Chapter

Prediction of Agricultural Contaminant Concentrations in Ambient Air

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Abstract

Monitoring ambient air to assess environmental exposure and risk for volatile agricultural chemicals requires extensive resources and logistical effort. The cost and technical limitations of monitoring can be mitigated using a validated air dispersion model to simulate concentrations of volatile organic chemicals in ambient air. The SOil Fumigant Exposure Assessment (SOFEA) model was developed to explore volatile pesticide exposure and bystander risk. SOFEA assembles sources and source strengths, uses weather data from the region of interest, and executes an air dispersion model (AERMOD, ISCST3) to simulate pesticide concentrations at user defined receptors that can be used in exposure and risk assessment. This work highlights SOFEA development from inception and modifications over the last 1.5 decades, to the current delivery within the public domain. Various examples for the soil fumigant 1,3-dichloropropene are provided.

Keywords: air dispersion modeling, SOil Fumigant Exposure Assessment tool (SOFEA), AMS/EPA Regulatory Model (AERMOD), 1,3-dichropropene, Gaussian plume

1. Introduction

The development of a numerical modeling tool for the soil fumigant 1,3-D started several decades ago using the Industrial Source Complex Short Term (ISCST3) air dispersion model [1]. Early work was extended by incorporating a soil fate modeling tool, the Pesticide Root Zone Model (PRZM3), to simulate the source strength used in ISCST3 air dispersion calculations [2]. This initial work was the forerunner of the SOil Fumigant Exposure Assessment system (SOFEA), a stochastic numerical modeling tool developed by Corteva Agriscience as a regulatory tool to evaluate and manage human inhalation exposure potential associated with the use of soil fumigants and other semi-volatile or volatile compounds [3]. There are no existing models for predicting pesticide exposure that can easily incorporate multiple fields throughout the year that mimic use rates and volatility that ultimately govern exposure. Even today, SOFEA has more attributes and functionality when addressing exposure risk from the use of volatile (or semi-volatile) pesticides than other agricultural models.

SOFEA calculates fumigant concentrations in air arising from volatility losses from treated agricultural fields for entire agricultural regions using multiple transient source terms (treated fields), Geographic Information System (GIS) information, agronomic specific variables, user specified buffer zones, and field re-entry intervals. The United States Environmental Protection Agency (USEPA) Gaussian plume models ISCST3 [4] and/or the AMS/EPA Regulatory Model (AERMOD) [5–6] are used for air dispersion calculations. Examples of ISCST3 simulations include modeling vehicle exhausts in urban areas [7] and modeling the ambient air concentrations at specified buffer distances for single fields in agriculture [8]. AERMOD simulations include estimates of mercury levels in air [9]), NO_2 and SO_2 predictions in Thailand [10], and air concentrations resulting from emissions from agricultural fields treated with the soil fumigant 1,3-dichloropropene [11].

This work provides a summary for SOFEA development and use in agriculture over the past decade. SOFEA uses field observed (or numerically generated) fumigant flux profiles from soil as transient source terms for both agricultural shank injection and drip-irrigation applications of a soil fumigant. Measured reference flux observations are scaled based upon depth of incorporation into soil and the time of year, to map the complete flux response surface from field/numerical observations, however a soil physics model can also be used to estimate flux from soil (e.g., HYDRUS [12], CHAIN_2D [13], etc.). Weather information, field size, application date, application rate, application type, depth of soil incorporation, pesticide degradation rates in air, tarp presence at the soil surface, ag-capable land, field re-treatment from 1 year to the next, buffer setbacks, and other sensitive parameters are varied stochastically using Monte Carlo techniques to mimic region and crop specific agronomic practices. Agricultural regions up to 49,210 km^2 (19,000 mi^2) can be simulated for temporal periods ranging from 1 day to more than 70 years for the purpose of addressing acute (24 h), short-term (72 h), sub-chronic (28 or 90 days) or chronic exposure. Multi-year, multiple field simulations are conducted using either random field placement in all agricultural capable areas, by selectively placing fields in historical or prospective areas, and/or placing fields of a specific size and spatial location if this information is available. Regional land cover, elevation, and population information cavn be used to refine source placement (treated fields), dispersion calculations, and exposure assessments. Both current and anticipated/forecasted fumigant scenarios can be simulated to provide risk managers with the necessary information to make sound regulatory decisions.

SOFEA has been used for regulatory decision making in California, was reviewed in the 2004 USEPA Scientific Advisory Panel (SAP) meeting [14], and is currently being used in the registration review process for 1,3-dicholopropene (1,3-D) with USEPA. Algorithms used by SOFEA to refine exposure predictions and manage acute, sub-chronic, and chronic risk associated with the use of soil fumigants on a local or regional basis are presented. Although SOFEA was originally designed specifically to describe air concentrations for the soil fumigant 1,3-D, the model is readily adaptable to generically describe the post-fumigation air concentrations of other soil fumigants and semi-volatile organic chemicals. SOFEA can now be executed in "retrospective" mode which allows the user to specify specific field locations where known fumigant applications are made and specific receptor locations where fumigant concentrations are measured which makes the model predictions available for comparison to field monitoring observations. Other enhancements to SOFEA include the option of importing flux (emissions) from soil simulated by a soil physics model (HYDRUS, CHAIN_2D) in lieu of flux obtained from field experiments. SOFEA will soon be in the public domain and can be obtained from Exponent Inc. (U.S. based consulting company) for use with all volatile or semi-volatile pesticides if parameterized appropriately. This manuscript summarizes SOFEA capabilities in both in prospective and retrospective mode, from inception to release of the model to the public domain.

2. Background

A generic methodology to determine fumigant concentrations in ambient air in large and diverse air sheds has been developed (**Figure 1**). Directionally averaged air concentrations within entire air sheds are determined using a multiple source Gaussian dispersion model that has been modified to include Monte Carlo sampling techniques, ties to GIS databases, and agronomic practices. Time averaged transient air concentrations simulated via a numerical model can be used to assess exposure and risk for an unlimited number of scenarios.

SOFEA enables the determination of "area-wide" concentration profiles for user specified distances that account for multiple field applications. Thus, the effect of fields "off-gassing" at different points in time and space are accounted for by SOFEA. The user can evaluate the impact of the buffer on the acute exposure for residents and by-standers by specifying a buffer distance from the edge of treated fields. The user can also determine the chronic exposure to individuals residing in the use area by specifying the total mass applied on an annual basis and running SOFEA for a full year or multiple years. SOFEA inputs and outputs are easily exported to other file formats or programs. Concentrations of soil fumigants in air

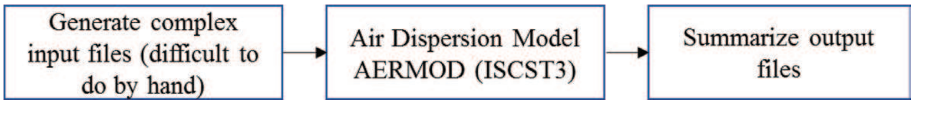

Figure 1.
SOFEA is an intelligent input file generator and output repository for agronomic use of the USEPA Gaussian plume model AERMOD (and formerly ISCST3).

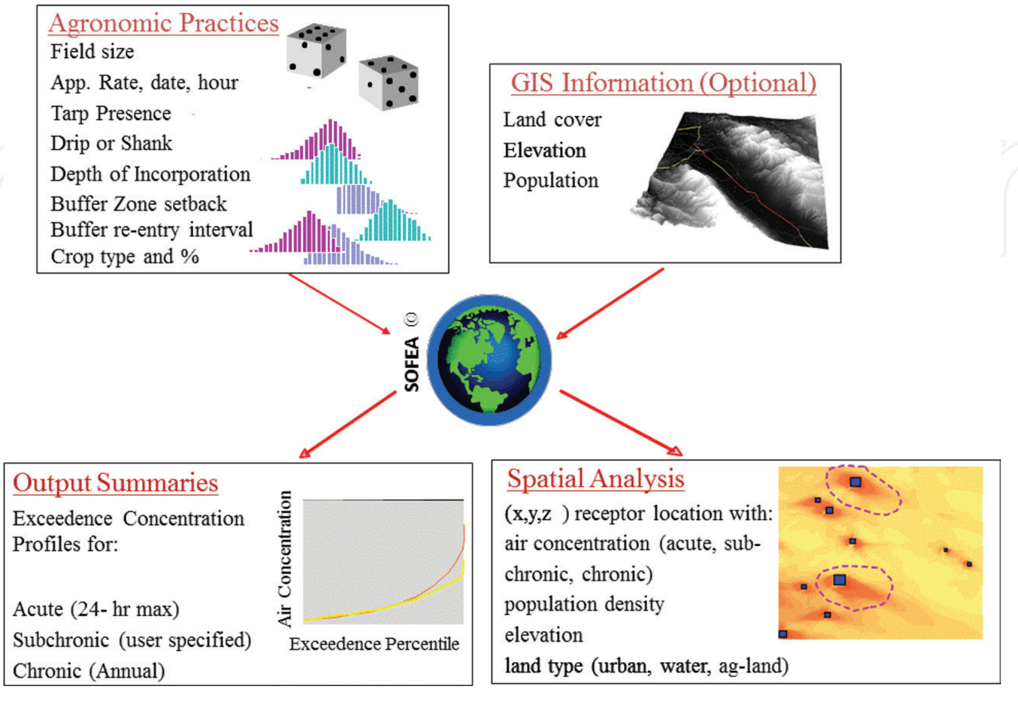

Figure 2.
SOil Fumigant Exposure Assessment Model overview.

are associated with x, y, z co-ordinates and associated with proximity to treated fields as well as human populations (if population census data is available). The SOFEA model is readily adaptable to generically describe the post-fumigation air concentration of other organic contaminants, **Figure 2**.

3. SOFEA refinements and use, past and present

3.1 Air dispersion model

The ISCST3 [4] and AERMOD [5, 6] models were developed by the USEPA as regulatory tools for predicting concentrations of air contaminants in diverse air sheds. Both are Gaussian plume models useful for estimating air quality surrounding contaminant release sites. AERMOD replaced ISCST3 by USEPA, although ISCST3 is still in use by some researchers and regulatory authorities. ISCST3 has been widely used to simulate probability distribution functions (PDFs) of fumigant concentrations in air within townships in California to estimate acute and chronic bystander exposure [15, 16].

3.2 Parameter representation

The complex terrain algorithms of ISCST3/AERMOD can account for the effects of elevation changes within specific regions should this information be available. Population information (if provided or known) can also be used in population-based risk assessments. The 2010 U.S. census data lists population densities by census blocks and is a good choice for population information. A township is defined

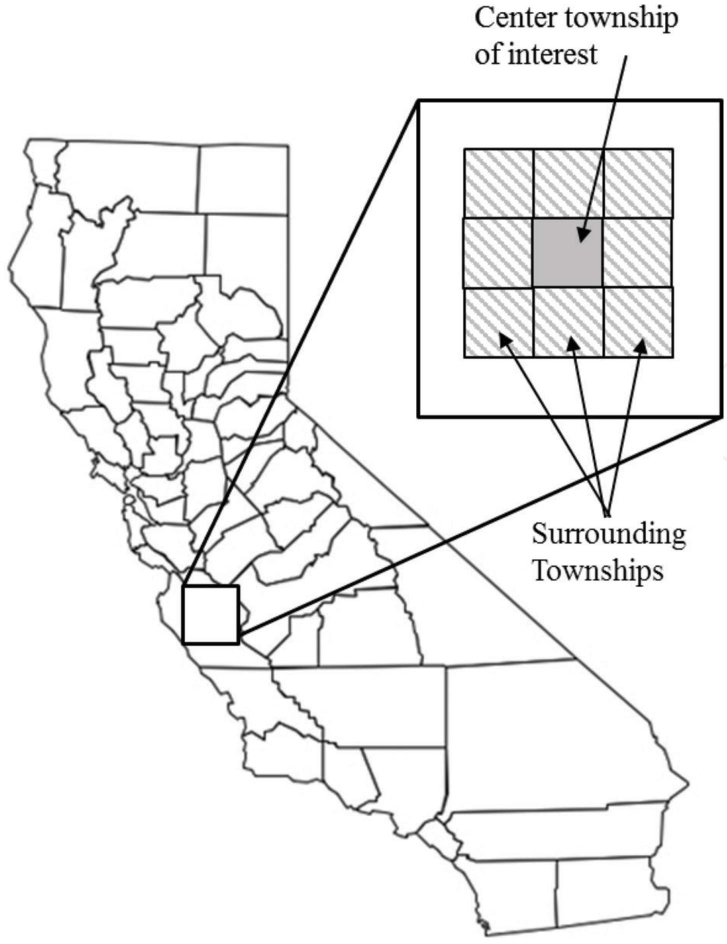

Figure 3.
Example of a 3 × 3 township air shed for SOFEA simulation from the state of California.

according to the Public Land Survey System (PLSS) and is nominally 6 × 6 mi (9.66 × 9.66 km) in area, **Figure 3**. The spatial locations for receptors placed uniformly or weighted in a central township are user specified, and appropriate land cover, elevation, and population data from GIS data bases are necessary inputs. Township information must include land cover such that ag-capable land can be quantified. Elevation and population information are optional. The impact of sources external to the central township domain will depend on the persistence and drift characteristics of the pesticide being simulated. However, a model evaluation for 1,3-D showed that 3 × 3 townships was adequate to account for edge effects [17].

3.3 Air shed simulation domain

An air shed is defined as a volume of air overlying a square surface area, where source terms (i.e., treated fields) throughout the air shed can contribute to overall air concentrations at specific locations. Although historical SOFEA simulations focused on air concentrations in either a single township or a 3 × 3 township domain, the model can be used to simulate concentrations across much larger airsheds. The complex terrain algorithms of ISCST3 or AERMOD can take advantage of elevation changes within specific regions. Receptors can be placed uniformly in a central township or over a multi-township domain. Source terms can be placed anywhere in the simulation domain, which can include up to 23 × 23 townships (49,210 km^2 = 19,000 mi^2). When running in prospective mode, the user need only specify the annual pesticide mass applied to any township within a 23 × 23 township domain, appropriate GIS information, receptor spacing and heights, as well as appropriate PDFs characterizing agronomic practices within the region.

3.4 Stochastic portrayal

Concentrations of a soil fumigant in air resulting from transient agricultural source terms are also dependent upon meteorological conditions, application timing, and other agronomic properties. A mechanism was required that could propagate parametric uncertainty in sensitive model inputs to air concentration predictions. Monte Carlo (MC) methods provide a straightforward technique to propagate such uncertainty in independent parameters to dependent output variables [18, 19]. PDFs can include fumigated field sizes, application rates, application dates etc. SOFEA can also be used in retrospective mode, where exact treated field locations and application parameters (mass applied, date applied, etc.), and receptor locations are known. Variability in input is described by PDFs that are randomly sampled to generate input parameter sequences. Stochastic variables for SOFEA include application rate, date, and hour of day initiated, pesticide depth of incorporation, presence of a tarp at the soil surface, application type (shank injection or drip irrigation), field size, weather year, and pesticide properties such as degradation rates in air. Output predictions are no longer deterministic, but rather a discrete distribution is generated from which exceedance probabilities and return frequencies can be calculated (e.g., 1-in-100-year exposure potential, and so on). Air quality modeling work is in accordance with the policy established by the U.S. EPA for Air Quality Models and follows the guidelines set forth by U.S. EPA for Monte Carlo Analysis [20].

The original version of SOFEA required the MS Excel add-on program Crystal Ball™ (Decisioneering, Inc.) to transform ISCST3 from a deterministic model into a stochastic/deterministic system; however, subsequent versions have been modified to include Visual Basic Applications (VBA) algorithms that obviate the need for Crystal Ball™. In SOFEA2, an ISCST3 input file is exported from Excel that is based upon appropriate selections from user defined PDFs that are derived from actual agronomic data. Excel, ISCST3, and VBA programs were coupled to allow the transparent integration of the Monte Carlo component in SOFEA3, which used, but $ISCST_3$ had changes in mixing height calculations under calm conditions such that simulation with parametric uncertainty more closed matched monitoring observations [21]. The latest version of SOFEA (SOFEA4) contains identical functionality as the original version but was rewritten in C++ and Qt to replace VBA programming, ISCST3 replaced by AERMOD, and results using SOFEA4 use are found elsewhere [11]. SOFEA4 provides automation, transparency, a Graphical User Interface (GUI), the use of AERMOD, and maintainability for future support.

3.5 Crop selection and simulation domain

Fumigants are used on a variety of high valued agricultural commodities. Each commodity/crop is potentially unique, with different agronomic management practices. The crops chosen can be based upon current or future forecasted fumigant uses, and currently up to five different crop types can be considered. Predominant crops where soil fumigants are used include tree and vine (TV), field crops (FC), nursery crops (NC), strawberries (SB) and post-plant vines (PP). The contributions of a soil fumigant to air quality from each crop are easily extractable by keeping the crop types/parameters unique during simulation. This aids in determining appropriate Best Management Practices (BMP's) by crop type. SOFEA uses the supplied PDFs to generate the agronomic variables (e.g., field size, application rate, etc.) for each crop type. Thus, if a region is dominated by one crop type, all five crop types in SOFEA can be parameterized with the same data (if desired) to minimize computer memory requirements.

3.6 Receptors

Receptors are specific (x, y, z) locations in the simulation domain where air concentrations are calculated. These receptors can be uniformly placed within the township for chronic exposure predictions, or at specific setback distances around treated fields if acute exposure assessment is required, **Figure 4**. Historical SOFEA simulations in CA have assumed a rectangular grid of 36 equally spaced receptors per township section (i.e., a 1 mi^2 area) which yields 1296 receptors per township at a spacing of 268.2 m (880 feet) [11, 21]. Receptors are typically placed at 1.5 m above the ground to mimic the breathing height on adult. Ultimately, any desired

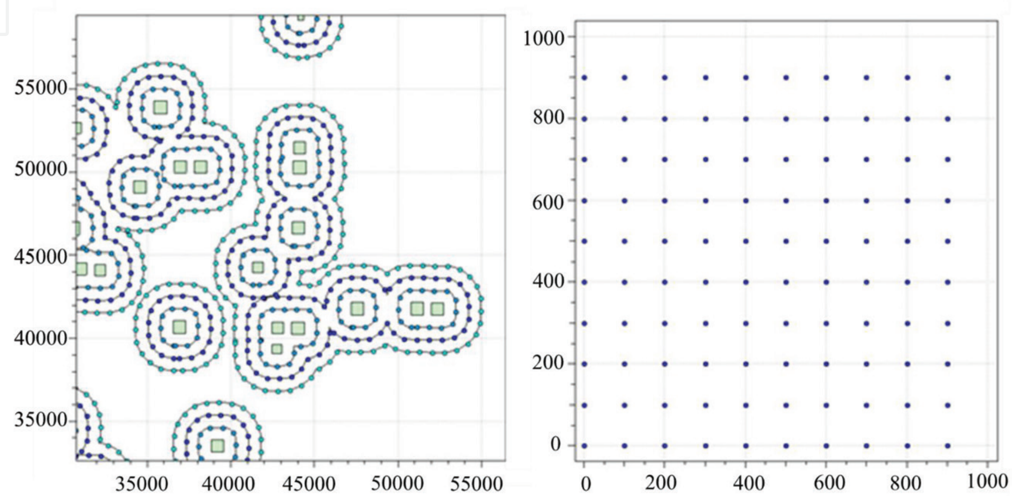

Figure 4.
Receptor placement at user specified buffer setback near treated fields (left) or uniform grid placement (right).

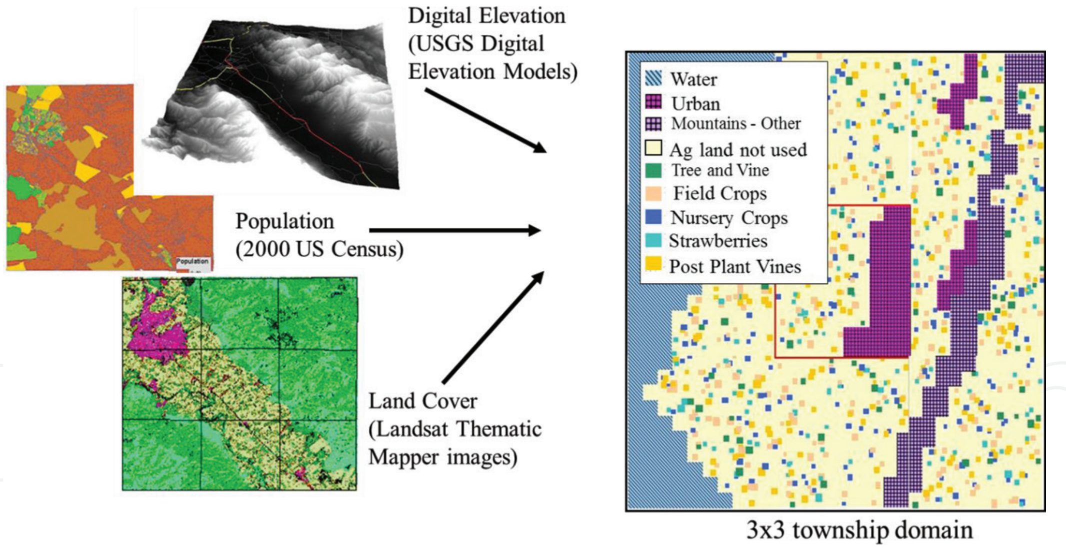

Figure 5.
Example of the continually updated public domain data bases available to the user of SOFEA.

receptor location and density, and height can be specified by the user, allowing individual receptors to be placed anywhere in the simulation domain.

3.7 GIS data layers

Many data bases and GIS software programs exist to extract appropriate information for use in SOFEA, **Figure 5**. SOFEA is not a GIS tool but rather uses GIS information that has been assembled using software such as ArcView™ (ESRI, Inc.). Land cover information is obtained by Landsat Thematic Mapper images (30-m resolution) that contain 21 unique land classifications [available from the National Land Cover Data (NLCD) database at http://landcover.usgs.gov/natllandcover.htm]. Elevation information is obtained from the USGS Digital Elevation Models (DEM) data at 1:24,000 scales. Population information is given by census blocks and populated with data from the 2010 US Census, and GIS information is used to parameterize the air shed for ISCST3/AERMOD simulations (e.g., ag-capable land where fields can be placed, etc.).

3.8 Meteorological data

A single location for weather data is used in SOFEA to represent weather conditions from the region of interest. Meteorological information includes hourly air stability class, wind speed, air temperature, wind direction and mixing and ceiling height for ISCST3, along with the Monin-Obukhov stability length for AERMOD. Wind speed and direction are critical parameters, and for larger simulation domains with potentially greater surface roughness length (z) (due to trees, buildings, fence rows, etc.), wind speed is preferable measured at a height of 10-m. A rule of thumb for determining the minimum height of the wind sensor is 7*z [22]. Flat fallow fields typically have a roughness length z < 0.1-m, and therefore an anemometer height of 2-m is adequate. The user creates a weather library for each year of weather and this library is assigned a uniform distribution when SOFEA is executed in prospective mode, or actual weather information for a specific time frame when running in retrospective mode. Weather data is available from public sources such as the California Irrigation Management System (CIMIS), the National Oceanic and Atmospheric Administration (NOAA), or the Florida Automated Weather Network (FAWN), or could be collected by a dedicated weather station installed in the simulation domain. The weather station should collect, at minimum, hourly precipitation, solar radiation, air temperature, and wind speed and direction (SOFEA requirements). Weather data must be pre-processed using PCRAMMET if the ISCST model is used, or the AERMET pre-processor if AERMOD is used. Pre-processing is conducted outside of the SOFEA model framework.

3.9 Source placement

In prospective mode, sources (treated fields) can be placed randomly or weighted to specific township locations, **Figure 6**. All ag-capable land (all land excluding urban areas, water bodies, barren, rock, quarries, and wetlands) is used and placement is based on a uniform probability of occurrence (known as random field placement). However, there are situations in high pesticide product use regions where treated field locations are known, and section weighting can be used to ensure that product use spatially represents historical needs. A township section is 1/36 of the township area and the user can specify the probability that these sections are locations where fields are placed. Receptors in these regions will register higher chronic soil fumigant air concentrations due to the increased field (i.e., source) density. Section-weighting probabilities can be based on expert judgment and/or historical product use records. When sections "fill up" and can no longer contain another treated field, a "spill-over" algorithm is introduced in SOFEA where the fields are then placed in sections surrounding the section that is "filled."

3.10 Township allocation of fumigant mass

In California, the amount of 1,3-D applied annually cannot exceed a mandated township allocation which is set based on acceptable levels of chronic exposure. Each township is assigned an allocation amount based on CA permit conditions (or some other a user-supplied amount), so this system can and has been applied in

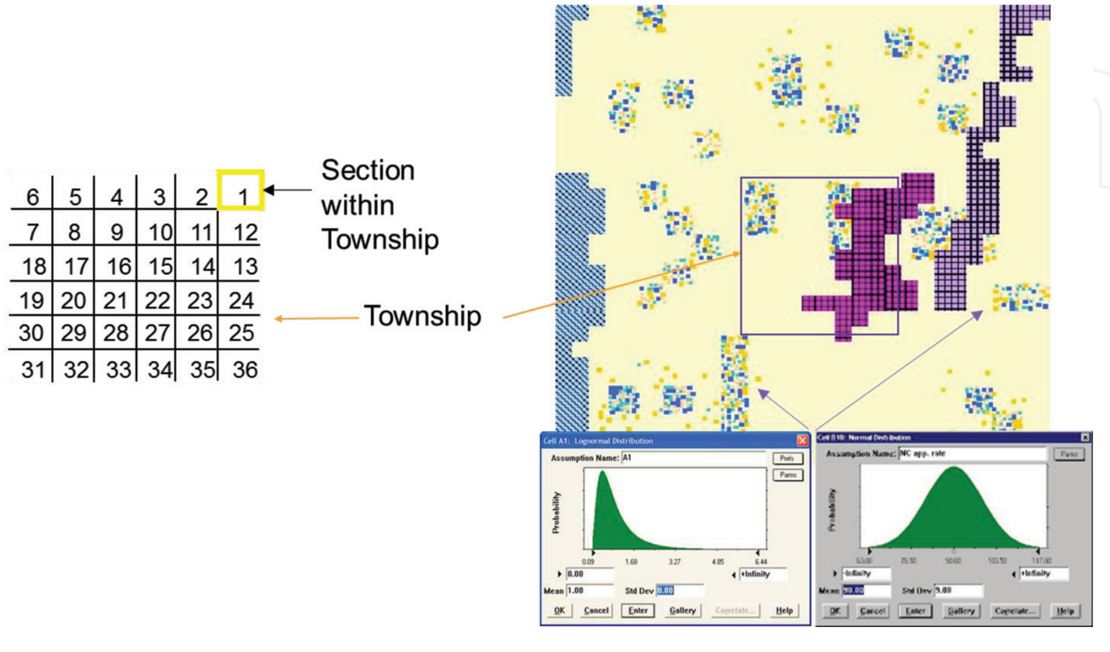

Figure 6.
Use of section weighted placement of treated fields within a township based upon specific sections having high fumigant use. Each field is assigned input based upon user specified PDFs.

other fumigant use areas across the United States. The amount of pesticide used in a given township is thus given as a fraction of this user specified township allocation.

3.11 Application scaling factor (CA only)

The California Department of Pesticide Regulations (CDPR) uses a simple procedure to account for seasonal and incorporation depth variability on pesticide volatility losses to represent the complete flux response profile. Volatility losses are sensitive to temperature and depth of soil incorporation [2] and a simple expression is used where the chemical flux from soil to the air is defined as.

$$Flux_i = R \times Fr_i \times S_{incorp} \times S_{yr} \quad (1)$$

where, $Flux_i$ = scaled hourly flux loss from soil into air for hour "i" based upon an actual field trial, Fr_i ($kg\ ha^{-1}\ h^{-1}$), R = pesticide application rate ($kg\ ha^{-1}$), Fr_i = observed flux rate (reference profile based on a field experiment, or modeling), S_{incorp} = scaling factor for depth of incorporation (dimensionless), and S_{yr} = scaling factor for time of year (dimensionless).

Although the CDPR approach only uses a single flux profile for each application type, these profiles are modified by soil incorporation depth and time of year. Also, models such as HYDRUS [23], STANMOD [24], CHAIN_2D [13] and PRZM3 [25] can also be used to develop flux profiles for different conditions.

3.12 Temporal representation S_{yr} (CA only)

California is sectioned into warm and cool seasons where increased emission to the atmosphere occurs under warm conditions and is arbitrarily increased by a factor of 1.6× by CDPR. Therefore, S_{yr} is assigned a value of 1.6 to account for gross seasonal temperature effects during the warm season. This warm season can be a specific time of the year (as for CDPR) or the SOFEA user can use a continuous sinusoidal function, where the amplitude and frequencies are daily average air temperatures based upon what day within the year a pesticide application is made (**Figure 7**, left). In addition, several constraints on the depth of incorporation are used for CA and are given in **Figure 7** (right). The user can specify how the pesticide incorporation depth in soil can alter the cumulative mass loss from the soil surface (linear, exponential, CDPR) by selecting from options in the drop-down

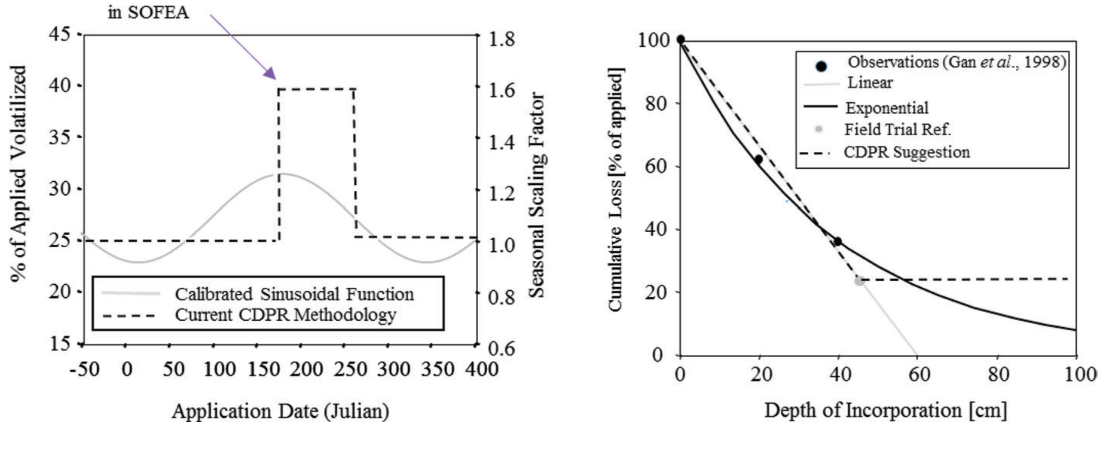

Figure 7.
Example of CDPR application factor or sinusoidal modeling for percent of applied volatilized (left) and impact of depth of pesticide incorporation (right).

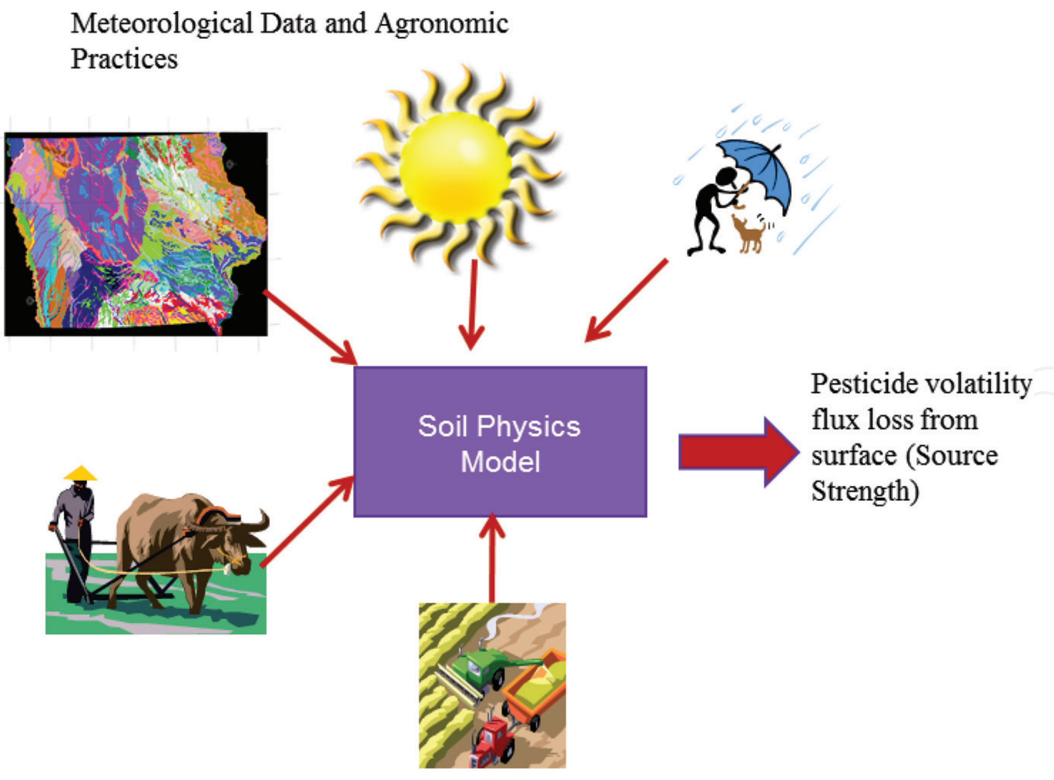

Figure 8.
Obtaining soil volatility flux estimates using a model such as CHAIN_2D or HYDRUS.

menu in the SOFEA GUI. The type of seasonal scaling (CDPR or sinusoidal) can also be selected by the user in the SOFEA GUI.

3.13 Model output characterization

SOFEA is used to execute the air dispersion models ISCST3 (historical) and/or AERMOD (recent). Hourly output from these models can be analyzed according to user selections for post processing output concentrations (e.g., 1-h, 1-day, 3-day, 15-day, annual, and so forth). Functionality for the current version of SOFEA is somewhat different than in the earlier versions, but the bulk of functionality for SOFEA are the same and found elsewhere [3].

In earlier versions of SOFEA, input and output were facilitated via a VBA interface that utilizes EXCEL spreadsheets containing user supplied PDF's of application parameters. Users could create inputs based on actual field data and pesticide use information, or generate hypothetical distributions of use parameters such as field sizes, application rates and timing, depth of injection, etc. Over the years, SOFEA has evolved from a VBA model using only ISCST3 to a C++ interface that can drive AERMOD simulations (e.g., SOFEA4). A user guide for the most recent version of SOFEA4 is currently in preparation and should be available sometime in 2019.

Chemical flux estimates can be obtained from a variety of different experimental sources but can also be estimated from soil physics models such as HYDRUS [23], STANMOD [24] and CHAIN_2D [13], **Figure 8**. Such models can and have been used to simulate both volatility from soil along with movement into the soil profile. Advantages of using a soil physics model to estimate pesticide flux loss deal with low cost and the semi-infinite parameter space that can be explored with simulation techniques. Field studies in five different states that explored atmospheric flux loss for chloropicrin and 1,3-dichloropropene were validated with CHAIN_2D and indicate the model can correctly capture both peak and cumulative emissions effectively for these two soil fumigants [17, 26]. Thus, CHAIN_2D and similar models are useful

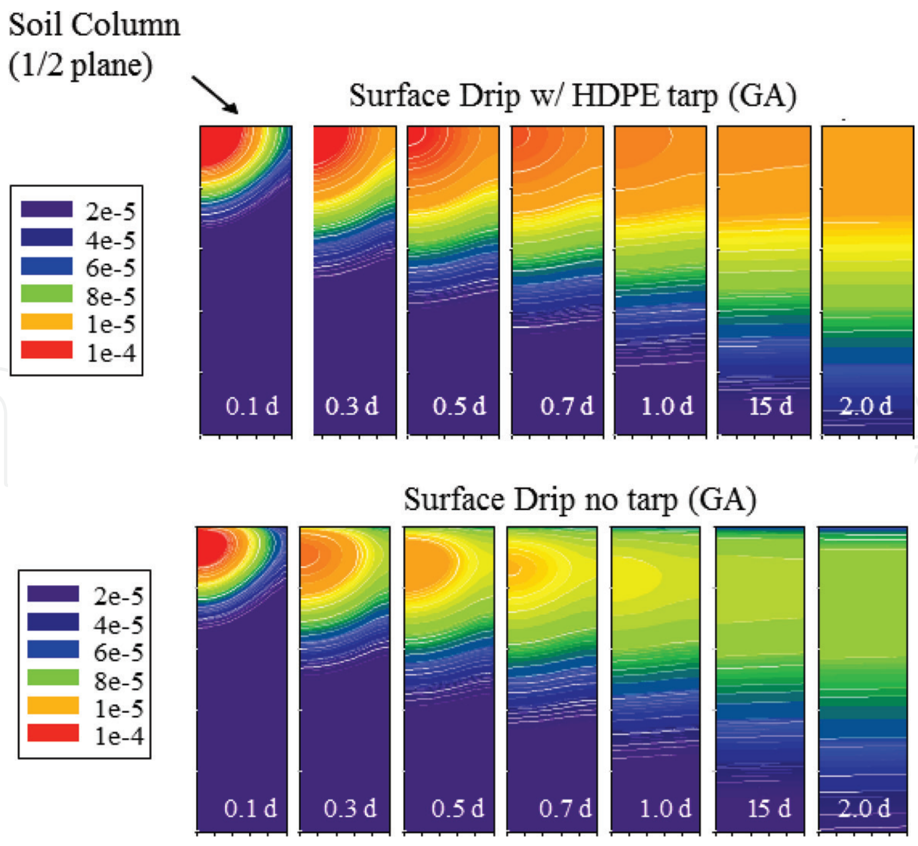

Figure 9.
Example use of soil physics model CHAIN_2D where exploration of multiple mitigations strategies such as water sealing, tarps, depth of incorporation, etc. can be simulated, as well as concentration by time (C × T) within soil for biological efficacy.

tools for extrapolating flux predictions to diverse scenarios where experimental observations are unavailable [27–29]. Examples of various mitigations strategies that can be explored using soil physics models include the use of agricultural films, increased soil injection depth for the fumigant, and under a near semi-infinite parameter combinations of meteorological, soil and agronomic properties, **Figure 9**.

Soil physics models should first be validated with field observations before being used to extrapolate to a variety of different conditions. Cryer and van Wesenbeeck [26] used CHAIN_2D to validate against field observations, and then coupled CHAIN_2D to several USEPA air dispersion models (ISCST3 [4] and CALPUFF [30]). Both cumulative and 1-h maximum air concentrations were simulated and compared against field observations with good success (the best observations and simulations results were between 6 and 8%). In addition, both ISCST3 and CALPUFF air dispersion models showed similar order of magnitude output predictions [17]. Chloropicrin and 1,3-D emissions through Totally Impermeable Film (TIF) were compared using HYRUS where the fumigant flux was simulated within a factor of ~2, though the timing of the peak was over-predicted by the model [29]. The authors suggest that field-based calibration should be conducted when tarps are used because of the lack of representative field effective permeability data for the tarps.

Most inputs can be specified as either discrete values, or as PDFs. If possible, PDFs should be used to maximize Monte Carlo capabilities of the SOFEA modeling system and encompass uncertainties and variability in model inputs. SOFEA can generate fumigant concentrations for each receptor in the simulation domain (up to 11,664 receptors have been simulated in a nine-township air shed), averaged over specific time intervals (24-h and yearly) or periods specified by the user. For example, the user could specify the output of 24-h average, 60-day average, and annual average concentration PDFs, for assessing acute, sub chronic and chronic risk to exposed populations.

3.14 SOFEA sensitivity analysis

A sensitivity analysis was conducted with earlier versions of SOFEA to determine which variables had the greatest impact on model predicted concentrations [3]. The dependent variable endpoint in the sensitivity analysis for Kern County, CA was the 15-D multi-direction average air concentration at 30.5 m buffer. Sensitive parameters were the crop percentage, application rate, application date and weather year, in addition to the amount of 1,3-D mass applied in a township and the proximity of a treated field to a monitoring location. Additional parametric sensitivity analysis for CHAIN_2D/ISCST3 showed several soil and irrigation parameters as consistently sensitive, including depth of incorporation into soil, tarp material, and initial soil water content [17].

3.15 Historical uses of SOFEA

A moderate overprediction in air concentrations was made by SOFEA when predicting regional air concentrations for Ventura and Merced counties in California [31] which included 25 contiguous townships and treated at 1.5 times the current township allocation using 1,3-D (or at maximum levels of 1,3-D used between 1999 and 2006). However, this work provided an example of how SOFEA could be used using actual agronomic practices to manage the use of soil fumigant products and long-term exposure and risk to residents located in high-use regions. This publication also discussed how high-use rural areas leading to the highest predicted air concentrations could be used in a formalized risk assessment. The observation that the high concentrations were surrounding the downwind locations around treated fields was first predicted by Cryer and van Wesenbeeck [1] before the SOFEA modeling tool was fully developed.

SOFEA was improved with the release of SOFEA2 which eliminated the need for the third-party software Crystal Ball™ while also incorporating the ability to specify unique agronomic fields and air monitoring receptor locations. Further refinement includes post-processing hourly concentration predictions for precise starting intervals, the capacity to incorporate specific field flux loss from soil physics modeling for each field in the simulation domain, and the ability to accommodate drip applications made to vineyards. SOFEA and SOFEA2 generated the same output distributions when identically parameterized (unpublished work of Corteva Agriscience).

A 1,3-D air monitoring study was conducted in a high fumigant use area in Merced, CA, where 3-day average air concentrations were measured continuously at the approximate center at each of nine townships over a 14½ month period [21]. This monitoring study was designed specifically for validating SOFEA. Although SOFEA2 predicted the general pattern and correct order of magnitude for 1,3-D air concentrations as a function of time, it failed to recover the highest observed 1,3-D concentrations of the monitoring study which typically occurred in December. It was found the atmospheric mixing height was a significant parameter affecting the modeled 1,3-D concentrations. An algorithm that adjusted the PCRAMMET mixing height based on measured wind speed and air temperature was found to improve the simulated concentrations significantly, however the inclusion of AERMOD in SOFEA3 improved the model fit to observed data without requiring any mixing height adjustment. Comparison of the output probability density functions (PDFs) for 72 h 1,3-D concentrations between monitoring observations and SOFEA4

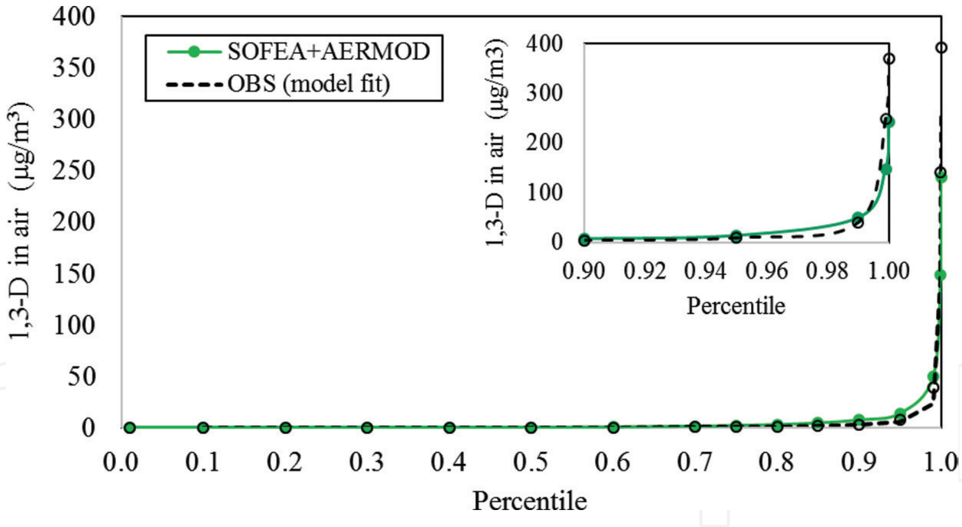

Figure 10.
Exceedance probability for Merced CA study from measured and simulated conditions when AERMOD replaced ISCST3 in SOFEA3 as the dispersion model for predictions.

simulation indicate that slight under-prediction of concentrations above the 99th percentile was off-set by slight over-prediction of the 1,3-D concentration distribution below the 99th percentile, resulting in the annual average 1,3-D concentration for the nine-receptor monitoring domain being slightly over predicted (<2%). This suggests that without further refinement, based upon field validation observations, SOFEA2 results are representative but conservative estimates of exposure for 1,3-D if border township contributions and mixing height (MH) adjustments for calm periods are considered. SOFEA2 proved a useful tool for estimating airborne levels of 1,3-D but showed some weakness when incorporating ISCST3 [21] and was renamed SOFEA3 when AERMOD was included.

AERMOD was used in conjunction with SOFEA2 after 2016 (now named SOFEA3), following the knowledge that MH was one of the most sensitive variables and that ISCST3 and its associated meteorological pre-processer over-estimated MH during stable air (calm conditions). Analysis showed SOFEA3, when using AERMOD in lieu of ISCST3 as the air dispersion model, improves the predictions of observed 1,3-D concentrations, and obviates the need for adjustments of the MHs in the processed weather file, as was required with SOFEA2. Improvements are a result of the refined algorithms in AERMOD for prediction of MH during calm conditions, based on updated understanding of Planetary Boundary Layer (BPL) dynamics, the use of the Monin-Obukhov length scale (L), and the calculation of a convective and mechanical MH, the latter which is used only for stable conditions (when $L > 0$). **Figure 10** shows SOFEA3 results compared to the 2010–2011 California (Merced) monitoring study, while **Figure 11** represents the same simulation predictions at a much finer resolution (11,664 receptors per township) such that contour plots for air concentration can be obtained.

SOFEA3 was rewritten using C++ and Qt to replace VBA, and now this latest version is denoted SOFEA4. SOFEA4 was used to simulate 1,3-dichloropropene (1,3-D) concentrations in ambient air in three agricultural areas in the USA where soil fumigation is a critical aspect of pest management and crop production. The regions explored by van Wesenbeeck et al. [11] are the Pacific Northwest, the mid-Atlantic coast, and the Southeast coastal plain, **Figure 12**. The Merced, CA monitoring study served to represent the southwest region of the U.S. SOFEA4 is the latest modeling tool of SOFEA that has been modified to use AERMOD, the EPA's recommended regulatory air dispersion model, to predict short-, medium- and long-term pesticide concentrations in air resulting

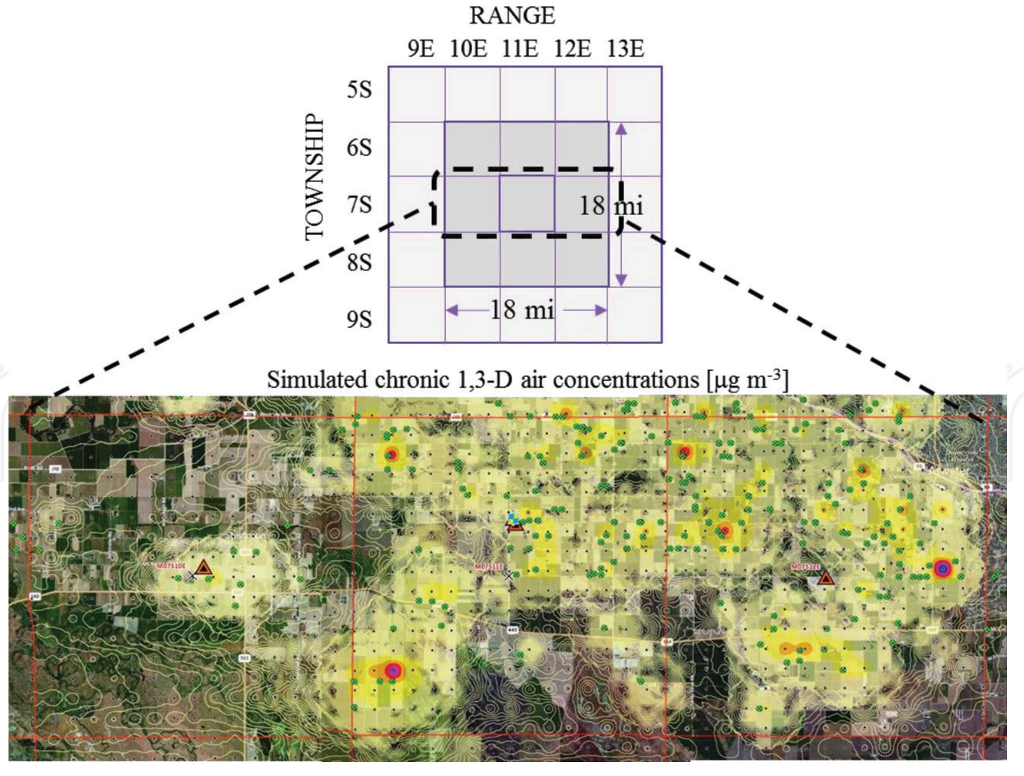

Figure 11.
Example of simulated SOFEA3 (i.e., AERMOD used) chronic air concentration predictions over a three-township area of Merced CA where field location, application rate and date are known and air concentrations at a central location in each township was monitored over a 14-month period.

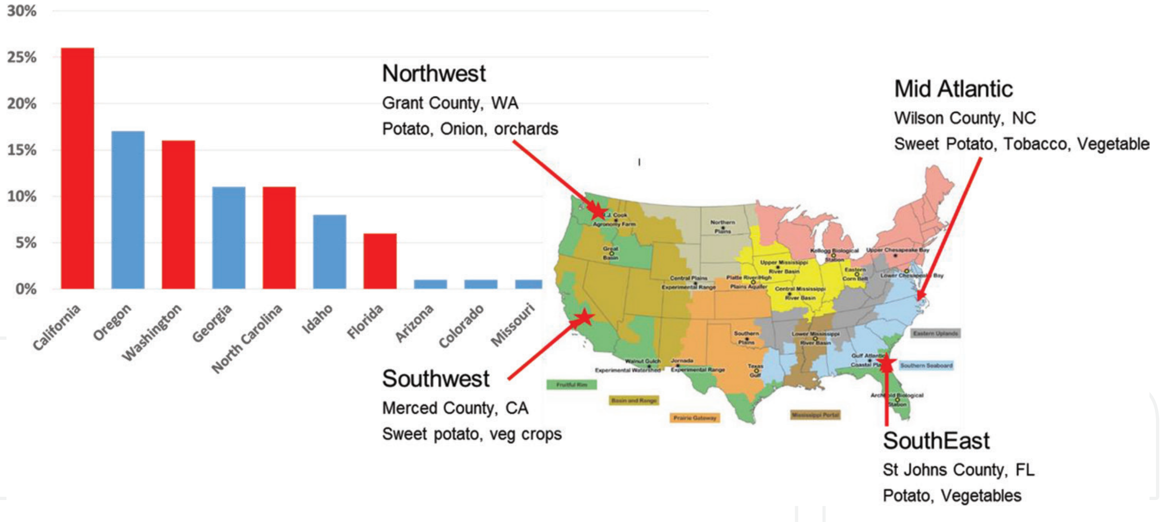

Figure 12.
Geographic region for SOFEA4 simulations for high 1,3-D use areas of the United States [11]. Results for the Southwest are found elsewhere [21].

from representative agronomic practices and large air sheds. SOFEA3/4 with AERMOD improved model predictions over what SOFEA2 with ISCST3 produced, due to the more realistic mixing height (MH) calculated by the weather pre-processor that subsequently resulted in higher concentrations during calm (stable air) periods. Advantages of using SOFEA4 to model fumigant concentrations over monitoring approaches for fumigant concentrations in air, include the ability to predict concentrations at a much greater temporal frequency (and spatial locations) than could be accomplished by monitoring alone. 1,3-D application data obtained from growers along with local weather data was used to parameterize SOFEA4, and it was found the Human Equivalent Concentrations

(HECs) for acute, short-term, subchronic, and chronic exposure for 1,3-D were not exceeded for four study areas with intense 1,3-D use [11, 21].

4. Discussion

The SOil Fumigant Exposure Assessment (SOFEA) model was originally developed in 2005 [3], expanded/refined multiple times over the last 14 years to explore volatile pesticide exposure and bystander risk (most recent version being SOFEA4 where C++ replaces VBA, and now with AERMOD the principle model used). Multiple publications using SOFEA have been documented since SOFEA was first developed [3, 11, 14, 17, 21, 31], with the most recent manuscript on SOFEA4 use for high use regions in the United States currently undergoing a journal review process for publication [11]. SOFEA assembles sources (agricultural fields), various management practices, source strengths (pesticide flux rates), weather data from the region of interest, and executes an air dispersion model [AERMOD, ISCST3 (historical)] to simulate pesticide concentrations at user defined receptors whose concentration predictions can be used in exposure and risk assessment procedures. This book chapter describes the historical development of SOFEA up to the latest version (SOFEA4) including all attributes that have been described over the years. SOFEA now uses AERMOD, the officially sanctioned USEPA regulatory air dispersion model, in lieu of ISCST3 for air dispersion simulations. Recent SOFEA simulation results were compared to the ambient air monitoring data collected in an intensive 1,3-D fumigation field trial in Merced, CA specifically designed to validate SOFEA against monitoring information. SOFEA4 (using AERMOD) was shown to improve the prediction of high concentrations (and thus the annual average concentration) compared to SOFEA2 (using ISCST3) and earlier versions of SOFEA. Better comparison against field observations using SOFEA4 was attributed to the improved characterization of the Planetary Boundary Layer (PBL) during calm period conditions (low wind), and more realistic Mixing Height (MH) calculations that are employed by AERMOD compared to ISCST3 [11, 21].

The validated SOFEA4 model was further used to simulate 1,3-D air concentrations in three study areas across the US having significant 1,3-D use [11]. These areas include Quincy, WA (representing the Pacific Northwest), Wilson, NC (representing the Atlantic coastal plain), and St. John's, FL (representing GA/FL). Including Merced, CA results [21], these four agricultural regions represent land areas that account for ~95% of the 1,3-D sold in the USA, **Figure 12**. The most recent publication (under review) of SOFEA deals with actual field locations and 1,3-D application parameters used for two annual product use cycles (2015–2016, and 2016–2017) in multiple high use regions in the United States (as documented by local growers in each study area [11]).

SOFEA has exceptional attributes and functionality compared to other similar modeling tools for addressing the exposure and risk from the use of volatile (or semi-volatile) pesticides. In a collaborative effort between Corteva Agriscience and Exponent, Inc. (an Engineering and Scientific Consulting company), SOFEA3 was upgraded to modern software engineering standards (renamed SOFEA4), and a new graphical interface was developed with C++ and Qt to provide users an Integrated Development Environment-like (IDE) experience in creating new simulation projects. Summary statistics, moving averages and quantiles can be calculated efficiently over millions of data points, comprising hourly concentrations over several years and thousands of receptors. A beta version of SOFEA4 is currently being tested and evaluated for release, and will be made publicly available online via Exponent, Inc. in mid-2019 for use with other volatile or semi-volatile chemicals for large-scale environmental and risk assessment procedures. Parties interested in using SOFEA4 can contact Exponent Inc. directly to obtain both the user's guide and the latest version of the model.

5. Conclusions

SOFEA is used to predict soil fumigant and semi-volatile pesticide air concentrations under actual or projected use. SOFEA, first released in 2005 [3], has over a decade of development and refinement and is a comprehensive numerical tool that has been validated against many field trials and monitoring studies using 1,3-dichloropropene as summarized in this manuscript. Both the timing and magnitudes for more than 450 1,3-D treated fields in a 5 × 5 township domain were followed over a 1.5-year period [11, 21] in a field trial in CA specifically designed for SOFEA validation.

Examples of a soil physics model, CHAIN_2D, for flux predictions has also been used for source strength predictions in SOFEA, in addition to using field observations that are scaled by depth of soil incorporation and the time of the year when the application is made. Comparison of SOFEA predictions against other field studies has been good. SOFEA is a powerful tool to simulate air concentrations for regional agronomic conditions when multiple fields are simulated under typical agronomic conditions. SOFEA is especially useful for regulatory risk managers and product stewards who often are required to make decisions when only limited or incomplete data is available.

Chemical exposure information generated by SOFEA can be and has been used in a formalized risk assessment where risk to human populations is addressed. Understanding how various agronomic BMPs affect acute, sub chronic, and chronic exposure is an essential requirement for proper stewardship of volatile and semi-volatile pesticides, and SOFEA can be used for validation purposes or when limited, or no experimental evidence is available. SOFEA4 is being released to the public domain later in 2019 such that any user wanting to simulate air concentrations for volatile and semi-volatile chemicals in large and diverse airsheds can be incorporated, in support of (or in lieu of) monitoring trials.

List of abbreviations

1,3-D	1,3-dichloropropene
AERMOD	USEPA Regulatory Model (Gaussian plume)
ArcGIS	GIS for geographic information by ESRI
ArcView	Entry level of ArcGIS Desktop, a GIS software by ESRI
BMP	best management practice
CDPR	California Department of Pesticide Regulations
CHAIN_2D	computer program for 2-D variability saturated water flow, heat, solute transport
C++	general purpose program language
Crystal Ball™	software add-on for MS Excel developed by Decisioneering, Inc.
ESRI	Environmental Systems Research Institute
Exponent Inc.	US-based consulting company
GIS	geographic information system
Hydrus	water, heat, solute transport in saturated porous media (modeling software)
ISCST3	USEPA Industrial Source Complex Model (Gaussian plume)
PDF	probability density function

PLSS	public land survey system
PRZM3	USEPA Pesticide Root Zone Model
Qt	cross-platform framework for developing application software with a graphical user interface
SAP	USEPA Scientific Advisory Panel
SOFEA	SOil Fumigant Exposure Assessment system
TIF	totally impermeable film
USEPA	United States Environmental Protection Agency
VBA	visual basic for applications

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