curve as described below has been found through testing during the development of FEMS to best represent endpoint distances when compared with isopleth analysis of the TOXST output:

Y = e ^ ((x – b)/a)

Where
Y = distance to endpoint from center of field
x = occurrences / year of reached endpoint in TOXST
a = (occurrences / year of ring 2 – occurrences of ring 1) ÷ (ln (ring distance 2) – ln (ring distance 1))
b = occurrences / year of ring 1- (a * ln (ring distance 1))

For example, using the example dataset below, the results can be calculated using the above equation to derive a distance of 685 meters from the center of the field.

Target Number of Occurrences / year (x) = 1.49
Ring Distance 1 = 500 meters
Ring Distance 2 = 750 meters
Occurrences of Concentration Threshold at Ring Distance 1 = 2.5
Occurrences of Concentration Threshold at Ring Distance 2 = 1.2

Therefore
a = (1.2-2.5)/(ln(750)-ln(500)) = -1.3/.4055 = -3.21
b = (2.5-(-3.21*ln(500)) = 2.5 – (-19.95) = 22.45
y = e ^ ((1.49-22.45)/-3.21) = e ^ 6.53 = 685 meters

- ***Output Data Supports Selecting Percentile for Compliance*** -- TOXST directly computes the average number of times per year concentrations are higher than user-specified thresholds at each receptor, with the user defining the basis for compliance. FEMS uses this information to display the maximum downwind distances, considering all directions around the compass, needed to reach user-specified threshold concentrations. The distances output from FEMS are computed based on the user-specified number of times per year concentrations are greater than the selected thresholds. These outputs also can be interpreted in terms of percentiles of concentrations, rather than times per year above thresholds, by simple conversions as described below.

  For example, when 4-hour averaging is used, there are [8,760 hours/year]/[4 hours per period] = 2,190 periods per year. The point of compliance could be set on the basis of the “x” percentile value out of 2,190 possible periods per year to consider frequency. For example, if 1.5 times per year above concentration thresholds were selected in FEMS as the basis for computation, the equivalent percentile would be computed as follows:

  Percentile = [(2,190 - 1.5) / 2,190] * 100 = 99.93

An alternative perspective on exposure would be to consider percentiles of exposure during the active off-gassing sequence. Using 1.5 times per year above concentration thresholds in this case would convert to percentile form as follows:

$$\text{Percentile} = [\ (24 - 1.5) / 24\ ] * 100 = 93.8$$

or if 1.0 were used instead of 1.5:

$$\text{Percentile} = [\ (24 - 1.0) / 24\ ] * 100 = 95.8 \sim 95$$

By selecting the percentile to match the scale of review of interest, the focus can be on either the active emissions (off-gassing) period or the annual perspective. Considering both perspectives, however, most realistically describes the magnitudes and frequency of exposures.

- ***Approach to Account for Regional Variability in Meteorological Data*** -- On a national basis, FEMS provides the user with the option of selecting a specific region for analysis, with the representative 5-year data sets being available for access within the modeling system. Special sub-regional adaptations also can be available, such as the subdivision of California into 5 or 6 sub-regions to meet California Department of Pesticide Regulation (CDPR) requirements. The prototype version of FEMS contains one sample 5-year meteorological data set for the Fresno, California sub-region. Attachment 5 provides a recommended methodology to address regional applications of FEMS to address the national perspective.

2.3 Selection of Specific FEMS Options

In addition to selecting the emissions sequence file representing the application/ sealing scenario of interest, users are provided with the option of selecting from among the inputs described in Tables 1 and 2. It is important to note that prior to using FEMS for a specific fumigant, the ".dat" files need to be set up to match the format of the kern2001.dat file used as the test case in FEMS. Once these files (one for each application and sealing method of interest) are copied to the FEMS subdirectory on the hard drive (where FEMS is installed), these distribution are then available to support exposure assessment for that fumigant.

Meteorological data for other regions will be populated in FEMS after the SAP review of the prototype.

2.4 Summary of Conceptual Model: Specific EPA-Recommended Model Documentation Elements

The following summarizes on a conceptual basis how the FEMS approach meets the EPA-recommended objectives in the development of a model for agricultural fumigants.

2.4.1 System Boundaries

Off-gassing from an applied field defines the source. The default modeling domain is set arbitrarily at 2,500 meters, well within the generally accepted applicability of Gaussian modeling in applied assessment. Applications can be modeled for anywhere in the United States, with emphasis to be placed on meteorological data representative of California, Pacific Northwest, Great Lakes, Florida, and the Southeastern United States. The prototype version of FEMS contains meteorological data from Fresno, California as the test case example.

2.4.2 Important time and length scales

The minimal modeling unit is a one-hour increment, consistent with standard EPA modeling practice and the development of the EPA ISCST3 and TOXST models (EPA, 1999; EPA 2003b, and National Research Council, 1994). The outer extent of the modeling domain will rarely exceed 25 km. In most cases, the critical area of the modeling domain will be within 2.5 km.

Table 1: FEMS Input Parameters

Name of Parameter	Description of Parameter	Minimum Value	Maximum Value
Area Source (IX & IY)	Length and Width of Applied Field in meters	1 meter	1000 meters
Receptor Grid	10 Polar Receptor Grid Rings (5 degree increments) in distances from the center of a field	Ring 1 of 10 (user defined or 50 meters)	Ring 10 of 10 (user defined or 2500 meters)
Simulation	Number of TOXST simulated years to run	200 years	100,000 years
Monte Carlo	Randomization Parameter for Wind Speed, Wind Direction, Atmospheric Stability, and/or Emissions	0 (No randomization)	1 (Randomized data)
Indoor	Ambient, Personal, and/or Indoor Exposures	0 (only ambient)	3 (all exposures)
Number of Applications/Year	Number of Application/year	Once every 4 years	Three times a year
Days	Days field off-gassing	1	100
Averaging Time	Averaging Time for Exposures[11]	1	24
Application Rate	Application Rate Percentage of Modeled Value	1%	200%
SPSS	Parameters to define emissions distribution[12]	User defined	User defined
Occurrences of Threshold Attainment	Number of times/year concentration threshold can be interpreted in terms of percentile	0.00 (0.01 threshold of sensitivity)[13]	100.00
# of Thresholds	Number of Thresholds to be modeled in TOXST	1	6

11 Averaging times are in integer units that 24 can divide into (1, 2, 3, 4, 6, 8, 12, and 24 hours).

12 These files need to be set up on a chemical-specific basis prior to making model runs with FEMS. The emissions distributions need to be computed by the user in the sample format shown for kern2001.dat in the FEMS subdirectory. Separate emissions distributions are needed for each application method, sealing method, and specific conditions of interest.

13 FEMS calculates the number of occurrences/year that concentration thresholds are reached down to the 0.01 level in increments of 0.01. FEMS has not been evaluated in terms of stability for frequencies less than 0.05 occurrences/year when concentrations are greater than threshold levels.

Table 2: Meteorological Datasets

Metam-sodium Use Region	Surface Meteorological Station	Upper Air Meteorological Station[14]	Years of Dataset
California	Fresno	Oakland	1987-1991
Pacific Northwest	To be added	To be added	To be added
Great Lakes	To be added	To be added	To be added
South East	To be added	To be added	To be added
Florida	To be added	To be added	To be added

2.4.3 Key processes

Although the methods of application and sealing may differ, and result in different emission rates and differing daily cycles in emissions, the only source modeled in FEMS is off-gassing associated with fumigating an agricultural field.

2.4.4 System characteristics

To process data in an efficient and timely manner, and to avoid potential memory limitations, it is necessary that FEMS be run on a computer system with the following minimum specifications:

- 2 GHz Speed (preferred)
- 512 MB of RAM memory
- 10 GB available on hard drive
- Windows 98/2000/XP with DOS PROMPT

14 Upper air data are used to enter mixing height term to ISCST3. For a ground-level source all typical modeling domains (< 5 to 10 km), this term has little effect, if any, on the results. For example, the potential artifact near sunrise from the EPA meteorological processor PCRAMMET is caused by assignment of neutral (D) stability within 10 minutes of sunrise -- some anomalous low mixing heights < 10 meters can be assigned by the preprocessor for non-stable conditions. This artifact produces low-level trapping of the off-gassing plume, which can lead to unrepresentatively high modeled concentrations. As an example of the unrealistic nature of this condition, consider a field with a surface roughness of 1 cm, a mean wind speed of 1 m/sec, and at a latitude typical of central California. The mixing height can be computed for neutral conditions using the relationship: mixing height = ~ (a)(u*) / f, where a = 0.2-0.3, u* = friction velocity, and f = coriolis force (Randerson, 1984; Panofsky and Dutton, 1984). This default estimate of mixing height during such conditions would be in the range of 150 to 225 meters, well above the conservative default used in the processing of meteorological data for FEMS.

2.4.5 Source description

The source can be considered in three dimensions to encompass the applied field to an application depth of typically 12 to 24 inches or more, depending on the fumigant and application method. The active ingredient is contained in some ratio of vapor phase over liquid phase, the magnitude of which depends on the fumigant's physical and chemical characteristics, as well as the soil type and conditions.[15] Movement of the active ingredient on a vertical basis can take place in the liquid or vapor phase, with ultimate release at the surface in the vapor phase. The total off-gassing rates to the atmosphere as a function of time are computed in an empirical manner typically based on field studies, either by ambient networks or flux monitoring on the field, often conducted under worst-case/upper-end conditions in terms of off-gassing potential.

2.4.6 Available data sources (quality and quantity)

The following categories are addressed:

- ***Emissions Data*** -- FEMS was developed using data collected from air quality monitoring networks (typically established approximately 150 to 700 meters from the edge of an applied field). These measured air quality data, in conjunction with normalized dispersion modeling, are used to compute emission rates in time steps (typically 4 to 6-hour increments) using least-squares analysis of the natural logarithms of measured and normalized modeled concentrations for each time increment evaluated. The use of alternative methods to estimate emissions as a function of time could be employed, such as on-field flux monitoring or potentially by remote sensing. The distributions of emission rates by time steps would need to be parameterized by a cubic function fit, however, to be used within the current coding in FEMS. Otherwise, minor coding changes would be needed to accommodate alternative emission fitting methods.

- ***Meteorological Data*** -- Standard meteorological data from the National Weather Service (NWS) or Federal Aviation Administration (FAA) are used to model exposure in FEMS, including readily available data for wind speed, wind direction, ambient temperature, and sky conditions (total opaque sky cover and ceiling height) needed to complete the required data to compute stability class for each hour. Hourly mixing height data are processed based on twice per day regionally available upper-air soundings through a standard EPA meteorological pre-processing program, PCRAMMET,[16] to create model input files that are suitable for the ISCST3 model. In terms of emission fitting procedures used for

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15 Methyl Bromide is an example of a gas-phase only application.

16 PCRAMMET is accessed in the FEMS run stream because the randomization of the uncertainty associated with wind speed also effects the computation of atmospheric stability.

the interpretation of measured air quality data, onsite meteorological data are collected concurrent with the field studies. Wind monitoring heights are typically set at 10 meters for Good Laboratory Practice (GLP) studies. Stability and mixing height data are computed by PCRAMMET.[17] The 5-year meteorological data sets are based on wind data typically collected at 6 meters (20 feet), which introduces a minor degree of conservatism in the exposure analysis.

2.4.7 Data Gaps

- ***Data Gaps in Default Emission Rates*** -- The most significant data gap in the use of FEMS involves establishing default emission rates for those periods where emission rates, including emissions distributions, cannot be specifically computed because of limitations in the available field data. There are two ways that these data gaps can be filled:

  - *Default Method*: The default method involves averaging the two adjacent emissions distribution to the average of the two nearby non-defaulted periods' emissions distribution, weighting as necessary by proximity to periods with non-default emissions data. If this is judged to be infeasible, the preceding diurnally matched period can be used as a default for the period in question. This would be a generally conservative estimate, because the amplitude of the emissions within the diurnal cycle typically becomes lower each day. In the event of missing data, standard procedures such as these are recommended, but should not override user judgment when an alternative approach is determined to represent best the site-specific conditions.

  - *Alternate Method*: Time series analysis provides a potentially more representative means of filling data gaps, using exponential smoothing with linear trends and additive seasonality (in this case diurnal) factors considered. On this basis, gaps are filled by first using interpolation from adjacent periods to produce a complete data set for time series analysis. Then, the interpolated values can be replaced by the corresponding data from the time series analysis.. The primary advantage of this approach is that it considers all of the available information, rather than the more subjective options of manual diurnal matching or linear (weighted) interpolation from adjacent points. This approach considers three primary terms: a smoothing factor; a trend term; and a seasonality factor. SPSS

[17] Mixing heights were adjusted to 10.1 meters if they were < 10 meters, per EPA guidance, because of modeling artifacts from modeling a ground level source with mixing heights of <10 meters. Although this artifact would not generally be a sensitive issue for routine analysis in FEMS, for any evaluation of very low frequency events (low probability events) it could become more of an influential factor.

software was used for the example provided in this background document. Other statistical software packages could provide comparable methods.

The specific steps taken to use time series analysis to fill data gaps are as follows:

1. All periods that do not have sufficient data to estimate the emissions term are initially interpolated based on linear interpolation weighted by the proximity of the adjacent periods with non-default coverage.

2. At least four complete cycles are needed to fit the time series. Defaulted data will be needed if by the fourth day concentrations are at or near the detection limits of the air quality sampling method. On this basis, it is preferable for in-depth, GLP studies to include a minimum of four diurnal cycles.

3. An iterative approach is used to fit the parameters in the time series, for example, using the grid search method in SPSS Version 12 (Trends package).

4. Data that were defaulted are then replaced with the corresponding values from the fitted time series.

Figures 6 and 7 present the four-day time series for metam-sodium field studies applicable to chemigation/intermittent sealing and shank injection/intermittent sealing, respectively, based on exponential time series analysis (linear trend and multiplicative seasonality component with 6-period periodicity) fit with the following parameters:

Application and Sealing Methods	**Alpha term**	**Gamma term**	**Delta term**
Chemigation Intermittent Sealing	0.00	0.050	0.053
Shank Injection Intermittent Sealing	0.00	0.20	0.00

As shown in Figures 6 and 7, the overall emissions pattern is reproduced, but in some cases the peaks in the time series are higher or lower than the directly computed emissions data. The analyst using FEMS will need to use judgment in interpreting the time series, and take suitable steps to help ensure that data gaps are not filled in a manner that would be likely to understate exposures on this basis. As mentioned earlier, however, it is more important that distributions of emissions and exposures are established on a daytime and nighttime basis than expecting a high level of accuracy on a period-by-period basis.

The current examples are based on the default approach, although the test data set for chemigation/intermittent sealing (kern2001.dat) did not require any data filling procedures. It is planned that future applications of FEMS will be processed with data gaps being filled by the time series approach.

- ***Data Gaps in Meteorological Data Coverage*** -- Meteorological data are used for two purposes in FEMS: (1) in the form of onsite meteorological data to support the computation of emission rates; and (2) for the exposure assessment based on five year, sequential meteorological data sets. If there are missing records during a field study, they are generally filled based on the most representative source of off-site data. The five-year data sets are generally based on data collected at NWS or FAA meteorological monitoring sites. The surface meteorological data generally have few data gaps, however, the twice per day soundings data more often have some missing data. Generally, these gaps are filled by interpolation based on adjacent hours. More extensive gaps can be filled by climatological means. For this application involving ground-based area sources with modeling domains of interest typically within a few kilometers or less from the source, mixing height is generally of little or no significance, however, for the exposure assessment.

2.4.8 Data Collection Programs (Quality and Quantity)

Attachment 1 summarizes the four GLP field studies that are serving as the initial databases in FEMS.

2.4.9 Mathematical Model

The core dispersion modeling algorithms in FEMS are based on the Gaussian plume model. The Gaussian assumption is widely used in applied, dispersion modeling and is well-accepted throughout the scientific community. There are, however, inherent limitations in the use of Gaussian modeling, most notably the Gaussian assumption to represent vertical dispersion during afternoon convective conditions (Lamb, 1978; Willis and Deardorff, 1974, 1976a, 1976b, 1978, 1981). In most cases, the conditions of most critical concern in terms of exposure to fumigants are nocturnal inversions, which are not affected by this limitation. The current approach used in FEMS is to minimize any mischaracterizations of exposures during convective conditions to ensure that the modeling used to fit emission rates also is repeated in the same fashion when actual exposure assessments are conducted using long-term meteorological data sets. On this basis, empirical compensation can help minimize Gaussian model limitations during convective conditions. Additional improvements may be achieved in the future by enhancing modeling methods to compute reasonably reliable estimates during convective conditions for receptors close to, or on the ground-level area sources being modeled. Convective period complications are not considered a significant issue in terms of the limiting conditions for bystander exposures. Rather, the scope of FEMS to also cover the model-based extrapolation of worker exposure data to broader scenarios (different cultural application practices or different field conditions) could be enhanced through refinement in the treatment of convective conditions. Workers are on or near the field typically during daytime periods when convective conditions most likely occur.

Figure 6: Time Series ($\mu g/m^2/sec$) Analysis for Chemigation/Intermittent Sealing (Merricks, 2002a)

(Note: time series was based on 4 days (4 complete cycles) and then forecast out to the 6th day)

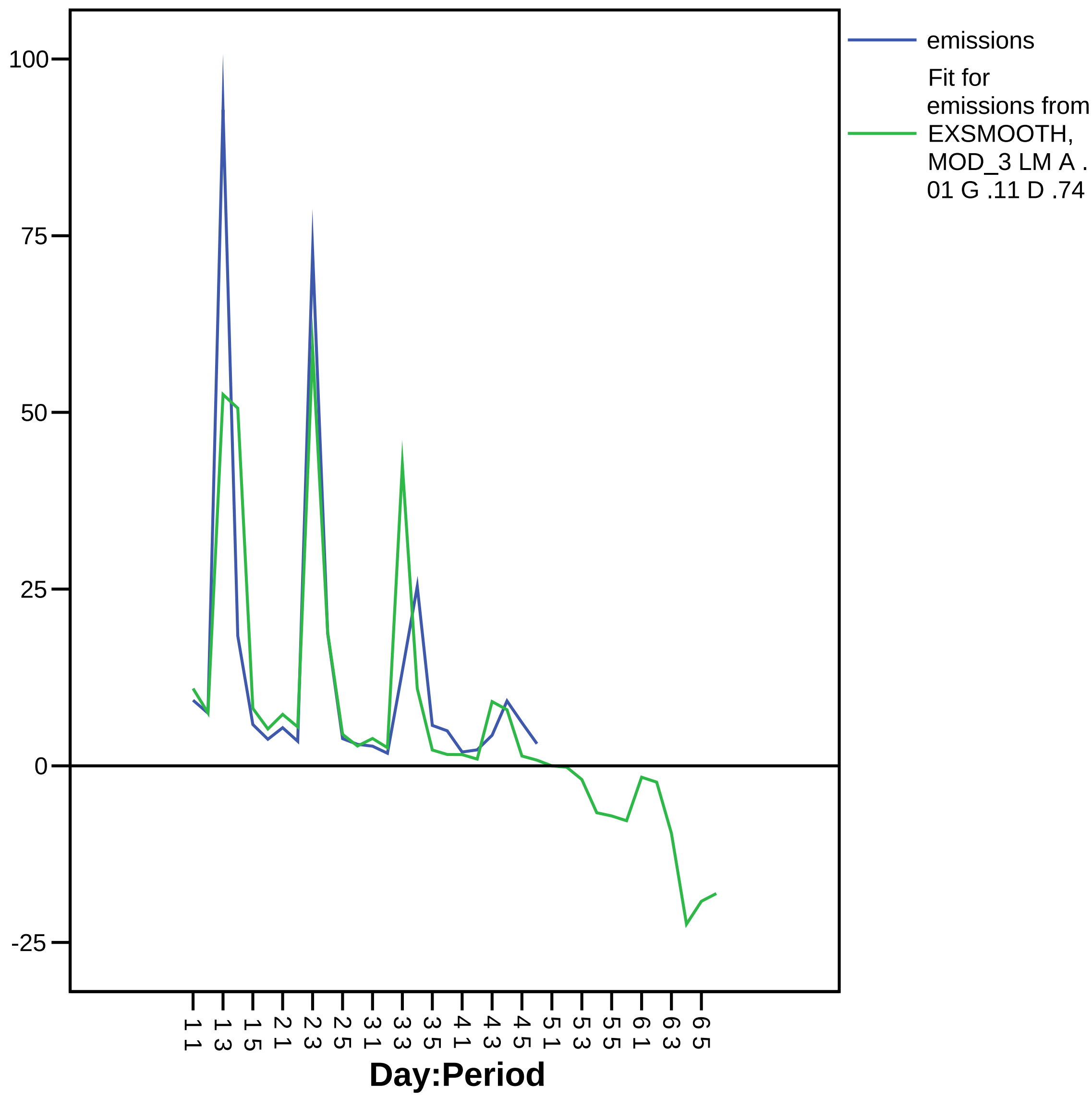
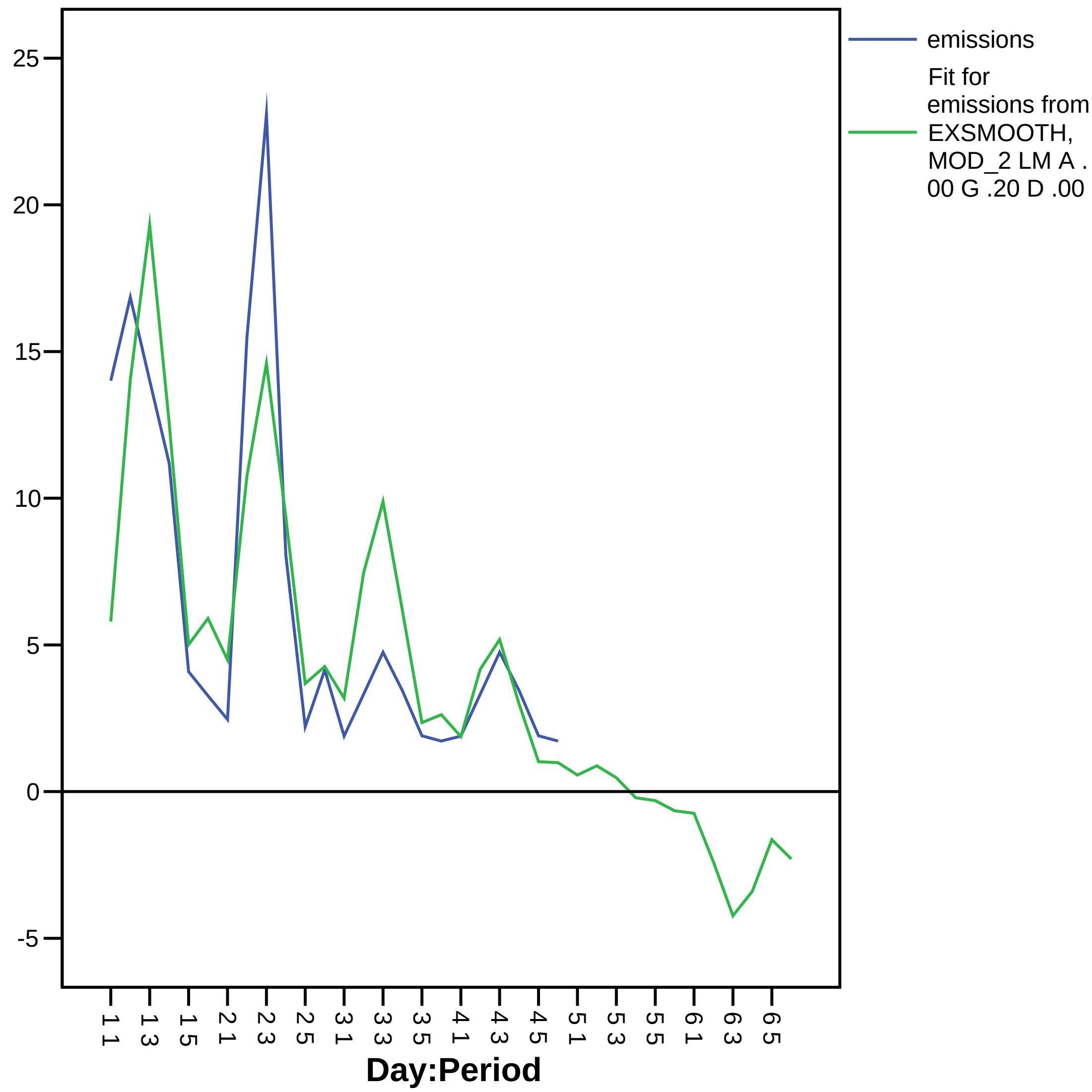


Figure 7: Time Series Analysis (µg/m²/sec) for Shank Injection/Intermittent Sealing (Merricks, 2001)

(Note: time series was based on 4 days (4 complete cycles) and then forecast out to the 6th day)



Limitations of the Gaussian model to represent the vertical profiles of concentrations for ground-level sources also have been noted (Turner, 1994; Nieuwstadt and van Ulden, 1978; and Gryning, van Ulden, and Larsen, 1983). These limitations, however, are not expected to be a significant limitation in the context of agricultural fumigant modeling. First, these limitations are restricted to neutral and unstable conditions, which often are not associated with worst-case, limiting exposures (especially for standard sealing methods). Second, the empirical fitting of emission rates using the same ISCST3 modeling treatments, as used when modeling multiple-year meteorological data sets in FEMS, provides empirical matching to represent model estimates at the monitoring height of approximately 1.5 meters above ground level. While it is probable that the vertical distribution above the 1 meter height may not be well characterized by the Gaussian fit for ground-level sources under neutral and unstable conditions, only the 1.5 meter level is used for subsequent analysis. This limitation, therefore, is not expected to be significant for this model application.

2.4.10 Important Assumptions

A summary of the important assumptions used in the development of FEMS include:

1. *Worst-Case/Upper-End Field Studies* -- Field studies conducted in Kern County, California (Bakersfield area) during summertime conditions represent worst-case, or high-end, emissions potential.

2. *Log-Transformed Data Are Needed to Fit Emissions Data* -- Emission fitting procedures are based on least-squares analysis of natural log-transformed measured and normalized modeled concentrations. There are well established precedents for conducting statistical analysis of concentrations with natural log transforms. For example, "*Lognormal distributions have a number of useful characteristics relevant to physical quantities . . . . For example, they assume only non-negative values in the common two parameter form. Also, the lognormal distribution describes random variables resulting from multiplicative processes. Further, the concentration of a chemical in the environment is often well-described by a lognormal because it results from dilution processes in water or air*." (Cullen and Frey, 1999, p.65).

   Another justification for a log-normal distribution would be the evaluation of the physical basis for concentrations/dilution processes in all environmental media to follow log-transformed treatments as described in Ott, 1990.

   Considering the above references, it would necessary to compute emission estimates using log-transformed measured and normalized modeled concentrations when using least squares regression to produce meaningful distributions of emission rates.

   Furthermore, based on review of existing field data (Merricks 2001, 2002a, b), it has been demonstrated that log-normal data produces much more ordered probability plots, and residuals based on least-squares analysis that are more normally distributed than in the original units. Probability plots were produced for the first six periods of the chemigation/intermittent sealing study to compare normal versus lognormal fitting of the measured data. Figures 8 through 13 clearly demonstrate that the air quality data are not normally distributed, and a log-normal transformation is much more appropriate to support subsequent statistical analysis.

Another consideration for using log-transformed data in this case, is the fact that emission rates cannot be negative. Especially considering the large magnitudes of the standard deviations of the measured air quality concentrations, the "rule of thumb" that the coefficient of variation should not exceed 0.3 is routinely violated if original units are used for emission fitting (Cullen and Frey, 1999). As an example, the following table, Table 3, shows the summary statistics for the first six periods (4-hour duration each) for the measured air quality concentrations for the chemigation/intermittent sealing study (Merricks, 2002b).

Table 3: Summary Statistics for First Six, 4-Hour Periods at the Chemigation/Intermittent Sealing Study (Kern 2001)

	N	Mean	Standard	Skewness		Kurtosis	
	Statistic	Statistic	Statistic	Statistic	Std. Error	Statistic	Std. Error
Period_1	15	65.1800	69.15929	1.240	.580	.599	1.121
Period_2	15	6.4733	12.54139	2.855	.580	9.035	1.121
Period_3	15	13.3600	37.50942	3.136	.580	10.018	1.121
Period_4	15	30.6800	64.64662	2.623	.580	6.571	1.121
Period_5	15	33.9267	39.35941	1.418	.580	1.845	1.121
Period_6	15	29.4800	30.12282	1.149	.580	.564	1.121

As shown in Table 3, in general, the magnitude of the standard deviations is similar to the means, with a high degree of positive skewness in the data. The coefficient of variation shows a minimum of 1.00, which is well above the recommended $\leq$0.3 to justify the use of a normal distribution, without log transformation, since negative emission rates are implausible. Non-transformed concentrations would therefore routinely produce anomalous, negative, emission rates for the lower portion of the emissions distributions, and understate the tails of the upper-end of the distributions, both of which would be problematic. As a point of reference for Table 3, normal distributions have a kurtosis of 3.0 and skewness of 0.0.

In summary, the use of log-transformed data in the computations of least-squares analysis provides the basis to match the skewness in the observed concentrations and avoid the computation of negative emission rates at the lower end of the distribution (unless the distribution was artificially truncated at zero emissions).

3. *Gaussian Modeling is Reasonable for This Application* -- Gaussian modeling of ground-based area sources represents a reasonable basis for the exposure assessment of vapor-phase agricultural fumigants during conditions most conducive to high impact conditions.

4. *Five Years of Base Meteorological Data is Sufficient* -- Five years of sequential, hourly meteorological data provide sufficient coverage to support the Monte Carlo-based extrapolation to 200 base years of meteorological data, which ultimately are used to account for uncertainty in the meteorological inputs to the exposure assessment.

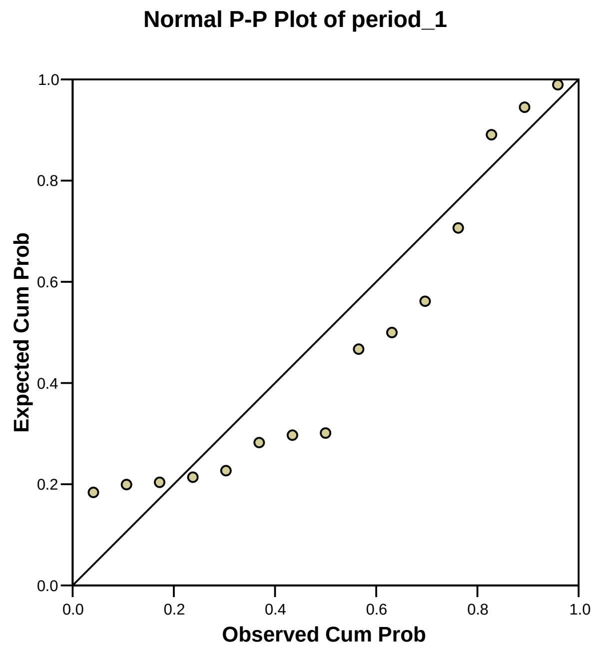
5. *Homogeneous Area Source Assumption is Suitable for Modeling Bystander Exposures* -- It is assumed for emission-fitting and modeling of exposure that the surface of the applied field uniformly emits throughout the total applied area. Although at the microscale level within the field, nonhomogeneity would be expected, in terms of the scale of the modeling analysis, the assumption of homogeneity at the composite source level is appropriate and necessary.

6. *Assumptions are Needed for Least-Squares Emissions Fitting* -- FEMS modeling procedures account for the intermittency, variability, and uncertainty in the emission treatments and meteorological input data. The methodology used to develop the distribution of emissions is based on two important implicit assumptions that are needed to make the problem tractable: (1) the measured data are reasonably accurate; and (2) the normalized modeling results are reasonably accurate.[18] In this manner, the standard error for the slope factor in the least squares regression can be isolated and used to estimate distributions of emissions. The compensation factor described in the footnote below is an important consideration in terms of implementing this method. In this sense, an advantage of ambient emissions fitting, relative to flux sampling, relates to the end use of the emissions data. If the goal is to conduct a mass balance of the active ingredient within the treatment zone, flux sampling may be the preferred technique to account for volatile losses. On the other hand, if the use of estimated emissions data is to serve as input to an exposure assessment, then the ambient approach provides a more direct representation of emissions in terms of this end use.

[18] In this case, if there are biases in the normalized modeling, the use of comparable modeling procedures for fitting the emissions distributions and conducting the exposure assessment would act to compensate, at least in part, for model tendencies to over or underestimate concentrations, since the emission rates are computed to provide the best match with measured air quality data.

Figure 8: Comparison of Normal and Natural Log-Normal Probability Plots for the First Six Periods of the Chemigation/Intermittent Sealing Test Case

Period 1
Kern 2001



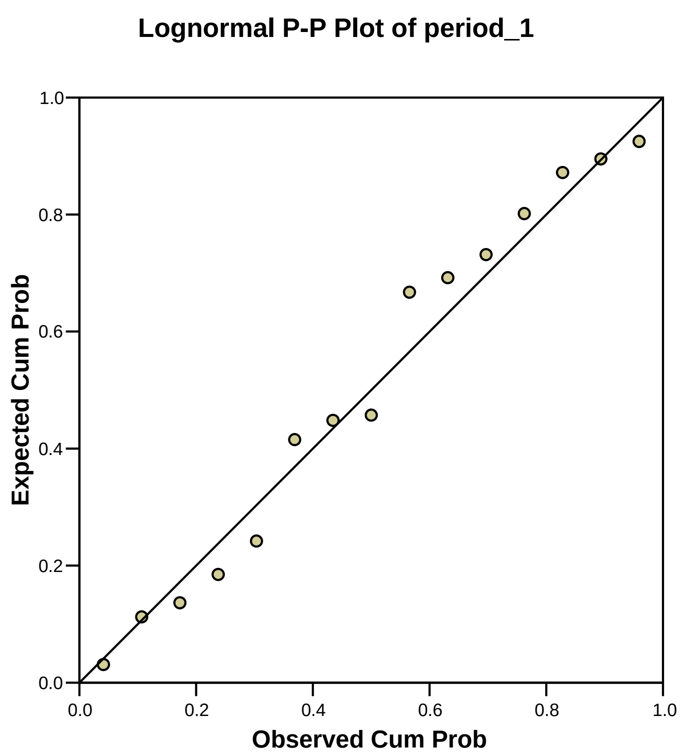
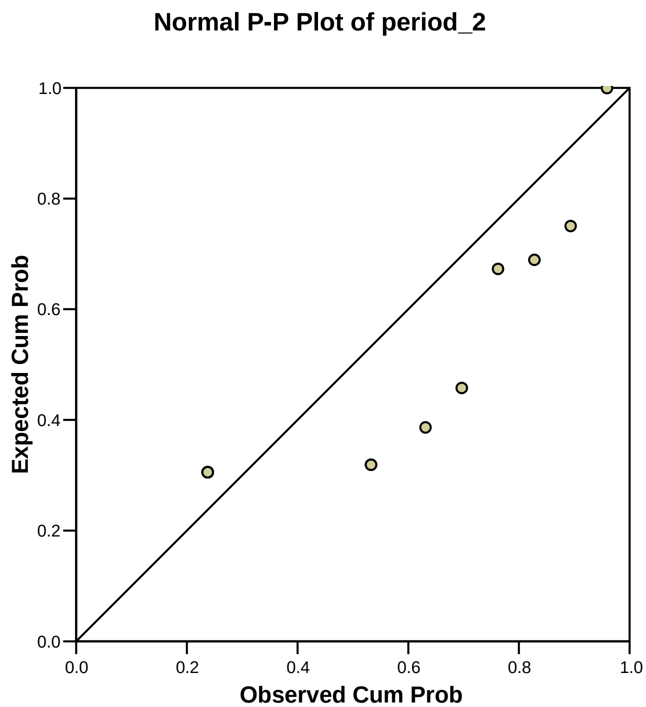


Figure 9: Comparison of Normal and Natural Log-Normal Probability Plots for the First Six Periods of the Chemigation/Intermittent Sealing Test Case

Period 2
Kern 2001



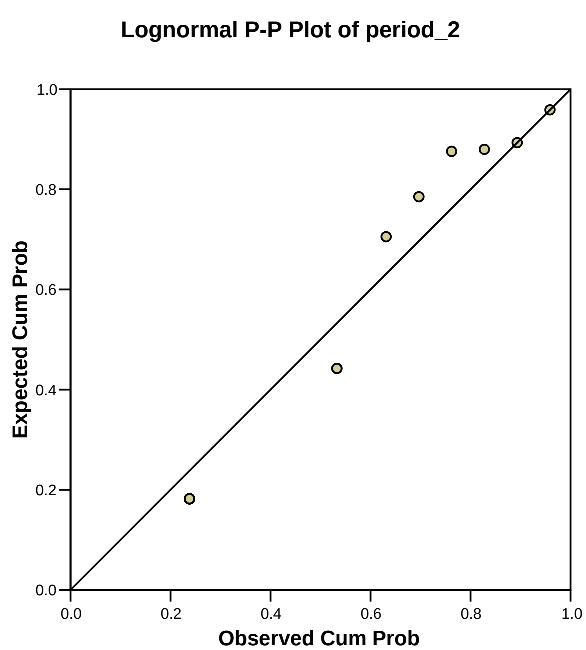
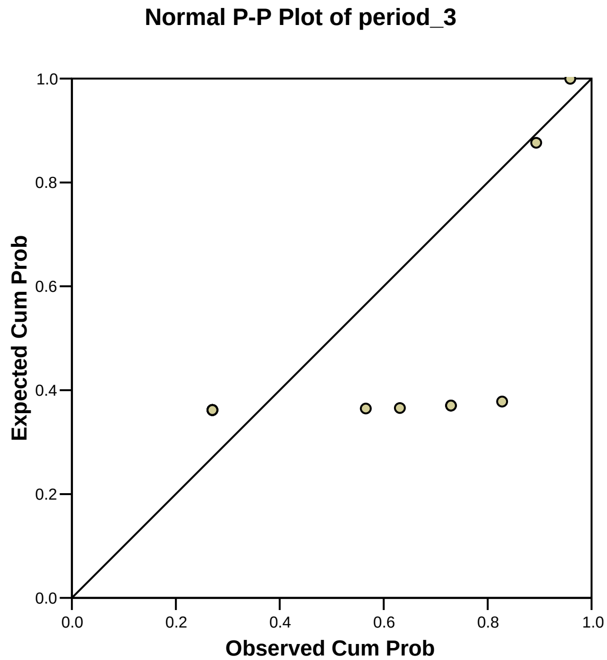


Figure 10: Comparison of Normal and Natural Log-Normal Probability Plots for the First Six Periods of the Chemigation/Intermittent Sealing Test Case

Period 3
Kern 2001



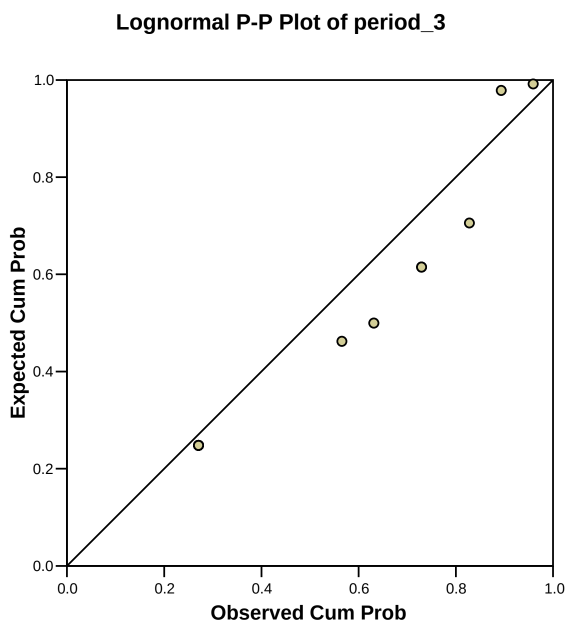
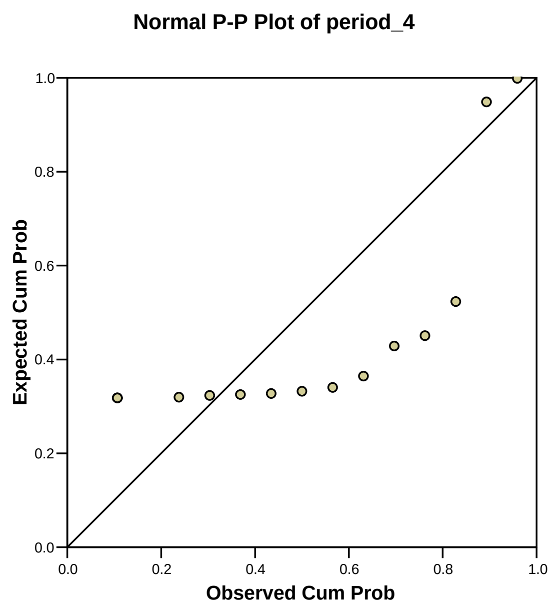


Figure 11: Comparison of Normal and Natural Log-Normal Probability Plots for the First Six Periods of the Chemigation/Intermittent Sealing Test Case

Period 4
Kern 2001



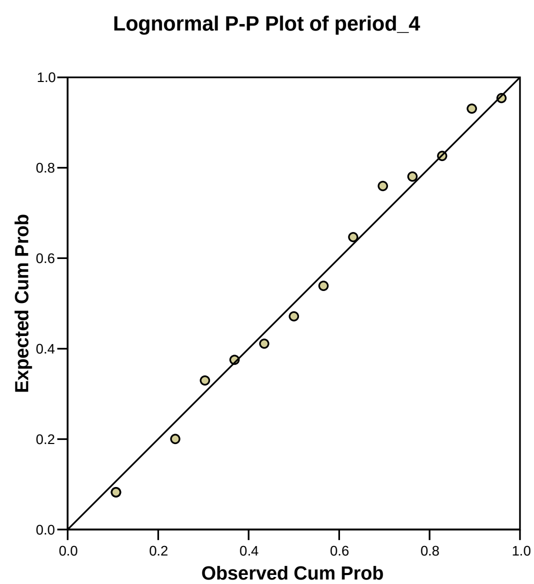
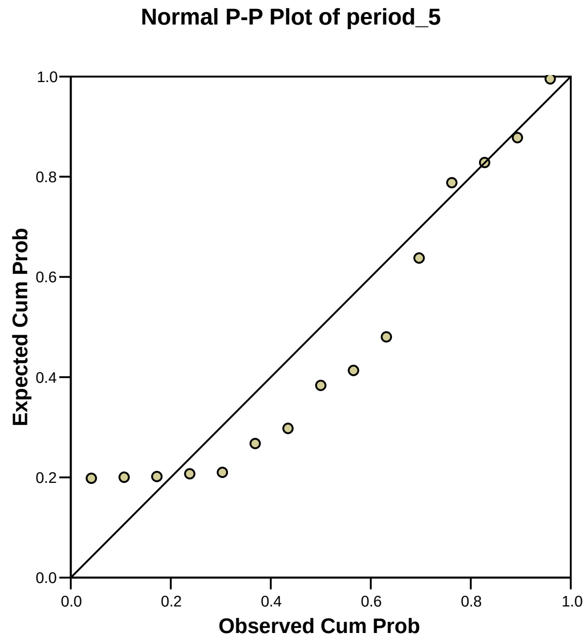


Figure 12: Comparison of Normal and Natural Log-Normal Probability Plots for the First Six Periods of the Chemigation/Intermittent Sealing Test Case

Period 5
Kern 2001



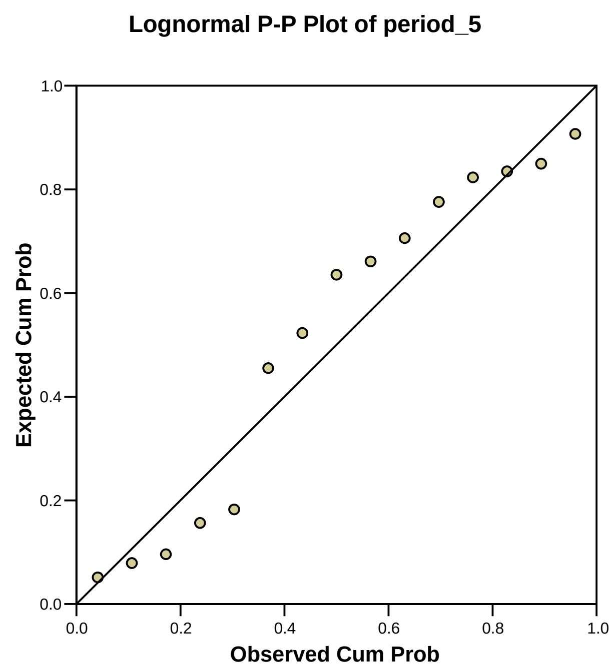
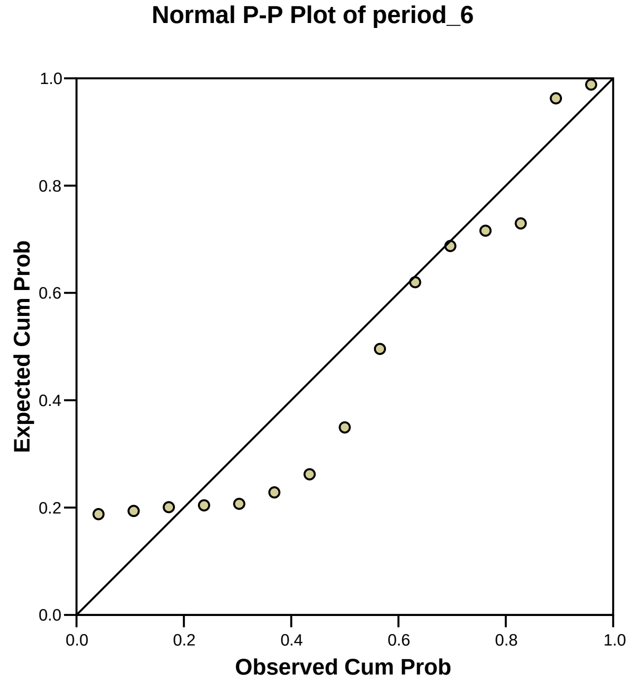
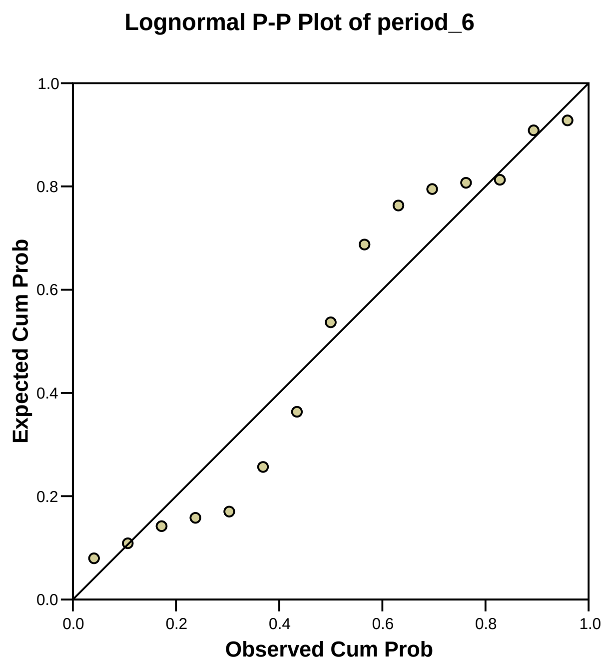


Figure 13: Comparison of Normal and Natural Log-Normal Probability Plots for the First Six Periods of the Chemigation/Intermittent Sealing Test Case

Period 6
Kern 2001





3.0 CHOICE OF TECHNICAL APPROACH

The published FEMS modeling and emissions processing procedures (Sullivan *et al.,* 2004 a, b) are contained in Attachment 1. The first paper describes how emission rates are determined using measured on-site meteorological data, air quality monitoring data, and normalized modeling data. The second paper summarizes the methods used in FEMS to calculate the distances to threshold concentration endpoints by using these calculated emission rates and Monte Carlo sampling techniques. These papers thoroughly document the technical approach used in FEMS, and provide suitable background material to support the review of FEMS. The following section summarizes the approach used in FEMS and also identifies refinements in these methods that have been made since the two technical papers went to press.

3.1 Summary of Technical Approach for Model Development

3.1.1 Meteorological Data Processing

FEMS requires sequential meteorological datasets to produce 200 years of meteorology data with uncertainty around the measured values represented by a probabilistic sampling approach. These datasets generally are based on five years of surface and upper air data acquired from NWS or FAA meteorological monitoring stations. FEMS will support the evaluation of regional differences based on input of representative regional data. The FEMS model is submitted for review using the Fresno NWS meteorological dataset (1987-1991) as the test-case example. Representative data for each major fumigant use region can be made available for utilization in the future, subsequent to model acceptance by EPA. FEMS can be applied to all use regions in the United States once meteorological data are processed for each region (subsequent to the review and acceptance of this prototype).

Meteorological data are processed within the FEMS run stream for each model run using the standard EPA PCRAMMET meteorological pre-processing program. FEMS requires the user to input the latitude and longitude of the region of interest so that the proper sunrise/sunset at that location can be inserted into PCRAMMET to calculate atmospheric stability for each hour. To avoid model artifacts near sunrise, mixing heights are not allowed to drop below 10.1 meters, *i.e.*, if mixing height is computed to be less than or equal to 10 meters, it is reset to 10.1 meters (Atkinson, D., EPA modeling guidance; email correspondence 2004). The actual hour-by-hour meteorological files[19] that are created for the 200-year simulations for each FEMS run are processed to account for uncertainty in the characterization of wind direction, wind speed, and atmospheric stability (and emission rates) on an hourly basis.

[19] Five-year meteorological data sets are the basis for the longer duration simulations in FEMS (200-100,000 simulated years).

3.1.2 Emissions Data Processing

3.1.2.1 Best Fit Emission Rates

The most important component of the FEMS emissions fitting approach is the collection of measured air quality concentrations that are representative of field conditions at the locations sampled. In terms of the number of samples needed to fit emissions data, the availability of a greater number of representative samples would act to reduce the uncertainty in the computed emission rates. Even with only several representative samples (two in the extreme), however, statistical analysis can provide input on the mean and uncertainty range of the mean. The uncertainty likely will be quite large with only a very limited number of samples, but a best fit and uncertainty range can still be computed and used to support an exposure assessment (Cullen and Frey, 1999). A more problematic situation would be to have many samples that were not representative of the conditions of interest.

Prior to presenting the details of the emission fitting procedures used with FEMS, the use of the EPA Industrial Source Complex (Short-Term Mode) model (ISCST3) is summarized below. ISCST3 is the dispersion model used for the emission fitting and the exposure assessment methodologies in FEMS. The area source treatment in ISCST3 is run, using onsite meteorological data for emissions fitting. Available meteorological data that are representative of the region of interest are input to the exposure assessment evaluations in FEMS. The most significant difference between the use of ISCST3 for emissions fitting compared to use for exposure assessment is the treatment of emission rates. Emission rates normalized to 1 $\mu g/m^2$ / sec are modeled when computing best-fit emission rates and emissions distributions. When used for exposure assessment, on the other hand, ISCST3 is run continuously cycling through the 24, 4-hour sets of computed emission rates that represent the empirically-computed emissions sequence for the 4-day off-gassing period that is representative of the application method and sealing method of interest. The cycled emissions data are diurnally matched with the meteorological data.

The following summarizes the differences in the model treatments:

Treatment	ISCST3 used for Emissions Fitting	ISCST3 used for Exposure Assessment
Receptor height	1.52 m Flagpole	0.00 m or 1.5 m Flagpole
Calm processing	Regulatory default	Regulatory default
Typical height of wind sensors (m)	10	6.1
Restrictions instability class changes	No restrictions	Case specific[20]
Area source geometry	Match to field study	Set by user
Receptors	Discrete: match sites	Ring distances set by user[21]

Least-squares analysis is used to compute best-fit emission estimates for each period. Attachment 1 provides further details on the general procedures that are followed. To account for the uncertainty of the computed mean emissions rates for each sampling period, a Monte Carlo approach is used to sample the distribution of mean emission rates within the 95 percent confidence interval around the mean to support this treatment. The computed best fit emission rate and the standard error of the mean are used in natural log units to calculate distributions of emission rates, which are finally recomputed in the original units (Land, 1972). FEMS randomly selects specific emission rates from the distribution of emission rates applicable to the elapsed time since application, with the emission distribution typically advancing in 4-hour increments depending on the temporal resolution in the field study (*refer to* Attachment 1 for more details). The following approach was used to avoid propagating obvious artifacts to the tails of the distribution, and also to seek a minimum number of exceptions:

- To avoid a mismatch between the measured and modeled pairs, the minimum model values are defaulted to 0.1 µg/m^3 if less than 0.1 µg/m^3. This default is necessary because the minimum measured concentration is set at one-half the detection limit, which generally results in 0.1 µg/m^3, for this example (or a 0.2

[20] The four metam-sodium GLP field studies used as examples for FEMS were conducted in Kern, County, California, during the summertime. These conditions can be characterized as a hot, dry climate, typically with sandy loam soils. This is a desert-like climate in many ways. As expected and observed in field studies, there is a very rapid transition from nighttime stable to daytime unstable conditions, and vice-versa near sunset. These rapid changes in temperature at the surface are attributed to the relatively low heat capacities of the soils. Rapid transitions in stability (no restriction) are used for emission fitting to best represent this observation. The specific treatment in the exposure model, however, should be considered on a region-specific basis.

[21] In this context, distances are set relative to the center of the field. The receptor selection and field sizes need to be compatible to generate useful output from FEMS. In the prototype mode, it is best to use the default set of receptors and default area source size as identified in the set-up prompts to avoid a mismatch.

µg/m^3 detection limit). This assumption can be considered similar to a background treatment for the measured and modeled components.

- A minimum of three pairs of measured concentrations greater than 0.1 µg/m^3 are recommended to support least-squares analysis for each averaging period.

- Only computed coefficients from the least-square analysis that are statistically significant are used.

- Mass balance is considered for each of the emission distribution values. In the example of metam-sodium, this chemical degrades primarily to MITC stoichiometrically by the following ratio: 73/129, which is equal to 0.56. Using the 75 gallon/acre application rate, with 100 percent stoichiometric conversion conservatively assumed as the maximum MITC on a square meter basis. If any selected emission rate produces a larger amount of MITC than the maximum potential MITC applied to the field (which would violate mass balance), the emission rate is defaulted to the maximum possible MITC emission rate (assuming the entire amount of MITC is emitted in a four-hour period).[22]

- Field fortification values document the losses of the off-gassing fumigant that may occur from the field sampling through the final analysis at the laboratory, such as during sampling and shipping, as well as through adsorption to sides of tubes. The measured concentrations are increased by scale-up factors based on measured recoveries of a known amount of chemical injected into the sampling tube in the field divided by the actual average recovery rate. Using MITC as an example, a factor of 1.05 to 1.16 is the range of recoveries from recent GLP field studies.[23]

An alternative procedure that could be employed would be to compute the least-squares analyses only using those paired concentrations where the observed (measured) concentrations were above the detection limit of 0.2 µg/m^3. This modification in the approach would serve to increase the standard error, especially during periods when winds are relatively

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[22] For shank injection into the bed, this generally would be 695 µg/m^2/sec at the maximum label rate of 75 gallons/treated acre. Chemigation would be 1,389 µg/m^2/sec at maximum label rate of 75 gallons/treated acre. These values become the maximum potential emission rates that are used as an upper limit to ensure that emission rates near the upper end of the 95 percent confidence range do not result in unrealistically high values that exceed potential mass that is available.

[23] The scale-up factor to account for incomplete sample recovery that is applied to the measured concentration can produce a small increase to the standard error of the mean when non-detect values (0.1 µg/m^3) are recorded, which serves to increase slightly the upper end of the emissions distributions. The final version of FEMS could remove this minor artifact if the SAP agrees.

steady, which usually results in a smaller number of sampling sites showing detectable concentrations. The increase in the standard error would increase the uncertainty in the computation of the mean, and thereby increase the range of emissions in the emissions distributions for these periods.

Figures 14 and 15 present the best fit emission rates for the example shank injection and chemigation data sets for metam-sodium, respectively. These figures show the variability in emissions over the diurnal cycle, the damping of the peak emissions on a daily basis, and the differences in the magnitudes and timing of peaks within the diurnal cycle as a function of application / sealing method.

Situations might occur for some periods where the model breaks down (*e.g.*, from low wind speeds, plume meander, large changes in wind direction within an hour, or low measured concentrations), or there is insufficient coverage of the plume to the point that there is no meaningful correspondence between the modeled and measured concentrations. In these situations, user discretion is recommended to appropriately default the emission rates. Two approaches have been identified in FEMS to fill missing data (*refer to* Section 2.1).

3.1.2.2 Calculation of Emissions Distributions

- ***Log-Normalized Approach* --** If a particular sampling period has at least three pairs of modeled and measured concentrations with concentrations > 0.1 μg/m^3, the Standard Error (SE) based on natural log-normalized data is $\leq$ 1.5, and the slope of the least squares fit is significant (< ~0.05), the natural log-normalized least squares approach is used to calculate the best fit estimate value, and the distribution is recalculated in the original units for the 2.5, 5, 10, 25, 40, 50, 60, 75, 90, 95, and 97.5 percent confidence values for the mean.

- ***Mean Measured/Mean Modeled Approach* --** If the SE is > 1.5 and the number of valid pairs are $\geq$ 3, the ratio of the (average of all measured values) over (average of **all** modeled values) is used to establish the best-fit emissions estimate. In this case, the SE is too large to compute a reasonable distribution, since the distribution could "blow up" to unrealistic levels. Because the ratios of each percentile in the distribution relative to the best fit mean are a function of the SE, the average of the SE values from the adjacent valid natural log-normalized periods is used to estimate the default SE for this period. The emissions distribution is then calculated using the default SE value.

- ***Interpolation Approach*** -- For periods with less than 3 pairs with both measured and normalized modeled concentrations > 0.1 μg/m^3, an interpolation method is recommended to calculate the emissions distribution. Interpolation at each of the standard 11 percent confidence levels of the mean is used as defaults, weighted by proximity, using the closest periods with $\geq$ three pairs that meet the > 0.1

μg/m^3 criterion. This approach uses the mean measured divided by the mean modeled data for the period as the best fit-estimate and then defaults the rest of the distribution through interpolation of SE from the nearest adjacent periods that used the log-normalized approach to calculate the distributions (*refer to* Attachment 1 for more details).

Figure 14: Emissions Sequence (Best Fit) for Shank Injection Applications

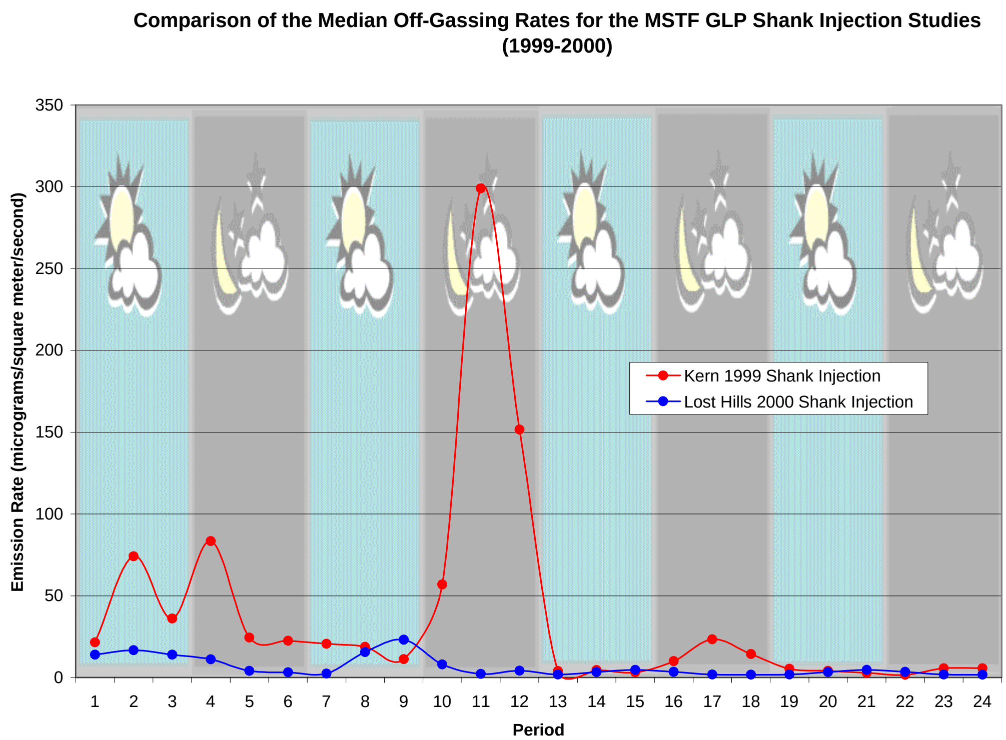
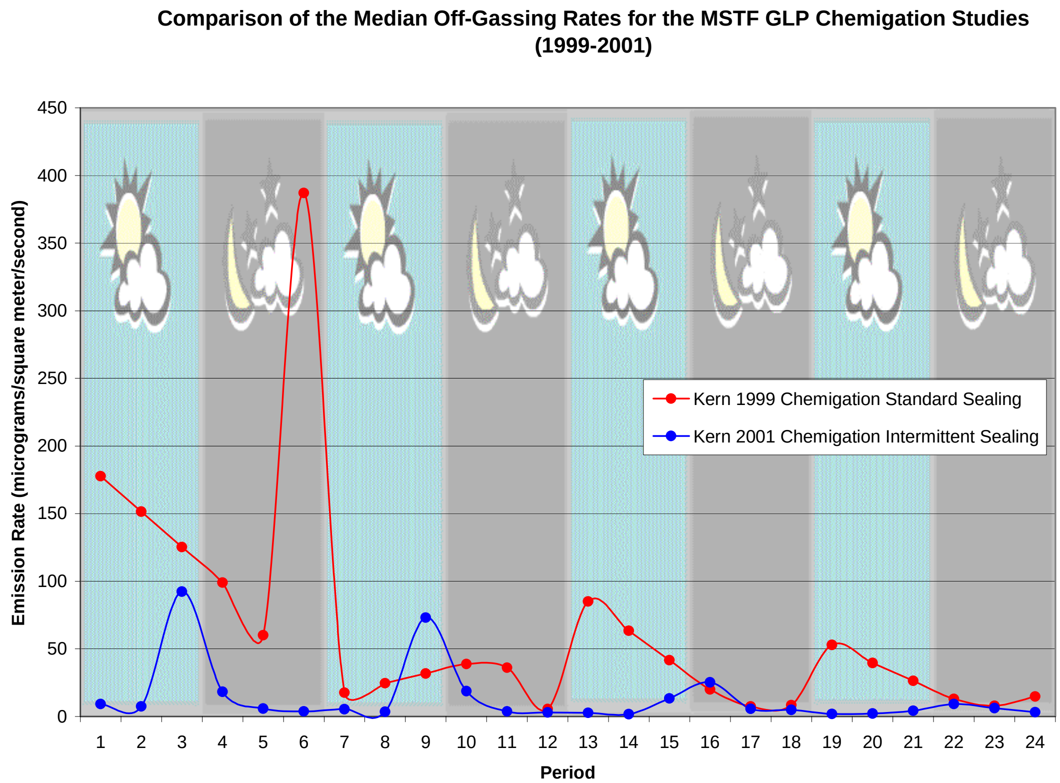


Figure 15: Emissions Sequence (Best Fit) for Chemigation Applications



The objective is to minimize the number of periods that require default data. This can be accomplished by carefully designing and implementing field studies to optimize coverage of the plume by the ambient air quality monitoring network.

Table 4 summarizes the approaches that are recommended for use based on considering the magnitude of the SE and number of pairs > 0.1 μg/m^3.

Table 4: Standard Error vs. Number of Pairs for Determination of which Emissions Calculation Method to Use

	3 or more Pairs > > 0.1 μg/m^3 [24]	2 or Less Pairs
SE > 1.5	Mean Measured/ Mean Modeled Method	Interpolation Method
SE < 1.5	Log-Normalized Least Squares Method	Interpolation Method

3.1.2.3 Parameterizing Emissions Distributions

The last step in the emissions assessment is to parameterize the emission distributions. A range of confidence intervals based on the standard error of the mean (as computed per Section 3.1.1.2 and as described in Attachment 1) is used to calculate the distributions of emission rates. *Refer to* Attachment 1 for description of the basic method. Once the emission distributions are calculated for eleven discrete values (2.5%, 5%, 10%, 25%, 40%, 50%, 60%, 75%, 90%, 95%, 97.5% confidence levels),[25] a cubic function is fit to the data to parametrically represent the cumulative probability distribution for subsequent Monte Carlo sampling. The emission rates for each hour of an active off-gassing event are drawn from the distribution, where "x" is a value between the 2.5 and 97.5 percent confidence interval of the mean:

$$Y = A + Bx + Cx^2 + Dx^3$$

The emissions distribution file for each specific application/sealing method is then fully described by a matrix of four computed coefficients for each sampling period times the number of sampling periods that comprise the off-gassing monitoring study. In the case of the metam-sodium GLP studies, the matrices are 4 coefficients by 24 periods. Figure 16 provides an example of a cubic function fit to the distribution of the mean emission rate by period, using a chemigation study as an example. Figures 17 and 18 present the emissions distribution sequences for shank injection/intermittent sealing and chemigation/intermittent sealing, respectively.

24 For example, a set of 5.0 and 0.10 would not meet this criterion, while a set of 1.1 and 0.11 would meet the criterion.

25 The 25, 40, 60, and 75 percent confidence levels were interpolated on a log-normal basis for the "H" values (Land, 1972), prior to fitting the cubic function.

Figure 16: Example of Parametric Fit to Emissions Distribution for Period 10 of the Chemigation Intermittent Sealed Study

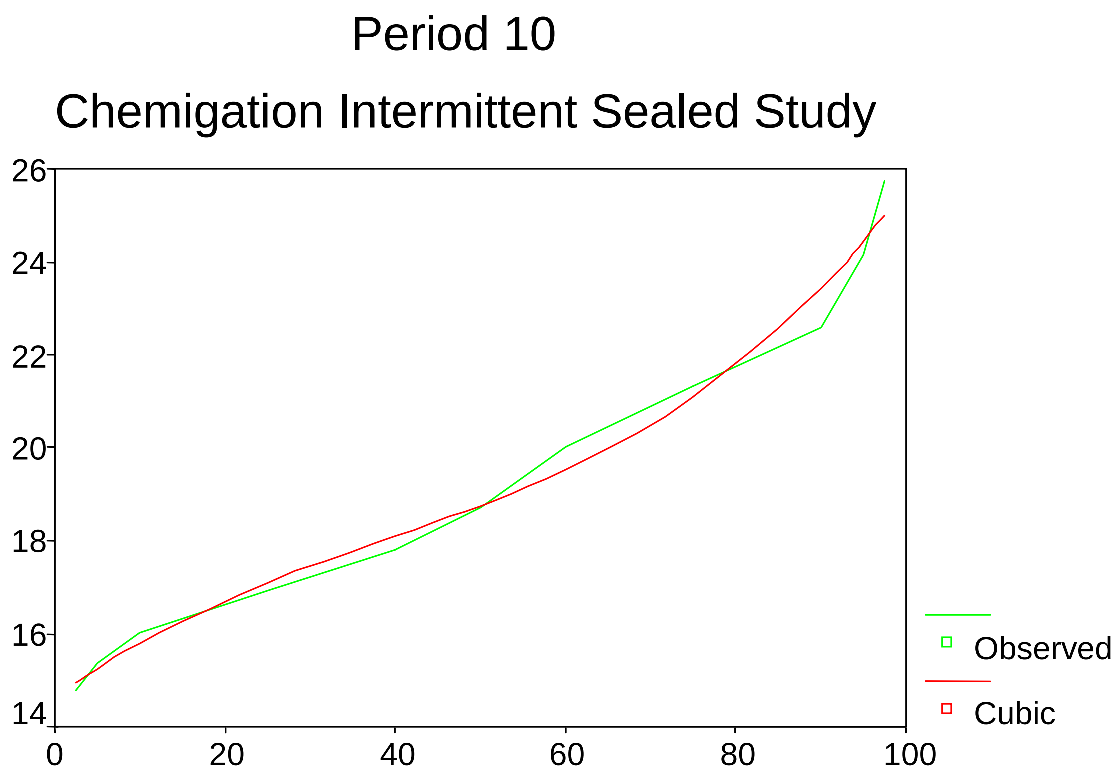


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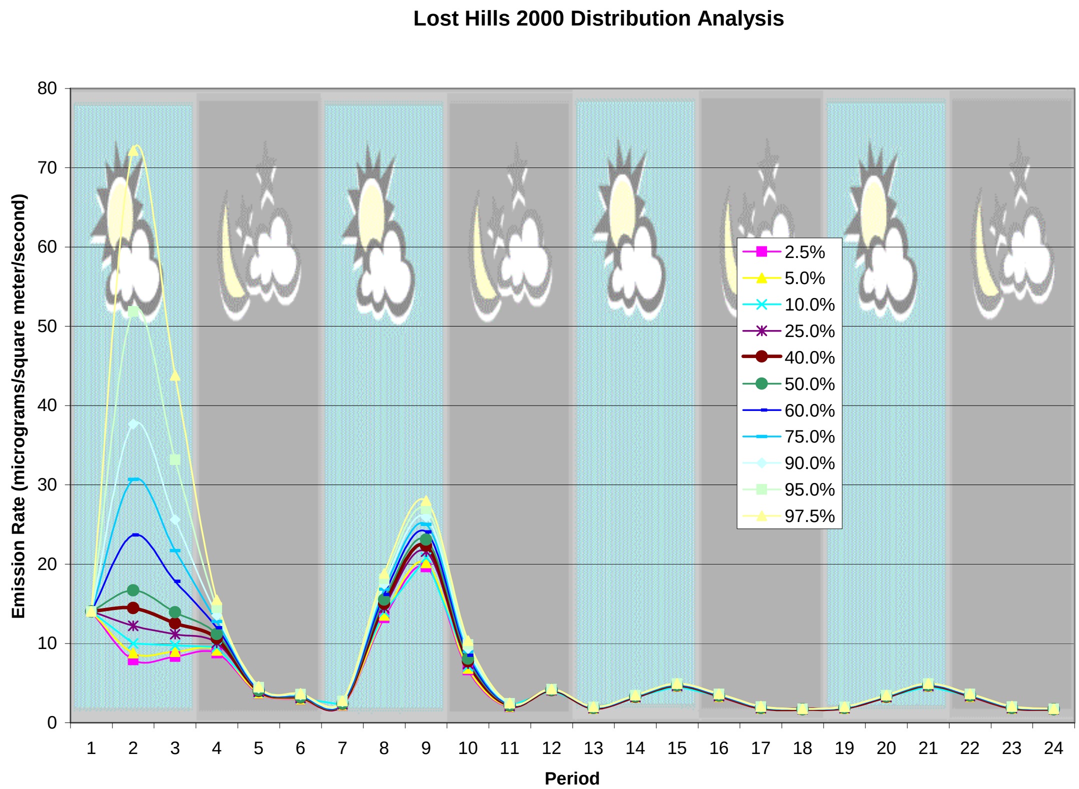
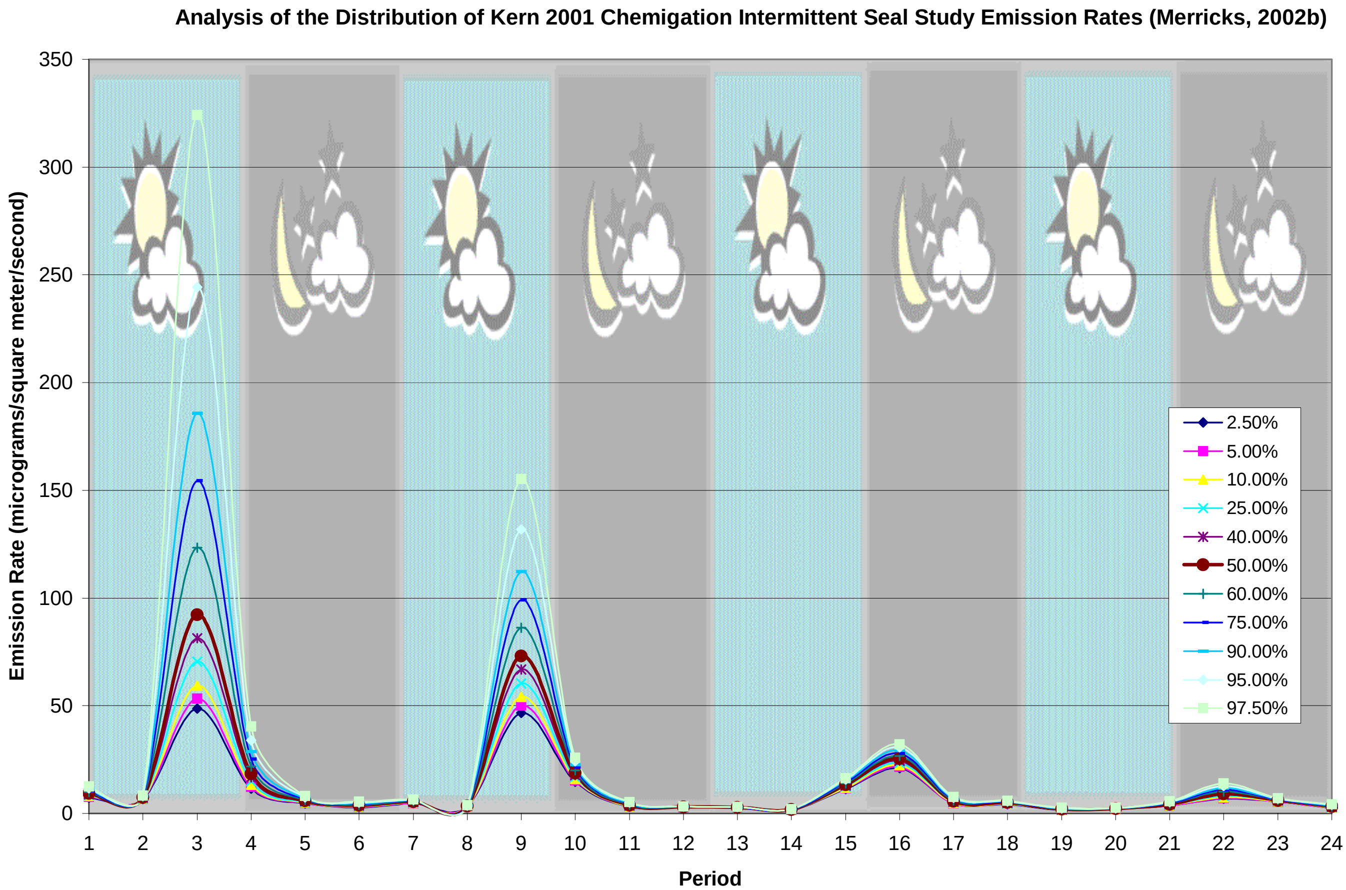
Figure 17: Emissions Distributions for Shank Injection/Intermittent Sealing[26]



26 Periods 1 through 3 needed to rely on off-site meteorological data to fit the emission rates. A larger amount of uncertainty was found in the fitted emissions data.

Figure 18: Emissions Distributions for Chemigation/Intermittent Sealing



3.1.2.4 Parameterizing Uncertainty in Meteorological Inputs to the Exposure Assessment

Expert elicitation techniques have been used to support the assessment of uncertainty in measured, sequential meteorological data that input to dispersion modeling analysis of air quality (Hanna *et al*.,, 1998; Hanna *et al*., 2001; and Hanna *et al*., 2002). Uncertainty of the measured meteorological data were parameterized using the distributions in Table 5.

Table 5: Distributions Used to Account for Uncertainty in Meteorological Inputs

Term	Shape of Distribution	95% confidence Range (+/- 1.96 sigmas)	Lower Limit	Upper Limit
Wind Speed	Natural log normal	+/- 1.5 m/sec	0	NA
Wind Direction[27]	Normal	+/- 45/wind speed (m/sec)	0	360
Stability Class	Normal	+/- 1 stability class	1	6

3.1.2.5 Monte Carlo Sampling Procedures

Simple random sampling within the 95 percent confidence interval of the best fit emission rates (2.5 to 97.5 percent confidence levels) was used to select emission rates, and to account for the uncertainty in the measured meteorological data. Because atmospheric stability is based in part on wind speed, the Monte-Carlo sampling of wind speed was done prior to the processing of stability data. All sampling to account for uncertainty in the input parameters was done on an independent basis (*refer to* Section 5.3 for a correlation matrix of model inputs, which shows "R" values of 0.20 or less among the inputs).

3.1.2.6 Rationale for FEMS Approach

The approaches taken in developing the current design of FEMS, as described to this point, were selected to meet specific objectives. The objectives include:

- ***Rely to the Extent Possible on Existing EPA Models*** -- EPA has developed a modeling method to evaluate acute exposures from batch operations, such as agricultural fumigants. The primary focus of FEMS is to prepare Monte Carlo-based inputs to support the two existing EPA models, ISCST3 and TOXST, which comprise the EPA methodology for batch sources. Downstream of the ISCST3/TOXST modeling, FEMS also post-process endpoint distances for each regulatory endpoint under review. Maximum use is made of unaltered

[27] Hanna *et al*., 2002.

computations from the ISCST3 and TOXST models, consistent with Section 2.3.2, Model Coding and Verification of the EPA Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models (EPA, 2003a), which states, *"Existing Agency models and code should also be reviewed to minimize duplication in effort."* Peer review of FEMS, therefore, can be focused on: (1) the coding in FEMS that facilitates data preparation (Monte Carlo sampling of emissions and meteorological parameters on an hour-by-hour basis); (2) the published computational procedures used to compile emissions distributions and conduct the modeling analysis (Sullivan *et al.*, 2004 a, b); and (3) the interpolation method to compute the distance to the endpoint concentration.

This design reduces the scope of additional peer review because FEMS is primarily based on maximizing the use of existing EPA models (*refer to* the flow diagrams (Figures 1 through 3) that identify the emissions processing (prior to FEMS) and the FEMS software components that need to be included in this review). Model validation, therefore, can be focused on the Monte Carlo sampling for the base input files and post-processing TOXST results, rather than on the validation of the ISCST3 or TOXST codes. As stated in the EPA Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models (Section 3.1.1) (EPA, 2003a), "*Models used for secondary applications (existing EPA models or proprietary models) will generally undergo a different type of evaluation than those developed with a specific regulatory information need in mind. By their nature, reviews of secondary applications models may deal more with uncertainty about the appropriate application of a model to a specific set of conditions than with the science underlying the model framework*." This statement directly reflects the review needs for the FEMS modeling system.

- ***Rely on EPA General Guidance for Conducting Probabilistic Exposure Assessment and Specific OPP Guidance*** **--** The modeling procedures used in FEMS are consistent with modeling policies and guidance as contained in (EPA, 1992, 1997, 1999, 2001, 2003b). On this basis, the methodology being employed for the Monte Carlo sampling procedures does not represent new methods, but rather the implementation of applicable existing guidance.

- ***Avoid Unrealistic Worst Case Assumptions that Distort the Distribution of Exposures*** **--** Agricultural fumigants produce off-gassing patterns that are best characterized as infrequent and highly variable. The technical approach in FEMS accounts for the intermittency through the EPA TOXST model, which "triggers" the start of applications based on probabilities set to match the application frequency identified by the model user. Frequency, variability and uncertainty are each specifically addressed in FEMS.

3.1.2.7 Reliability and Acceptability of Approach

The methodologies employed in FEMS are consistent with the EPA Guidelines on Air Quality Models and General Principles for Assessments (EPA, 1997, 2001, 2003 a, b).

All of the methods used in FEMS are based on sound scientific methods (Berthouex and Brown, 1994; Hanna *et al*., 1998; EPA, 1992, 1997, 1999, 2001, 2003 a, b). All of the key assumptions are summarized in Section 2 of this background document.

In summary, FEMS was designed to adapt model inputs to promote realistic representations of airborne exposures for agricultural fumigants through the use of existing EPA models, ISCST3 and TOXST. Probabilistic sampling of uncertainty in key input variables to these models are addressed through Monte Carlo sampling. EPA has identified the use of Monte Carlo sampling in many documents as an appropriate way to quantitatively account for the influence of uncertainty on the exposure assessment, as long as the probabilistic assessment are conducted consistent with stated EPA modeling policy (EPA, 1997, 2001, 2003 a, b).

The following lists each of the "*conditions for an acceptable risk assessment that uses probabilistic analysis techniques*" (EPA, 1997) and a description of how each item is addressed in FEMS:

1. *"The purpose and scope of the assessment should be clearly articulated in a 'problem formulation' section that includes a full discussion of any highly exposed or highly susceptible subpopulations evaluated (e.g. children, the elderly, etc.). The questions the assessment attempts to answer are to be discussed and the assessment endpoints are to be well defined.*"

   Section 1.0 of this background document clearly specifies the problem being addressed by FEMS. In summary, FEMS was developed to evaluate bystander exposures to agricultural fumigants as realistically[28] as possible within data limitations, by using probabilistic sampling methods to account for the distribution of concentrations as a function of distance from a field applied by an agricultural fumigant, including quantitative consideration of uncertainty in all major inputs of the modeling analysis. With the exception of creating Monte Carlo-based input to the analysis, FEMS was designed to have all computations made by existing EPA models, namely ISCST3 and TOXST, which minimizes the scope of additional peer review necessary.

2. *"The methods used for the analysis (including all models used, all data upon which the assessment is based, and all assumptions that have a significant impact upon the results) are to be documented and easily located in the report. This documentation is to include a discussion of the degree to which the data used are*

[28] Realistic within the context of using upper-end emissions data (empirically fit) because of current limitations in the coverage of a wide range of conditions and soil types.

representative of the population under study. Also, this documentation is to include the names of the models and software used to generate the analysis. Sufficient information is to be provided to allow the results of the analysis to be independently reproduced (Principles 4, 5, 6, and 11)."

Two published technical papers are presented in Attachment 1, which document in detail the methods used for the emissions and modeling assessments in FEMS. A test case example has been provided in Attachment 2 and Section 6 of this background document, including sample intermediate results, to support the independent confirmation of the results. As explained earlier, the emissions data err on the side of being protective because of the design objectives involved with initial collection of empirical field data (*refer to* Attachment 6). The steps to be taken to ensure that the meteorological data suitably represent each region are shown in Attachment 5.

3. *"The results of sensitivity analyses are to be presented and discussed in the report. Probabilistic techniques should be applied to the compounds, pathways, and factors of importance to the assessment, as determined by the sensitivity analyses or other basic requirements of the assessment (Principles 1 and 2)."*

   Section 5.3 of this background document presents sensitivity analyses showing sensitivity to the number of simulations, emissions data, and the meteorological parameters of wind speed, wind direction, and atmospheric stability. These results document the sensitivity of these terms.

4. *"The presence or absence of moderate to strong correlations or dependencies between the input variables is to be discussed and accounted for in the analysis, along with the effects these have on the output distribution. (Principles 1 and 14)."*

   Monte Carlo sampling is used in FEMS to account for the uncertainty around the mean of computed emissions and measured meteorological input parameters. Each of these terms is needed to support dispersion modeling analysis through the ISCST3 dispersion model. The Monte Carlo-based sampling of uncertainty within the 95th percent confidence interval of the means would be uncorrelated across input parameters in accordance with the sampling procedures used. In addition, preliminary testing showed correlation coefficients among input parameters to be << 0.2, which support the decision to maintain Monte Carlo sampling of uncertainty on an independent basis.

5. *"Information for each input and output distribution is to be provided in the report. This includes tabular and graphical representations of the distributions (e.g. probability density function and cumulative distribution function plots) that indicate the location of any point estimates of interest (e.g. mean, media, 95th percentile). The selection of distributions is to be explained and justified. For*

both the input and output distributions, variability and uncertainty are to be differentiated where possible. (Principles 3,7,8,10, 12, and 13)."

Attachment 1 contains the technical papers that document the basis for each of the distributions. Variability is addressed through the use of sequential meteorological and emissions data matched on a diurnal basis. Attachment 2 contains the cumulative probability distributions for each of the four GLP field studies that are used within FEMS as the current basis for modeling metam-sodium. The distributions for meteorological inputs are described in Attachment 2.

6. *"The numerical stability of the central tendency and the higher end (i.e. tail) of the output distributions are to be presented and discussed (Principle 9)."*

   The stability of the results (in this case distances to hypothetical regulatory endpoint concentrations) is shown as a function of the number of simulations for two scenarios 95th percentile concentration during the active 4-days of off-gassing period (or the 99.93 percentile on an annual basis) and the 20-year recurrence intervals[29] to evaluate the stability near the extreme upper tail of the distribution (*refer to* Section 5.3 of this background document for these results).

7. *"Calculations of exposure and risks using deterministic (e.g. point estimate) methods are to be reported if possible. Providing these values will allow comparisons between the probabilistic analysis and past or screening level risk assessments. Further, deterministic estimates may be used to answer scenario specific questions and to facilitate risk communication. When comparisons are made, it is important to explain the similarities and differences in the underlying data, assumptions, and models. (Principle 15)."*

   Sensitivity testing includes comparisons with unmodified ISCST3/TOXST results, without the additional Monte Carlo sampling of uncertainty, which is referred to as the benchmark treatment (*refer to* Section 5.3 of this background document). This review demonstrates that FEMS is generally more conservative than the existing EPA modeling procedures for handling batch sources such as agricultural fumigants (*i.e.*, ISCST3 and TOXST). The reason is that the coincidence of the upper ends of the various input distributions produces higher concentrations than would be computed through deterministic treatment of the model inputs, as is done in the benchmark comparisons shown in Section 5.3 of this background document (sensitivity testing).

8. *"Since fixed exposure assumptions (e.g. exposure duration, body weight) are sometimes embedded in the toxicity metric (e.g. Reference Doses, Reference*

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29 Presented as a sensitivity test per EPA, 1997.

Concentrations, unit cancer risk factors), the exposure estimates from the probabilistic output distribution are to be aligned with the toxicity metric."

FEMS output can be post-processed through custom runs to show concentration distributions, with up to six concentration thresholds to be evaluated per model run. The output can be further processed however, based on the standard ambient runs, or the personal exposure and indoor runs once fully tested, to show distributions of mg/kg/day based on post-processing the FEMS results and using Monte Carlo sampling to assign breathing rates and weights to each receptor. A database, such as NHANES II or III, can be used as the basis to sample by age, weight, and the associated breathing rates. Since body weight and breathing rates covary, the following approach could be done to post-process FEMS results to estimate mg/kg/day: (1) it would be assumed that there was a residence at each of the 720 receptors modeled in a FEMS run; (2) 2 adults and 2 children would be randomly sampled; (3) the database would be grouped by body weight, with distributions of breathing rates compiled for each grouping; and (4) by sampling on the basis of weight, and then sampling the breathing rate from the applicable distribution for the weight group, receptor data also could be evaluated on a Monte Carlo basis to support the assessment of mg/kg/day processing of the FEMS ambient, or in the future indoor and personal exposure estimates.

4.0 PARAMETER ESTIMATION

4.1 Data Used for Parameter Estimation

- ***Size of Area to Be Treated --*** There are two approaches that are usually followed in modeling agricultural fumigants: (1) treat the equivalent area of a typical field as a square area source; or (2) match the dimensions of the area to be treated to the typical orientation for the region in question. For example, in California, a typical 20-acre application on a major commercial tract (*e.g.*, working a quarter-section tract) would be approximately 100 meters wide (east-west) and 800 meters long (north-south), which is the recommended default in FEMS. The general recommendation of the FEMS developers is to run the model for the typical cultural practice in the region. There is sufficient flexibility in the input features, however, to accommodate analysis by either approach (or both if multiple runs are to be run and compared). Table 6 provides the recommended default specifications for various size fields.

Table 6: Approximate Widths and Lengths for Area Sources in Meters

Acres to Be treated	Default Source		Square Source	
	Width	Length	Width	Length
20	100	800	280	280
40	200	800	400	400
80	400	800	565	565
160	800	800	800	800

- ***Receptor Grid* --** Evaluation during the development of FEMS has been performed to determine the most suitable default receptor grid. It has been determined that 10 rings of receptors placed at the following distances from the center of a field (50, 100, 200, 300, 500, 750, 1000, 1500, 2000, 2500 meters) every 5 degrees of the compass generally are sufficient to determine accurate distances to exposure endpoints for most applications. In some cases, however, convergence can be achieved more quickly, in terms of the number of simulations, and accurately if preliminary runs are done to first identify the priority distance ranges for assessment, and then the receptor coverage is increased within the identified range, especially for unusually shaped fields. This is the recommended procedure when using FEMS. Similarly, for analysis of endpoint distances greater than 2,500 meters, expanding the coverage beyond the initially computed endpoint is recommended to improve the accuracy of the extrapolation calculations.

- ***Number of Simulations* --** As shown in Section 5.0, sensitivity testing has shown that to achieve a resolution of 10 meters in endpoint distances, a computational goal of the FEMS model, 5,000 to 10,000 simulated years, or more, is recommended. For review near the extreme upper-tail, as also shown in Section 5.3, a greater number of simulated years is needed to promote stable output results. In these examples, 100,000 simulated years were evaluated. Runs for 4-hour averaging show that on a 2.2 gigahertz desktop computer that approximately 8 hours is required to run the 200 base-year ISCST3 model runs. Table 7 shows the approximate run times for various number of simulations per model run using the 200 base year output files from ISCST3 and TOXST.

Table 7: Number of Simulations vs. Run Time[30]

Number of Simulations	Approximate Run Times 8-Hour Averages (Total Hours)
200	8.0
2,000	8.25
5,000	8.50
10,000	9
20,000	10
50,000	12
100,000	16

- ***Parameters To Be Randomized*** -- User options are provided to randomize uncertainty about the 95th percent confidence interval of the mean for any one of the following input terms on an hour-by-hour basis: emission rates, wind speed, wind direction, and atmospheric stability. For the inputs that are not selected to account for randomization, the best-fit emission rate and directly measured meteorological parameters are used without modification. It is recommended at this time that atmospheric stability be nonrandomized to avoid potential concerns with decreasing stability during the nocturnal inversion periods (although interludes of less stable conditions have been shown to occur during nocturnal periods associated with ground-based inversion conditions (Panofsky and Dutton, 1984). This recommendation needs further evaluation in the future. *Refer to* Attachment 1 for a more detailed description of the distributions used to account for the uncertainty in each of these inputs.

  The stochastic uncertainty in the wind direction term, relative to use in representing transport in a dispersion model, also needs further clarification. Review of a wind trace on strip chart paper shows most clearly the stochastic nature of wind direction variability. These fluctuations are caused by a wide spectrum of turbulent eddies with wave lengths ranging from centimeters to many miles. As wind speed decreases, a horizontal meander component becomes pronounced. Although the average wind directions from hour-to-hour may indicate general flow in a similar direction, there are likely to be very wide swings in the trajectories over the course of an hour during periods of low wind speeds. During such conditions, there clearly is less connection in a spatial sense between the meteorological monitoring station used to represent the region, and specific

30 Shorter or longer run times can be anticipated because run time is a function of both averaging time and the magnitude of the concentration thresholds, which affects the magnitude of concentrations above the ISCST3 output and TOXST processing thresholds, and of course the computer specifications.

trajectories from Point A to Point B that are modeled, in this case near an agricultural field. FEMS represents this uncertainty through a distribution that is an inverse function of wind speed to account for the greater uncertainty in characterizing wind direction under low wind speed conditions (Hanna *et al.*, 2002). For multiple-hour assessments, on the other hand, such as 8-hour averaging, for example, accounting for wind direction uncertainty can better represent the uncertainty in flow that can have a more substantial effect on the results, including the greater likelihood for encountering over a long period of simulated years high percentile occurrences of wind persistence within some averaging periods. As with all of the stochastic treatments in FEMS, however, the model user has the discretion to select those parameters for stochastic treatment that in his or her judgment best represent the application scenario at hand.

- ***Indoor/Personal/Ambient*** -- FEMS contains the option of including indoor and/or personal exposure estimates, for perspective, in addition to the routine computation of ambient exposures. In many cases, this option will not be selected for regulatory analyses, but it could be useful to provide perspective. The mechanism to provide this resolution is in place in FEMS. Ambient exposures, however, are the focus of the current SAP review at this time. The initial assumptions and methods in the initial coding of indoor and personal treatments can be refined, and linked to probabilistic treatments of subject weights and breathing rates to support the estimation of the distribution of mg/kg/day as a function of distance from the applied field.

  The benefits of sheltered environments in terms of buffering the peak concentrations are more pronounced for shorter averaging times (*e.g.*, 1-hour averaging) and as the tightness of the structure increases. Open/Closed window assumptions are used to account for differing tightness of buildings and the potential for having windows open by time of day and season to be realistic as shown in Table 8. These initial default assumptions are automatically applied when running personal exposures to account for the differing exposures between being outdoors and indoors. Indoor exposures only use the windows open and windows closed option.

Table 8: Initial Default Assumptions for Indoor/Personal/Outdoor Exposure Characteristics

Condition	Window Open (%)	Window Closed (%)	Indoor (%)	Outdoor (%)	Outdoor far away or in transit (%)
Daytime spring/summer/fall	20%	80%	87%	3%	10%
Daytime winter	1%	99%	89%	1%	10%
Nighttime spring/summer/fall	10%	90%	99%	1%	0%
Nighttime winter	0%	100%	100%	0%	0%

- ***Number of Applications/Year*** -- For most fumigants, including metam-sodium, applications to a particular field generally are done once per year or less. The user has the option to select the application frequency to match the crops/cultural practice under review. Custom runs can be conducted, however, on a seasonal basis with application probabilities set accordingly. In that case, the seasonal runs would contain only meteorological data suitable for the season in question, with runs executed one season at a time, and results merged to produce annual distributions, such as occurs in scenarios with multiple crops in key regions and seasons.

- ***Number of Days of Off-gassing*** -- The emission files for the metam-sodium GLP field studies are based on 4-days of off-gassing. Depending on the number of days for any particular field study, this value could increase or decrease. The selected value must match the emission files periods. For now, 4-hour averaging is used such that 6 periods per day need to be input in the emissions files, with four days of coverage in each file. FEMS can be modified to accommodate alternative averaging times. The prototype version of FEMS requires 4 days of off-gassing, but this value can be generalized in the final version of FEMS to provide the flexibility to meet the needs of any fumigant.

- ***Averaging Time***[31] -- Options for averaging time include any hourly period that can be evenly divided into 24-hours (*i.e.*, 1, 2, 3, 4, 6, 8, 12, and 24-hour averaging). This criterion is a requirement of TOXST. This level of resolution is needed, plus consideration of the diurnal variability in emission rates, for FEMS to be generally useful for the range of agricultural fumigants. Such resolution is

31 Although model averages can consider any of the times listed above, the FEMS coding is currently based on 4-hour field study sampling over four days. Alternative averaging times can be assessed in the future, but will require minor coding modifications to accommodate flexibility.

necessary because of the differences in toxicological data that require consideration of different averaging times from 1 to 24 hours in duration.

It should be noted that when averaging times of interest are less than 4 hours, the fitted emissions data will not directly show the distribution of 1-hour emission rates during each 4-hour period. It is infeasible at this time to collect hourly-resolved emissions data. Although rapid changes within a 4-hour period, for example, would not generally be expected, in the future this factor could be considered through either a remote sensing component, which for some fumigants (including the transformation product of metam-sodium, MITC), may provide supplemental data to evaluate more fully rates of change on this basis. Another option may be to use soil modeling procedures to address relative differences in expected off-gassing rates as a function of changes in soil moisture and temperature within a multiple-hour averaging period such as 4 hours.

- ***Application Rate*** -- For simplicity, the emissions data sets used to represent the application methods/scenarios of interest must be applicable to the maximum label rate (preferably through direct emission fitting based on field studies applied at maximum rate, or through emissions data scaled up to represent maximum application rate, as necessary and as appropriate). The user then has the option of identifying the percent of full application rate for the FEMS run to be made from (1 to 200 percent of the maximum application rate as selected).

- ***Emissions Files*** -- FEMS is designed to have all application/sealing scenarios of interest represented by parameterized emissions distributions. The current prototype includes example emissions distributions for metam-sodium for: shank injection/standard sealing, shank injection/intermittent sealing, chemigation/standard sealing, and chemigation/intermittent sealing. There is one record per 4-hour averaging period in each of these files, which contain the four coefficients needed to parametrically define the emissions distribution for each period based on a cubic function.

- ***Number of Thresholds To Be Modeled*** -- The number of thresholds for which FEMS (actually TOXST) will track concentrations above thresholds are determined by the regulatory requirements of the application at hand. Typically, there will be only one regulatory endpoint considered for any particular averaging time. If a range of values is under consideration, however, up to six separate endpoints can be considered in any single FEMS model run, with the endpoint distances identified separately for each. This field simply identifies by integer the number of threshold concentrations that will be entered in the record that follows (and is prompted next by FEMS). If a range of percentiles of exposure are of interest, custom runs of FEMS (multiple runs) can be made and TOXST outputs processed to show endpoint distances as a function of a range of percentiles, and concentration distributions on an annual and active off-gassing basis as a function of distance from the field.

- ***Thresholds*** -- The specific regulatory endpoints (air concentrations in μg/m^3) are entered here. FEMS will prompt the user the same number of times as the "number of thresholds to be modeled" was entered above.

- ***Allowable Number of Times/Year Concentration is Greater than the Threshold Concentration* --** This input, the average number of times per year concentrations are greater than the user-defined concentration thresholds,[32] is used to identify the percentile of concentration to estimate the distance to the endpoint concentration. The default value used in FEMS is 1.49. If the number of occurrences the computed concentration is at or above the threshold is greater than or equal to 1.49 at a distance from the edge of a field, the endpoint distance is increased in FEMS until compliance with the target endpoint distance is met. Across the full year, this represents the 99.93 percentile value using 4-hour averaging as an example, and approximately the 95th percentile of the 4-day period following application (based on 4-hour averages). Table 9 provides examples of the correspondence between the allowable times/year the concentration is greater than the concentration threshold and the associated percentile based on using 4-hour averaging.

Table 9: Percentile vs. Allowable Times per Year Threshold Concentration is Reached

Scenario	Allowable Times Per Year > Threshold Concentration	Allowable Times Per Active Off-gassing Period > Threshold Concentration[33]
90th percentile	219.6	2.4
95th percentile	109.8	1.2
99th percentile	22.0	0.2
99.5th percentile	11.0	
99.9th percentile	2.2	

- ***Region*** -- FEMS has been structured to include coverage for up to 8 regions. In terms of metam-sodium, the initial chemical that is being set up for FEMS, there are five major use areas that will need to be represented: California; Florida; the Great Lakes; the Pacific Northwest; and the Southeast. Substantial overlap with other fumigants is expected.

  The user is provided in FEMS with a list to select the region of interest for the run in question. **FEMS is provided in the demonstration mode with coverage only for Fresno, California (Option #1 in FEMS).** Attachment 5 describes the

32 This is labeled in FEMS as the number of exceedances of the threshold.

33 For this example, it was assumed there were four days of off-gassing and 4-hour averaging.

procedures that will be used to identify suitable, representative meteorological data for each of these regions when FEMS is fully implemented to meet requirements on a national basis.

- ***Latitude/Longitude/Time Zone --*** FEMS automatically processes the specific meteorological data to be used for each run, and on this basis accounts for the uncertainty in the meteorological parameters specifically each time, sampling within the 95 percent confidence of the measured values. The latitude, longitude, and time zone prompts are used collectively as input to the meteorological processing of atmospheric stability in the meteorological files within the EPA PCRAMMET meteorological processing program. The general recommendation would be to use the centroid value to represent the region of interest being addressed in the model run. For the prototype version of FEMS, it is recommended that the defaults shown on the on-screen prompts be used.

4.2 Rationale For Estimates In The Absence Of Data

4.2.1 Filling Emission Data Gaps

Emission rate is the most significant term in the context of data gaps (*refer to* Section 2.1 for a description of how missing emissions data are filled).

4.2.2 Filling Gaps in Meteorological Data Coverage

Standard interpolation procedures are used in filling in missing mixing height data, as necessary, to support the use of the EPA PCRAMMET meteorological data processor (*refer to* Section 2.1 of this background document for a description of these procedures).

4.3 Reliability of Parameter Estimates

4.3.1 Emission Rates

The emissions estimates, the most significant inputs to FEMS in terms of uncertainty, were described in Section 3.1 of this background document. As noted, these estimates are based on fitting log-normalized modeling and ambient monitoring results to identify best-fit emission rates, and also the distribution of mean emission rates, as a function of time. Through the use of upper-end empirical emissions data, and the quantitative inclusion of uncertainty in the analysis through Monte Carlo sampling of the emissions distribution, the emissions data in FEMS represent a realistic representation of expected emission rates, with an expected bias towards overestimation of emission rates, and thereby, exposures because of the use of upper-end empirically fit emissions data at this time, pending the availability of greater resolution at the regional level and by season. Considering the mean modeled concentrations and mean measured concentrations across the sampling network, with the data diurnally matched with 4-hour periods during the 4-day field studies,[34] it is anticipated that the average best-fit

34 It is more relevant to the end use of the data that the averages and ranges of the measured and modeled concentrations are reasonably consistent than the unnecessary and probably

emission rate generally would be within a factor of 2 of actual emissions (EPA, 2003b). It is likely, however, that in some individual periods, there may be larger differences.

4.3.2 Meteorological Data (Onsite and NWS/FAA Long-Term Data Sets)

Meteorological datasets that are used are as follows:

- Onsite for emissions fitting; and
- NWS or FAA for long-term meteorological data analysis.

The specifications for the meteorological data sources are described in Section 5.0.

5.0 UNCERTAINTY/ERROR

Accepting the premise that Gaussian modeling via ISCST3 is a reasonable assumption for this type of source, which represents acceptable practice based on the EPA Guideline on Air Quality Models and the guidelines for the ISCST3 model (EPA, 1993b, 1999), the most critical factors that affect the quality of the model output from FEMS are the quality of the emission rates and meteorological inputs to the system. The following specific steps are taken to ensure that high quality inputs are used with FEMS, with defined error tolerances, and with uncertainty in the input values specifically and quantitatively propagated through the exposure assessment.

5.1 Emission Rates

As described in Sullivan *et al.* (2004 a, b) and augmented in the previous sections, criteria have been established to promote high quality emission inputs (*refer to* Attachment 1).

5.2 Meteorological Data

Meteorological data to be used in FEMS are selected to be representative of the major agricultural regions based on available data from NWS and FAA meteorological monitoring sites. These monitoring programs have known specifications for the instrumentation in use and documented quality control/quality assurance to enhance the confidence in the reliability of the data.

Similar to the emissions discussion above, there is uncertainty in the measured meteorological data in terms of both the accuracy of the measurements themselves, as well as the representativeness of the data to describe transport and dispersion conditions from a given field to the downwind receptors being modeled. Also as shown in Attachment 1, the results of an expert elicitation survey (Hanna *et al*., 1998) is used to quantify the probability density function

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unachievable constraint that the model should match observed concentrations in time **and** space.

from which Monte Carlo sampling is performed, also from 2.5 to 97.5 percent confidence values for the means to account for this uncertainty.

The most critical meteorological data for modeling exposures are wind speed and wind direction. The wind speed data are accurate to the nearest knot, with wind speeds less than 2 knots being represented as calm. Wind speed is accurate to the nearest 10 degrees.[35] Based on meteorological monitoring systems used for the metam-sodium GLP field studies, Tables 10 and 11 provide examples of the specifications for the collection of onsite meteorological data that are routinely used to fit the emissions data.

Table 10: Met Data One Weather Station

Parameter	Threshold or Range	Accuracy
034B-ET Wind Speed Sensor	0.4 m/s	±0.11 m/s when < 10.1 m/s ±1.1 m/s when >10.1 m/s
034B-ET Wind Direction Sensor	0.4 m/s	±4°
CS500-ET Air Temperature Sensor	-25°-50° Celsius	±1.5° Celsius
CS500-ET Relative Humidity Sensor	10-100%	±3% for 10-90% range ±6% for 90-100% range
LI200X-ETM Solar Radiation Sensor	0.2 kW m^{-2} mV^{-1}	±3% typical, absolute error in natural daylight is ±5% maximum
TE525-ET Tipping Bucket Rain Gage	0.25 mm (1 tip)	±1% @ 50.8 mm per hour or less

35 Personal correspondence with the National Weather Service (Ronald C. Jones, NWS to Mark Holdsworth, Sullivan Environmental, June 9, 2004).

Table 11: ET106 Weather Station

Sensor	Accuracy	Threshold or Range
Met One 034B Anemometer	±0.11 m/s when < 10.1 m/s ±1.1% when > 10.1 m/s	0.4 m/s
Met One 034B Wind Vane	±4°	0.4 m/s
LI-200X Silicon Pyranometer	±5% maximum; ±3% typical	0.2 kW m^{-2} mV^{-1}
HMP45 Temperature Probe	±0.2°C at 20°C ±0.3°C at 0°C or 40°C	-39.2° to +60°C
HMP45 Relative Humidity Probe	±1%	0.8-100%
CS615 Water Content Reflectometer	±2.5% volumetric water content	0%-50%
Soil Temperature Probe 107	±0.1°C over -24° to +48°C range	-35° to +50°C
TE525 Rain Gage	±1% up to 1 inch/hour +0, -3% 1 to 2 inches/hour +0, -5% 2 to 3 inches/hour	0.01 inches

5.3 Sensitivity Analysis

5.3.1 Sensitivity of Concentration to Key Model Input

The metam-sodium chemigation/intermittent sealing study was used as the primary test case example to assess the sensitivity of the modeling to the key input terms, as well as to evaluate the potential for covariance among the key model inputs. First, a correlation matrix was produced to identify correlations between model input parameters, and also to evaluate correlation between the output concentrations and each input term. The sensitivity analysis was based on a 1,000 year simulation with 1 application per year by chemigation with intermittent sealing. The sole receptor that was used for this review was located 150m due North of the Center of a 19-acre field. First, as shown in Table 12, the "R" values were 0.2 or less among the inputs, which supports the position that the uncertainty in these inputs can be represented by independent probabilistic analysis. In addition, it was shown that the emission term accounts for nearly two-thirds of the variance in concentration. Stability accounts for approximately another five percent, which totals approximately 70 percent of the variance as being attributable to these two factors. Figures 19 through 22 present scatter plots for concentration and the various input parameters for chemigation with intermittent sealing. Figure 23 presents a scatter plot of emissions based on Period 3 for the chemigation/intermittent sealing field study based on running the Monte Carlo sampling for 1 year using the standard 4-day cycle.

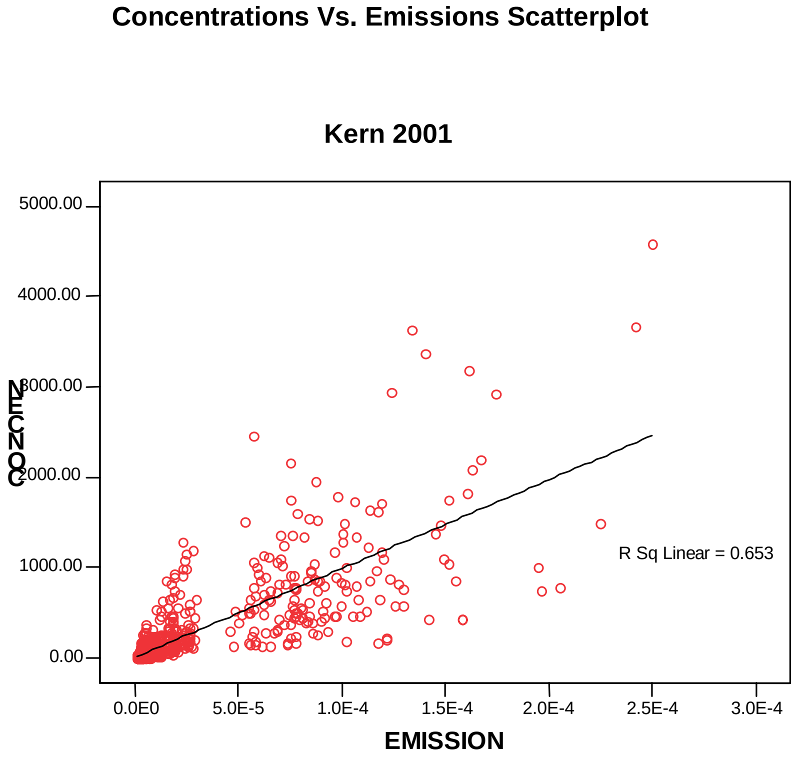
It is interesting to note that for the chemigation/intermittent sealing study the maximum concentrations were associated with neutral conditions. This is due to the fact that maximum emission rates for the soil conditions associated with intermittent sealing for chemigation occur during the afternoon, which is conducive to neutral through unstable conditions. The peak concentrations in this example are shown for conditions with flow from the South, with low wind speeds, and high emission rates, as would be anticipated. These plots demonstrate that there are very few hours over a long-term period when all of the conditions align to produce peak values at a receptor.

Table 12: Chemigation/Intermittent Sealing Study Correlations

		CONCEN	EMISSION	WD	WS	STABILITY
CONCEN	Pearson Correlation	1	.808(**)	.012	-.101(**)	.246(**)
	Sig. (2-tailed)	.	.000	.576	.000	.000
	N	2114	2114	2114	2114	2114
EMISSION	Pearson Correlation	.808(**)	1	.005	.093(**)	.106(**)
	Sig. (2-tailed)	.000	.	.820	.000	.000
	N	2114	2114	2114	2114	2114
WD	Pearson Correlation	.012	.005	1	-.059(**)	-.039
	Sig. (2-tailed)	.576	.820	.	.007	.075
	N	2114	2114	2114	2114	2114
WS	Pearson Correlation	-.101(**)	.093(**)	-.059(**)	1	-.014
	Sig. (2-tailed)	.000	.000	.007	.	.518
	N	2114	2114	2114	2114	2114
STABILITY	Pearson Correlation	.246(**)	.106(**)	-.039	-.014	1
	Sig. (2-tailed)	.000	.000	.075	.518	.
	N	2114	2114	2114	2114	2114

** Correlation is significant at the 0.01 level (2-tailed).

Figure 19: Chemigation/Intermittent Sealing[36]
Scatter plot of Emission Rate (μg/m²/sec) vs. Output Concentrations (μg/m³)



36 There is a gap in this scatter plot just below 5.0×10^{-5} μg/m²/sec. Coincidentally, none of the 2.5 to 97.5 percent confidence in the mean emissions produces emission rates within this gap. Figure 24 for the shank injection/standard sealing example, does not show this feature.

Figure 20: Chemigation/Intermittent Sealing
Scatter plot of Wind Speed (m/sec) vs. Output Concentrations (µg/m^3)

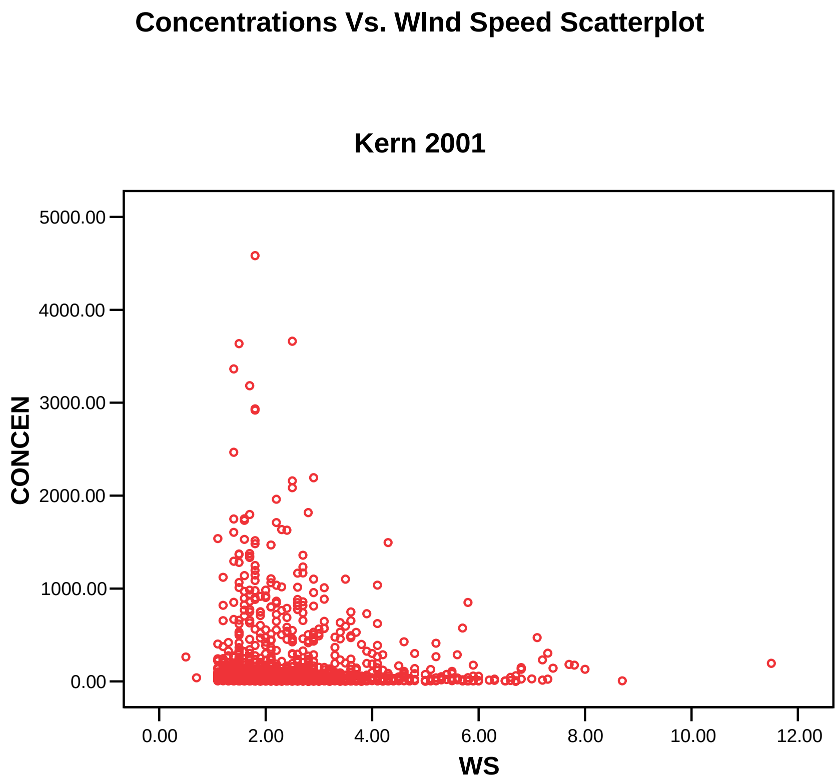


Figure 21: Chemigation/Intermittent Sealing
Scatter plot of Wind Direction (degrees) vs. Output Concentrations (μg/m^3)

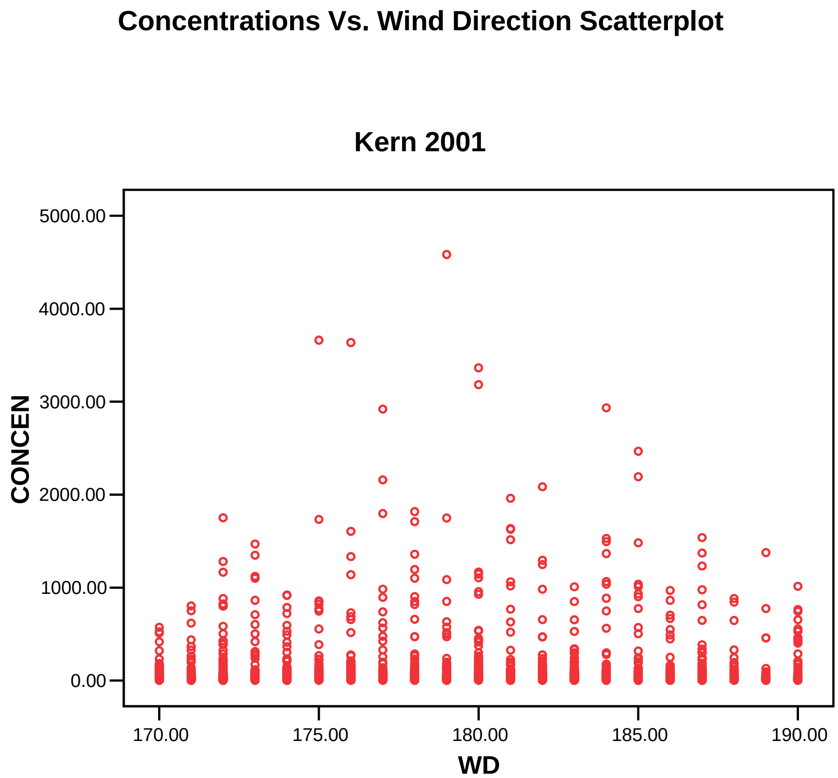


Figure 22: Chemigation/Intermittent Sealing
Scatter plot of Wind Speed (m/sec) vs. Output Concentrations (µg/m^3)

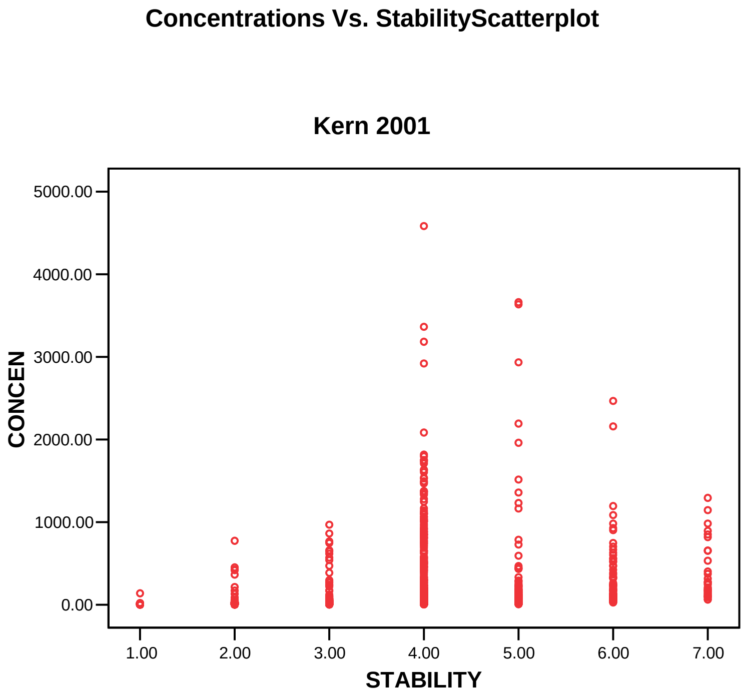
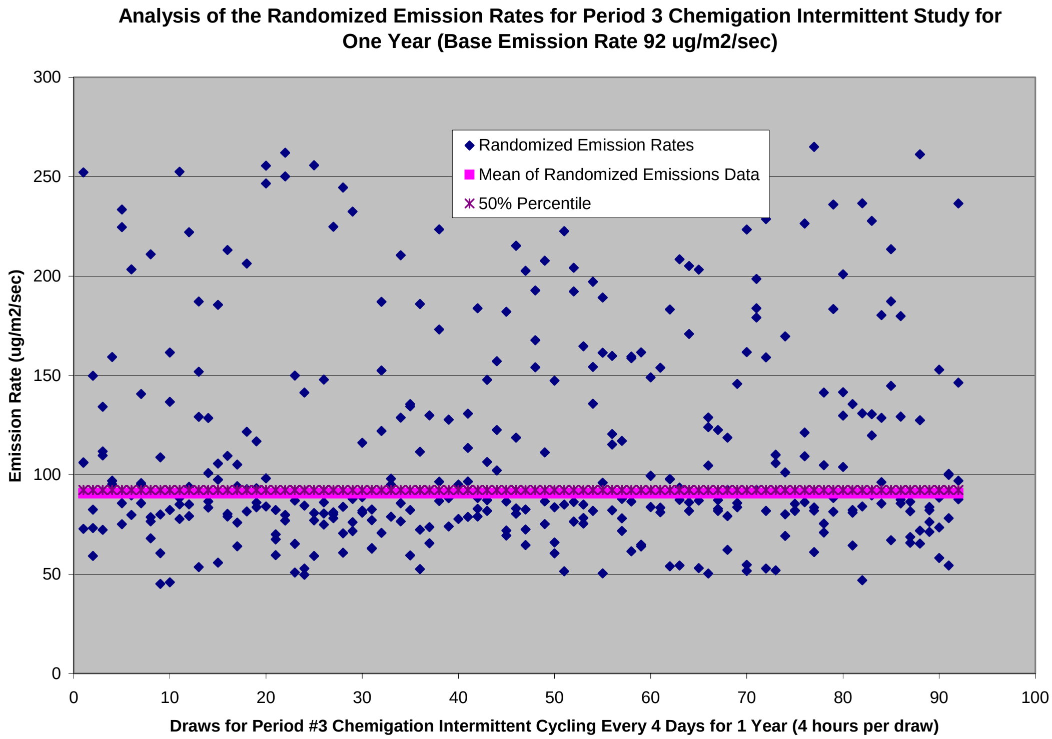


Figure 23: Scatter plot of Emission Rates for Period 3 for Chemigation/Intermittent Sealing



The following example of shank injection/standard sealing (maximum emissions during nighttime periods) provides a contrast in terms of sensitivity with the preceding results for chemigation/intermittent sealing, which had peak emissions during daytime periods. In this example of shank injection/standard sealing shown in Table 13 and Figures 24 through 27, the maximum impacts occur during stable conditions, rather than neutral stability, as expected. Approximately 62 percent of the variance in concentrations is explained by emissions and stability. Again, there is very low correlation among the input parameters, which supports the independent stochastic sampling of uncertainty for each input parameter.

Table 13: Shank Injection Intermittent Study Correlations

		CONC	EMIS	WD DDI	WS	STABLITY
CONC	Pearson Correlation	1	.731**	.021	-.142**	.302**
	Sig. (2-tailed)	.	.000	.341	.000	.000
	N	2134	2134	2134	2134	2134
EMISSSS	Pearson Correlation	.731**	1	.018	.000	.113**
	Sig. (2-tailed)	.000	.	.406	.986	.000
	N	2134	2134	2134	2134	2134
WD	Pearson Correlation	.021	.018	1	-.024	-.020
	Sig. (2-tailed)	.341	.406	.	.263	.350
	N	2134	2134	2134	2134	2134
WS	Pearson Correlation	-.142**	.000	-.024	1	-.053*
	Sig. (2-tailed)	.000	.986	.263	.	.015
	N	2134	2134	2134	2134	2134
STABLITY	Pearson Correlation	.302**	.113**	-.020	-.053*	1
	Sig. (2-tailed)	.000	.000	.350	.015	.
	N	2134	2134	2134	2134	2134

**. Correlation is significant at the 0.01 level (2-tailed).

*. Correlation is significant at the 0.05 level (2-tailed).

Figure 24: Shank Injection/Intermittent Sealing
Scatter plot of Emission Rate (µg/m²/sec) vs. Output Concentrations (µg/m³)

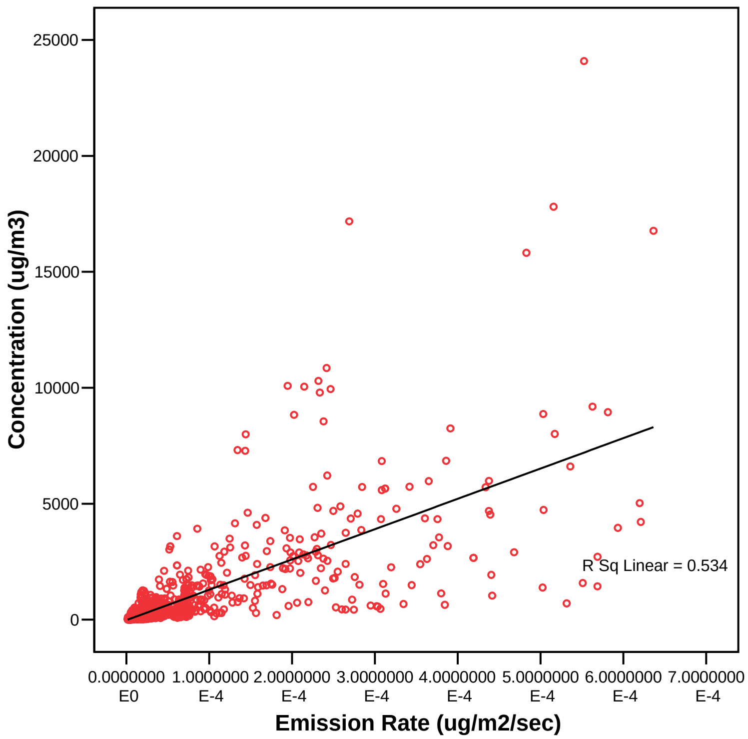


Figure 25: Shank Injection/Intermittent Sealing
Scatter plot of Wind Direction (degrees) vs. Output Concentrations (μg/m^3)

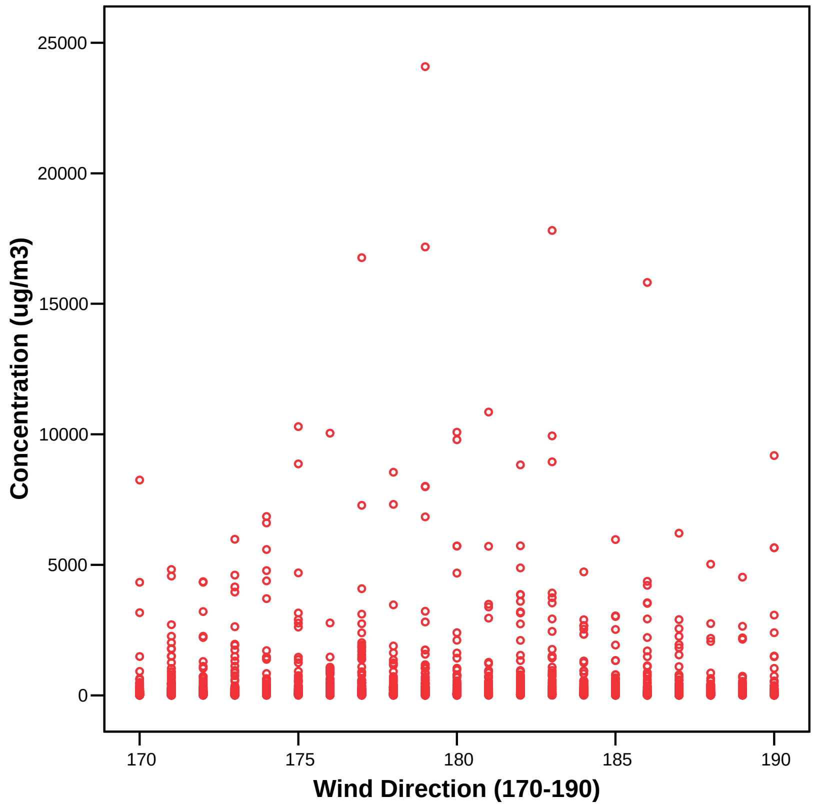


Figure 26: Shank Injection/Intermittent Sealing
Scatter plot of Wind Speed (m/sec) vs. Output Concentrations (µg/m^3)

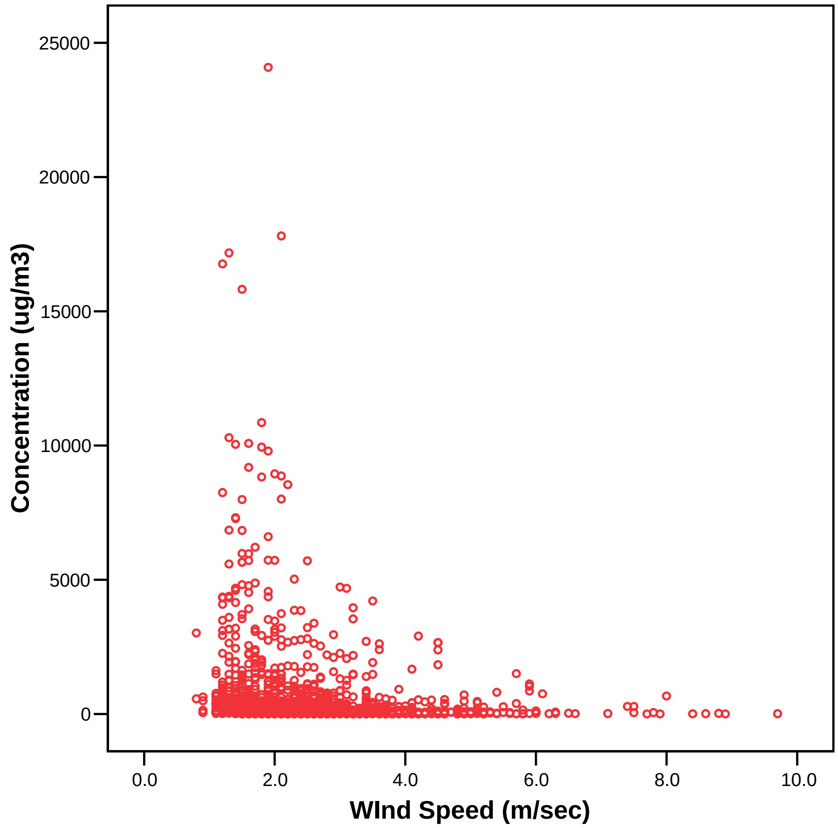
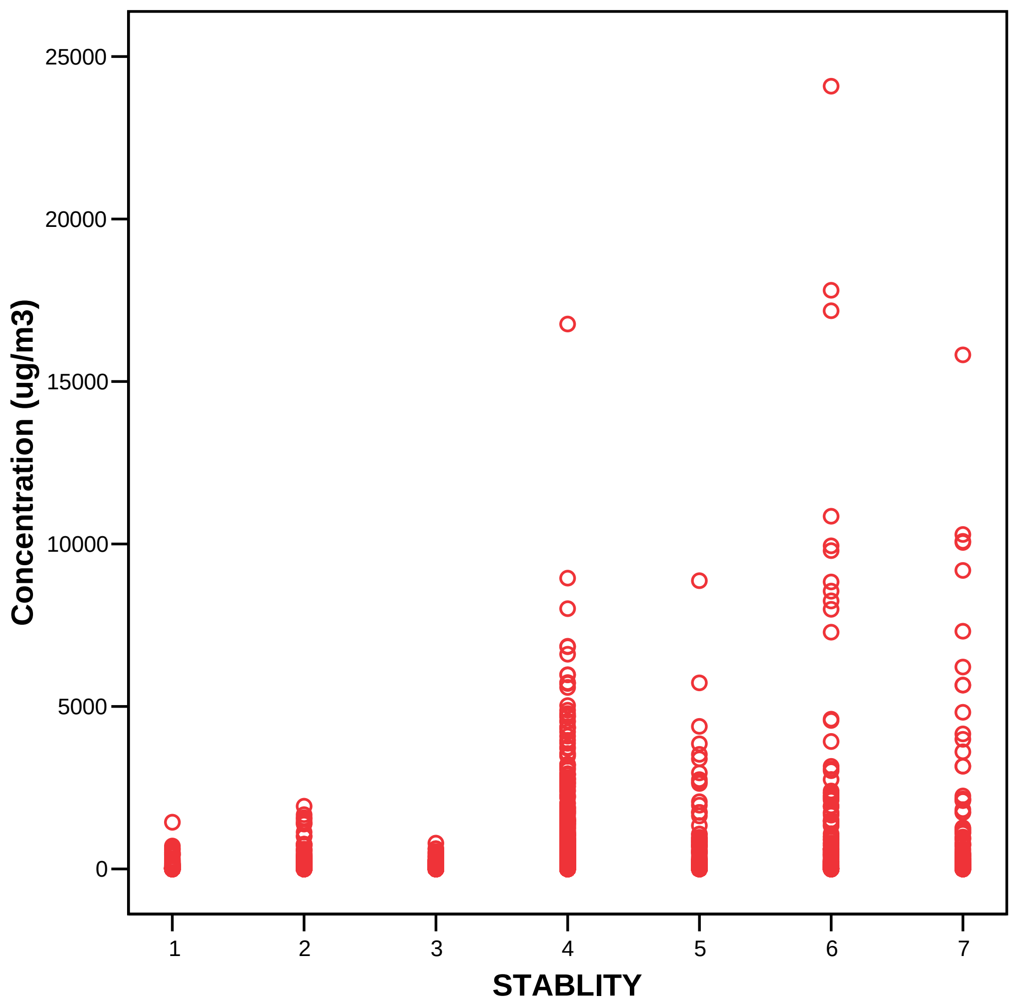


Figure 27: Shank Injection/Intermittent Sealing
Scatter plot of Atmospheric Stability vs. Output Concentrations (µg/m^3)



The following can be observed in the preceding sensitivity runs:

- The highest concentrations are shown to occur infrequently during periods with emission rates associated with the upper-end of the emission distributions.

- Relatively high concentrations are modeled during neutral through unstable atmospheric conditions for chemigation/intermittent sealing because nocturnal emissions were substantially reduced relative to daytime emissions. The highest modeled concentrations for shank injection/standard sealing, on the other hand, are shown for stable conditions associated with ground-based nocturnal inversions, which is consistent with the differences in sealing procedures.

- The area source associated with this sensitivity testing is a hypothetical 19.8-acre field 100 meters east-west and 800 meters north-south. As would be expected, even for an area source of this magnitude, the maximum impacts at this receptor 150 meters due north of the center of the field occurs within a relatively narrow band of wind directions, clustered from 175 to 180 degrees.

- With very few exceptions over the 1,000 year simulation, maximum concentrations were shown to occur with wind speeds $\leq$ 3 m/sec (with most of the highest concentrations shown for wind speeds $\leq$ 2 m/sec).

Figure 28 shows the sensitivity of FEMS to the number of simulations for the test case emissions file for the chemigation/intermittent sealing study (kern2001.dat), which was used as the test case example in this report. This example is based on hypothetical endpoint concentrations ranging from 25 to 750 µg/m3. A summary of FEMS sensitivity to the model input terms that can be addressed through probabilistic sampling to account for uncertainty in the mean around the best-fit value for each hour is presented in Table 14, also for the chemigation, intermittently sealed study. Figure 29 repeats the sensitivity testing to a number of simulations for shank injection/standard sealing, which is an application method with higher emissions than for chemigation/intermittent sealing, and nocturnal peaks. A similar convergence as a function of number of simulated years is shown. Table 15 presents other available sensitivity testing results for the shank injection/standard sealing example.

Analysis of the sensitivity of FEMS to the number of simulations indicates that more rapid convergence occurs as a function of the number of simulations for higher regulatory endpoints. The objective of +/- 10 meters computational accuracy generally can be with 5,000 to 10,000 or more simulated years. For lower endpoints, or for evaluation of recurrence intervals for very infrequent events, it is recommended that more simulations be run to achieve good stabilization of the distances from exposure source, such as up to 100,000 years.

Figure 28: Sensitivity to the Number of Simulated Years: Chemigation/Intermittent Sealing

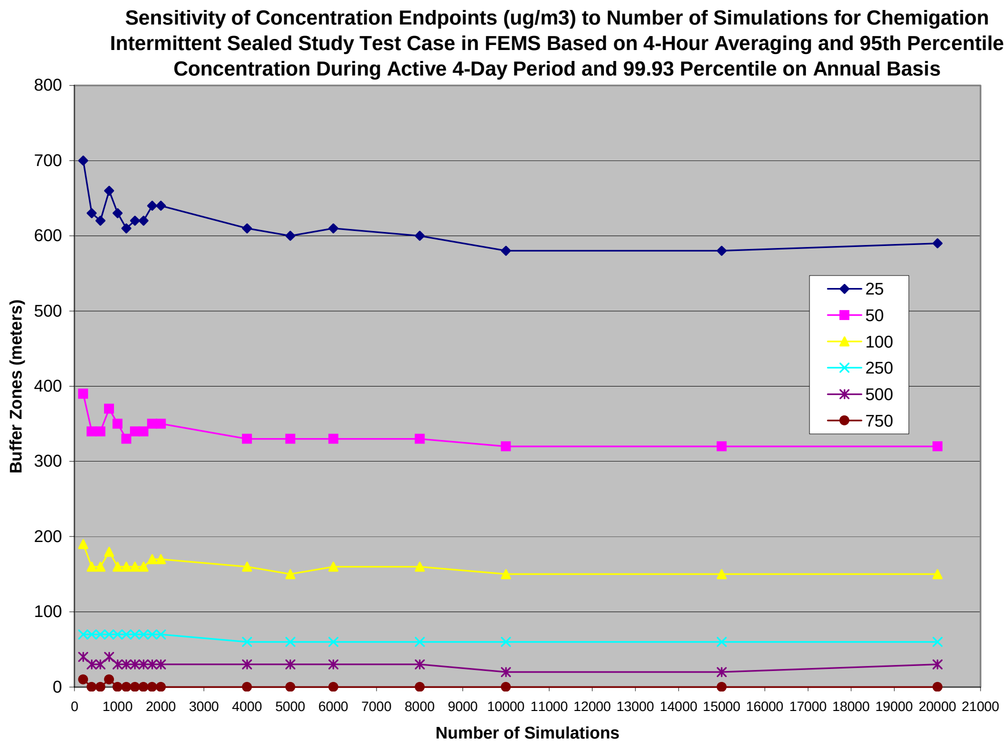


Table 14: Chemigation Intermittent Seal Study: Sensitivity to Stochastic Treatments of Input Terms

4- Hour Chemigation Intermittent Sealing Study Sensitivity Runs (5000 Simulations and 1.49 Exceedances)

Emissions	Wind Speed	Wind Direction	Stability	25	50	100	250	500	750
				micrograms/cubic meter endpoints					
X	X	X		600	330	150	60	30	0
X	X	X	X	590	330	160	60	30	0
	X	X	X	550	310	140	60	20	0
X		X	X	580	330	160	60	20	0
X	X		X	650	350	160	60	30	0
				630	**320**	**140**	**60**	**20**	**0**
X				670	340	160	60	30	0
	X			630	320	140	60	20	0
		X		570	300	140	60	20	0
			X	620	320	150	60	20	0

Endpoint distances shown in bold are with the benchmark run.

Figure 29: Sensitivity to the Number of Simulated Years: Shank Injection / Standard Sealing

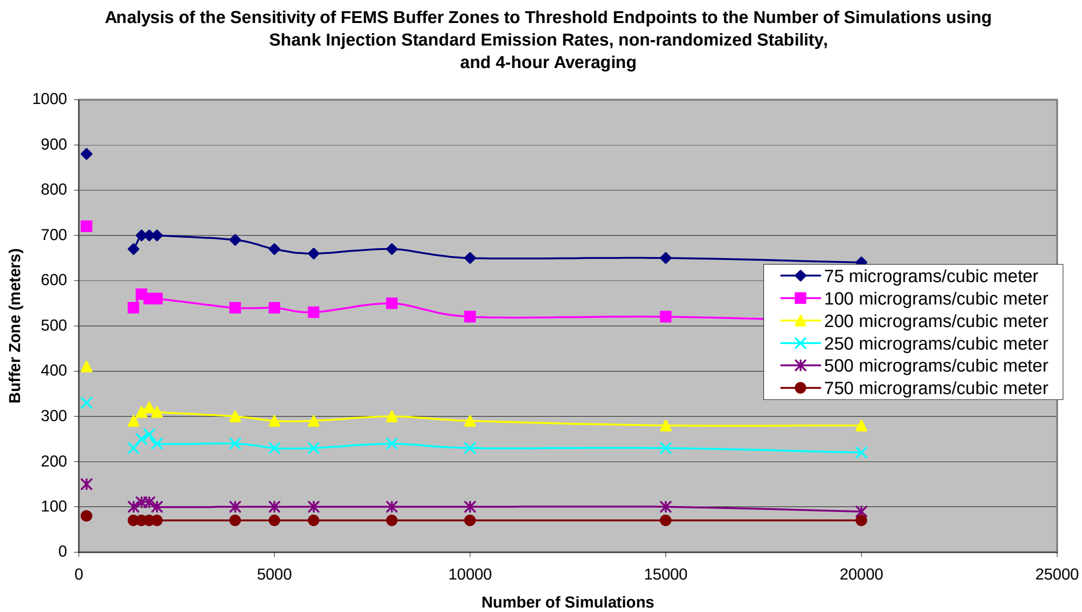


Table 15: Shank Injection/Standard Sealing Study: Sensitivity to Stochastic Treatments of Input Terms

4-Hour Shank Injection Standard (SHANK99.DAT) Sensitivity Runs (1.49 Exceedances & 10,000 Simulations)

Emissions	Wind Speed	Wind Direction	Stability	75	100	200	250	500	750
				micrograms/cubic meter endpoints					
X				720	540	300	240	100	60
	X			600	470	220	180	70	60
		X		510	410	210	160	70	60
			X	460	360	170	130	70	60
X	X	X		650	520	290	230	100	70
				560	**440**	**220**	**170**	**70**	**60**

Benchmark run in bold

Distances to endpoints < 50 meters were not determined with precision. Extra sets of runs would be needed to refine specific distances based on a finer-scale receptor grid.

The sensitivity analyses relative to key model inputs (emission rates, wind speed, wind direction, and atmospheric stability) were done two ways: (1) showing each term individually; and (2) holding out each term one by one.[37] On this basis, it is shown that emission rates is the most sensitive term, which acts to promote a more conservative analysis than relying on a deterministic assessment of emission rates. This shows that randomizing uncertainty in emission rates acts to increase modeling of peak acute exposures, as would be expected. Accounting for the uncertainty in the meteorological parameters for this scenario has an influence on the distances to the regulatory endpoints that are calculated, but not generally as great as the consideration of the uncertainty in the emission calculations (*refer to* Table 15 of this background document). This was not an unexpected finding.

It should be noted that the uncertainty in the meteorological input terms includes errors associated with instrument error as well as the representativeness of the data to account for transport within the modeling domain.

5.3.2 Sensitivity of FEMS Near the Extreme Upper Tail of Concentration

Alternate sets of sensitivity runs were done to show the sensitivity of the results for rare events. With relatively long recurrence intervals, however, the sensitivity to the meteorological and emission terms becomes more significant. To further test the stability of the FEMS results, a recurrence interval of 20 years was evaluated (concentrations/year greater than thresholds are $\leq$ 0.05/year) to test the stability near the extreme upper-tail of the distribution. For these tests, the shank injection/standard seal metam-sodium GLP field study was used (Merricks, 2002b) because it showed a larger variability in emission rates across the distributions. The results are shown in Table 16

The benchmark results for comparison with the FEMS treatments are the ones associated with all blanks in Table 16. These results are based on existing EPA modeling methods without Monte Carlo enhancements through FEMS. As shown, FEMS generally is more protective than the existing EPA modeling methods developed for batch sources such as agricultural fumigants without a probabilistic treatment for uncertainty in the model inputs. This is an important consideration for model review because the results can be referenced to existing methods as part of the validation procedure.

37 Complete evaluation of this matrix is in process and will be available for review at the SAP meeting.

Table 16: Upper-Tail Sensitivity Analysis (based on 20-year recurrence)

Chemigation / Intermittent Sealing

1-Hour Averaged Chemigation Intermittent (KERN2001.DAT) Sensitivity Runs (0.05 Exceedances & 100,000 Simulations)

Emissions	Wind Speed	Wind Direction	Stability	micrograms/cubic meter endpoints 1000	2000	2500	3000	4000	5000
X				270	70	50	50	<50	<50
	X			240	50	50	<50	<50	<50
		X		250	50	50	<50	<50	<50
			X	230	50	50	<50	<50	<50
X	X	X		290	80	60	50	<50	<50
				240	**50**	**50**	**<50**	**<50**	**<50**

Benchmark run in bold

Shank Injection / Standard Sealing[38]

Benchmark run in bold

1-Hour Averaged Shank Injection Standard (SHANK99.DAT) Sensitivity Runs (0.05 Exceedances & 100,000 Simulations)

Emissions	Wind Speed	Wind Direction	Stability	micrograms/cubic meter endpoints 2000	2500	5000	10000	15000	20000
X									
	X								
		X							
			X						
X	X	X							

Benchmark run in bold

[38] Results to be available for SAP hearing.

6.0 RESULTS

The test data set provided for review involves a 19.8-acre application of metam-sodium applied by chemigation and sealed by intermittent water sealing. The cover of the CD case for this disk provides a summary of the model options needed for the test run, which also are summarized as follows:

- Name of file - -(*whatever you want*)
- East – west dimensions of field = 100
- North-south dimensions of field = 800
- Default receptor grid? (enter 2 - - NO)
- At receptor prompts, enter (50, 100, 150, 200, 250, 300, 400, 500, 750, & 1000 meters - - 1 number for each of 10 prompts)
- Simulations = 5000
- At prompt for which parameters to randomize - - select 0
- Emissions, wind speed, wind direction randomized (enter 1 @ prompts)
- Stability non-randomized (enter 0 @ prompt)
- Indoor exposures option = 0 (ambient exposures only)
- Applications / year = 1
- Days of off-gassing = 4
- Averaging time = 4
- Percentage of maximum application rate = 100
- Name of emissions distribution file = kern2001.dat
- # concentrations thresholds = 6
- At concentration threshold prompts, enter (25, 50, 100, 250, 500, 750 - - 1 number for each of six prompts)

- Number of times / year > concentration threshold[39] = 1.49

- Meteorological region = FRESNO, CA

- Latitude = 30

- Longitude = 110

- Time zone = 8

The following, as provided in Attachment 2, provides the results of all key steps of FEMS, as used in the test case example in this background document, including:

- The model input files and meteorological data needed to replicate the test model run (on CD);

- Example interim output of FEMS, *i.e.*, converted binary output from the ISCST3 model that serves as input to TOXST (on CD and hard copy form); and

- Quantitative output (average times per year concentrations exceed thresholds) from TOXST, which can be reviewed to confirm the adequacy of the interpolation method contained in FEMS to compute radial distances to regulatory endpoint concentrations (on CD).

Table 17 shows the output file from the test case FEMS run. Figure 30 presents the FEMS TOXST output (per above) in the form of an isopleth analysis showing the average number of concentrations greater than the threshold concentration/year.

---

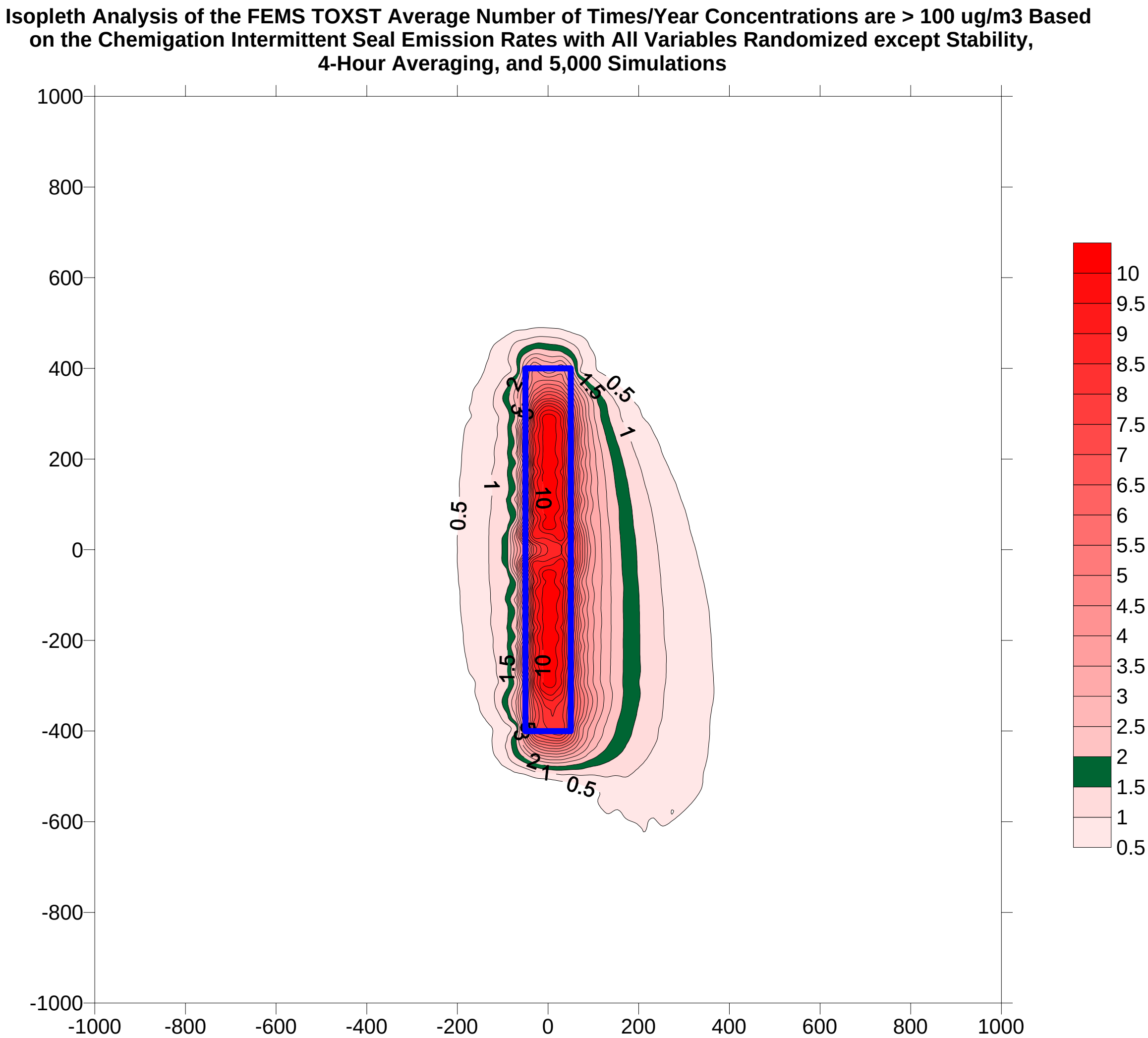
39 ~95th percentile concentration during active 4-day off-gassing period, based on 4-hour sampling as shown in the FEMS prototype.

Table 17: FEMS Output of Test Case File[40]

```
TEST CASE - 5,000 SIMULATIONS - KERN2001.DAT
200-Year and 5000 Simulations Randomized
Monte Carlo Exposures Assessment Using

Randomized Emission Rates
Randomized Wind Speeds
Randomized Wind Direction
Non-Randomized Stability

Acres Modeled  Averaging Time  Exceedances
-------------  --------------  -----------
   19 Acres       4 Hours          1.49

Using a Polar Receptor Grid Centered at the
Center of the Field with Ring Distances of

   50 Meters
  100 Meters
  150 Meters
  200 Meters
  250 Meters
  300 Meters
  400 Meters
  500 Meters
  750 Meters
 1000 Meters

Distance(s) (meters) to Concentration
Thresholds (micrograms/cubic meter)
Threshold  Distance
---------  --------
   25        600.
   50        330.
  100        150.
  250         60.
  500         30.
  750          0.
```

40 Some small differences (*e.g.*, 10 meters) can be expected in different runs.

Figure 30: FEMS Output Plot of Average Number of Times/Year Concentrations > Threshold Concentration[41]



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41 These values are used to compute percentiles of exposure during the active off-gassing period and on an annual basis.

The accuracy of these results can best be presented by displaying the model-based estimates of the concentration fields relative to the field data. Figures 31 through 36 present scatter plots of modeled concentrations based on the fitted emissions data for the six highest periods in terms of measured concentrations for the chemigation/intermittent sealing (test case) field study for metam-sodium. These concentration fields were based on emission data fit from the same measured data, so in this sense, these displays are not true indications of model performance. These figures do, however, provide an indication of the uncertainties associated with matching modeled concentration fields for the same sites and times to the observed spatial display of directly measured concentrations. Across the multiple periods and considering network ranges versus modeled ranges, the modeling is shown to be consistent with the generally accepted factor of two accuracy expected from the use of ISCST3, again with the understanding that the factor of two cannot be constrained in time and space (EPA, 2003b). It is anticipated, however, that with the use of the same emissions data (established for worst case conditions) that the use of 5-year meteorological data sets, with Monte Carlo sampling to account for uncertainty in key model inputs, should provide a reasonable representation of the concentration fields, generally erring on the side of overstating concentration through the use of worst-case / upper-end empirical emissions data based on summertime applications in the vicinity of Bakersfield, California where the soil conditions are hot, dry, and typically sandy loam. Most importantly, the **distribution** of concentration can be reasonably estimated through Gaussian modeling methods, such as used in FEMS.

7.0 CONCLUSIONS OF ANALYSIS IN RELATIONSHIP TO MANAGEMENT OBJECTIVES

The modeling methods employed in FEMS represent a scientifically sound basis to use existing EPA-approved models (ISCST3 and TOXST) to promote informed and sound risk management decisions that are based on a realistic representation of the annual, or active off-gassing period, distributions of concentrations for potentially exposed bystanders. The results appropriately include consideration of intermittency, variability, and uncertainty in the model inputs of emissions and meteorological data, which promotes consistency with the guidance of the EPA Office of Pesticide Programs (EPA, 1997, 2001, 2003a). As a modeling system to be available for general use, FEMS also will help promote consistency in the assessment of exposure for all agricultural fumigants because of the feature to address all averaging times from 1 to 24 hours,[42] and the capability to address multiple field scenarios (independent or common ownership).

Recommendations for Additional Analysis

The following identifies several areas where additional analysis in the future would be useful to expanding the scope of FEMS to meet the regulatory needs of agricultural fumigants:

[42] All averaging that are less than or equal to 24 hours and can be evenly divided into 24 (1, 2, 3, 4, 6, 8, 12, and 24 hours) can be modeled with FEMS.

- ***Adapt for Worker Exposure*** -- As stated in this background document, the most significant limitation to Gaussian modeling is the force fit of the Gaussian assumption on the distribution of concentrations along the vertical axis during convective atmospheric conditions. Although the next-generation EPA dispersion model, AERMOD (EPA, 1998), contains mixed-layer scaling to represent more specifically vertical dispersion during convective conditions, AERMOD's treatments for convective conditions do not include ground-level releases . Through either a theoretical extrapolation of existing results to cover surface releases, or preferably through future field research on this topic, improvements of modeling convective conditions could help promote a greater reliance on modeling methods, such as FEMS, to evaluate more fully worker exposures for a wider range of application methods, application practices, and field conditions. FEMS contains sufficient resolution in diurnal coverage to support model-based extrapolation of worker exposure data in the future, subsequent to the identification of a suitable theoretical or empirical basis to reasonably represent near-source exposures during convective conditions. Model-based worker exposure evaluations also would need to consider the complication of track-in (for shank injection enclosed cab scenarios).

- ***Enhanced Coverage of Field Study Data*** -- The degree of overestimation in FEMS for fumigants, including metam-sodium could be reduced in the future with greater coverage of heavier soils and cooler conditions in empirically-estimated emission rates, with reduced reliance on worst-case emission conditions to represent a wide range of sites and conditions.

Figure 31

Period 1 Chemigation / Intermittent Sealing

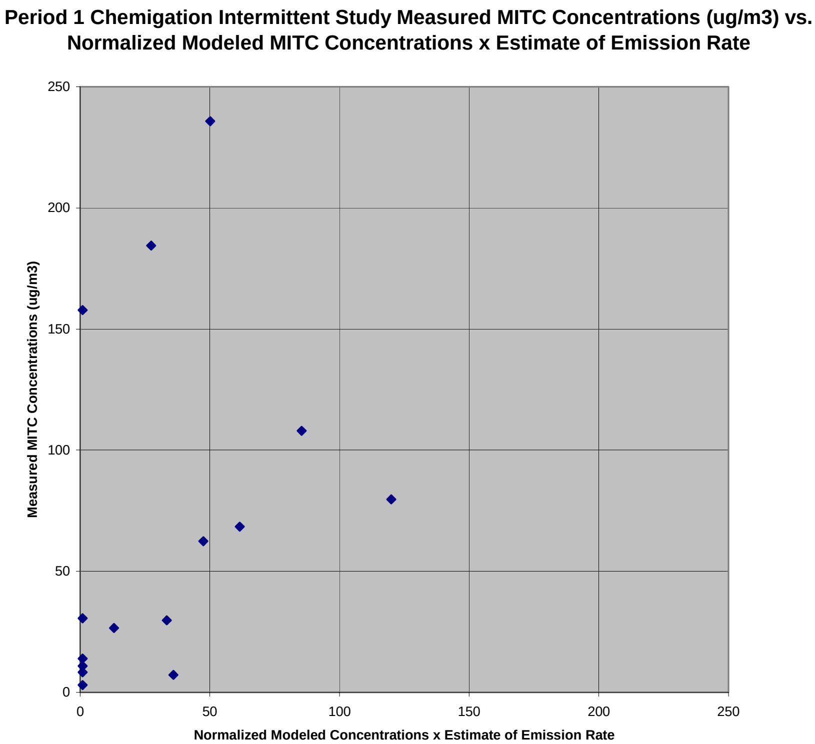


Figure 32
Period 2 **Chemigation / Intermittent Sealing**

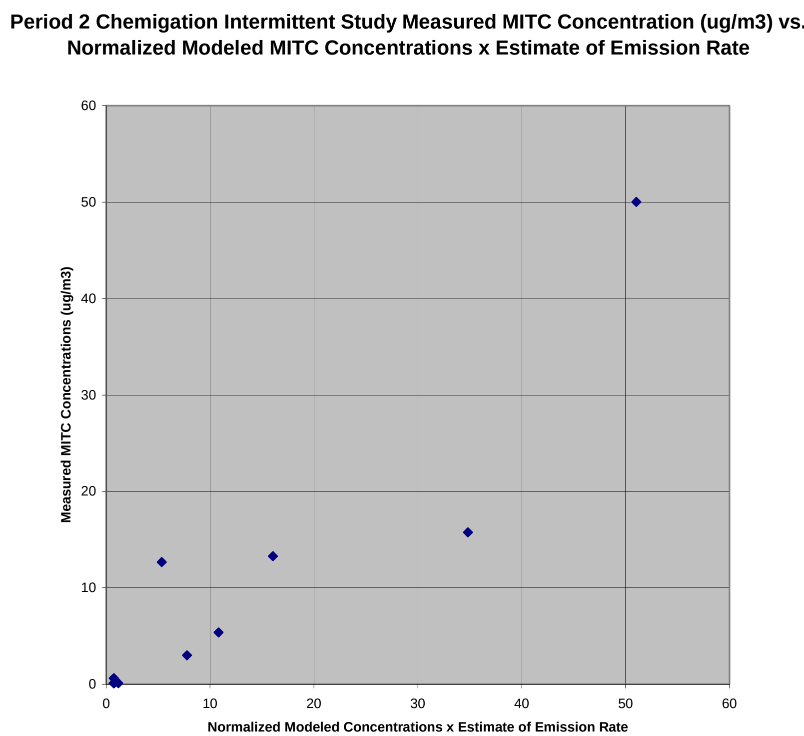


Figure 33
Period 3 Chemigation / Intermittent Sealing

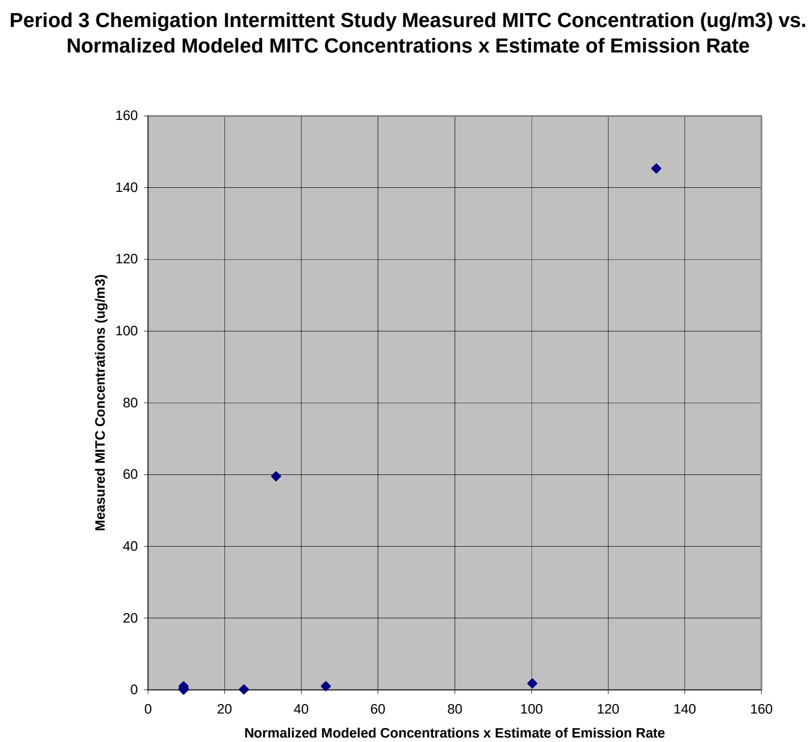


Figure 34

Period 4 **Chemigation / Intermittent Sealing**

Period 4 Chemigation Intermittent Study Measured MITC Concentration (ug/m3) vs. Normalized Modeled MITC Concentrations x Estimate of Emission Rate

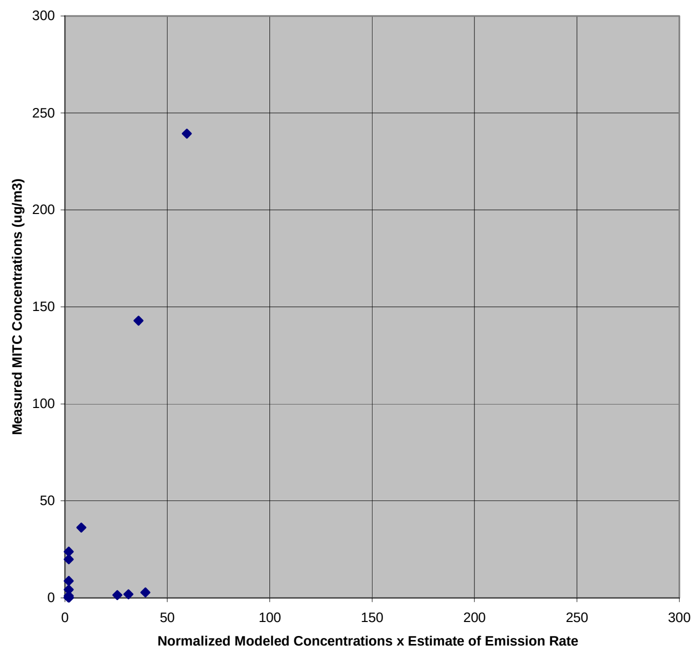


Figure 35

Period 5 **Chemigation / Intermittent Sealing**

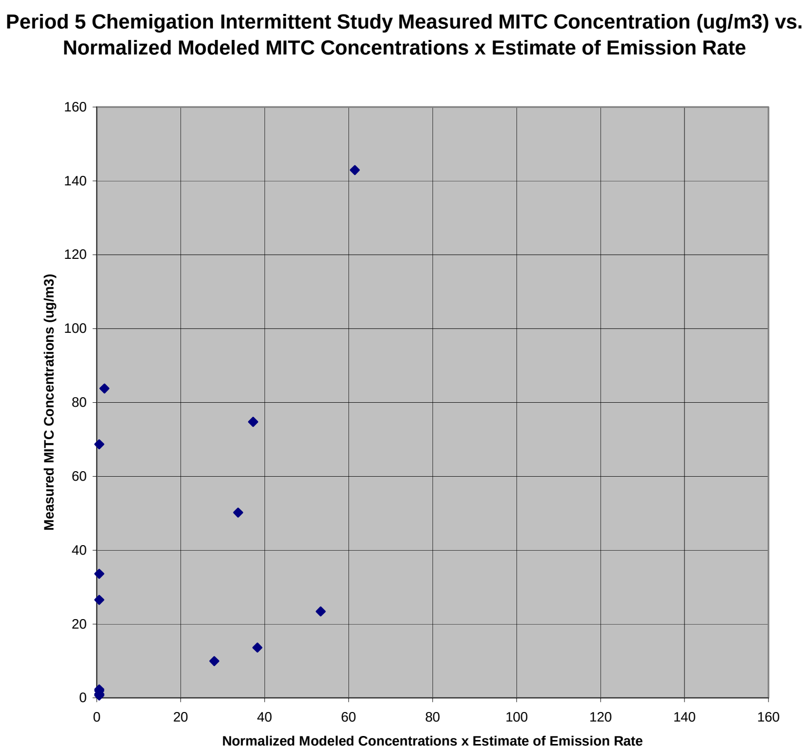
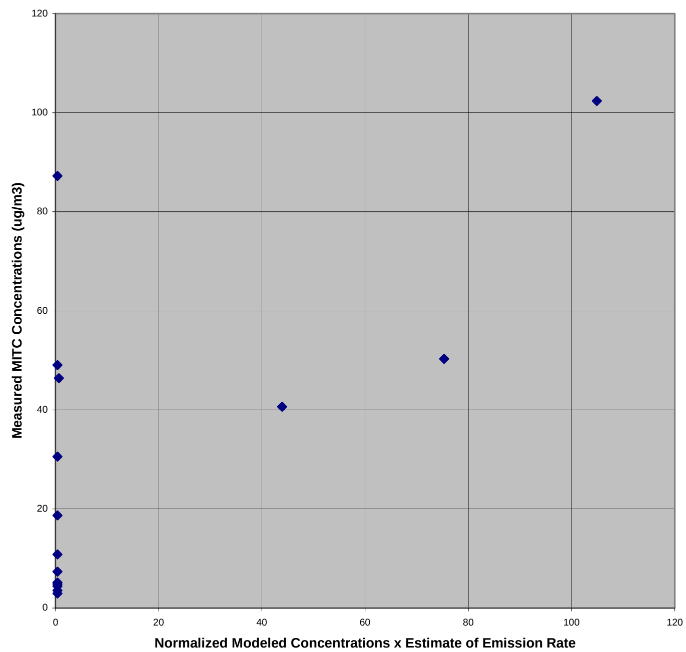


Figure 36

Period 6 **Chemigation / Intermittent Sealing**

Period 6 Chemigation Intermittent Study Measured MITC Concentration (ug/m3) vs. Normalized Modeled MITC Concentrations x Estimate of Emission Rate



Period	Plot Explanation
1	Three monitoring stations nearby Metam-Sodium tank. Possible contamination explains high measured/modeled ratios for these stations.
2	Good fit with only minor variability
3	High modeled/measured ratios can be explained by the fact that 1-hour averaged wind directions were very similar increasing modeling results.
4	Good fit with only two high measured/modeled ratios perhaps due to early evening wind direction variability.
5	High measured/modeled ratios explained by wind direction variability at nighttime. Hourly averaged wind direction missing plume.
6	High measured/modeled ratios explained by wind direction variability at nighttime. Hourly averaged wind direction missing plume.

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