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Modeling 1,3-D Concentrations in Ambient Air in High Use Airsheds of the United States

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ABSTRACT: Soil fumigants, such as 1,3-dichloropropene (1,3-D), are used on a variety of different crops in high use areas in the United States, including the Pacific Northwest, the mid-Atlantic coast, and the Southeast coastal plains. Contaminant concentrations in air are often required for environmental exposure and human risk assessment. The *SO*il *F*umigant *E*xposure *A*ssessment (SOFEA) model, originally developed to explore volatile pesticide exposure and bystander risk, has recently been upgraded using AERMOD, the US Environmental Protection Agency's (EPA) recommended regulatory air dispersion model to predict short-, medium-, and long-term pesticide concentrations in air resulting from representative agronomic practices in large airsheds. Modeling air concentrations has several advantages over monitoring such as the ability to predict concentrations at multiple locations and airsheds at a much greater temporal frequency than could be practically accomplished through monitoring alone. The agricultural modeling tool presented herein was parameterized using 1,3-D application data (mass, date, and depth applied, location, etc) obtained from growers in each study area, and local weather data and hourly concentrations of 1,3-D in ambient air were simulated for large airsheds. The human equivalent concentrations (HECs) for acute, short-term, sub-chronic, and chronic exposure of 1,3-D were not exceeded in any of the study areas investigated. These simulated 1,3-D concentrations are used to assess human exposure and risk, which considers human-life-stage-specific exposure factors, including residential mobility, time-activity patterns, and age-specific inhalation rates and body weights.

KEYWORDS: Air dispersion model, 1,3-dichloropropene, SOFEA, ambient air

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Introduction

Gaussian plume air dispersion models such as Industrial Source Complex Short Term (ISCST3),[1] American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD)[2], and California Puff (CALPUFF)[3] have been used extensively to simulate concentrations of volatile agricultural products in air for estimating bystander exposure.[4-6] The ISCST3 model has been used to simulate probability distribution functions (PDFs) of 1,3-D concentrations in air within townships in California to estimate acute and chronic bystander exposure.[6,7,8] Air dispersion model inputs include a flux profile ($M/L^2/T$) for either shank or drip applications of 1,3-D (obtained from field study observations), and local weather for the airshed being modeled.

The ISCST3 model has been widely used in regulatory air dispersion modeling of area point source contaminants such as farm fields. The PERFUM model[7] and FEMS model[8] are both graphical user interface (GUI) tools to parameterize ISCST3 model inputs and display model outputs required to conduct probabilistic risk assessments and establish safe buffer zones. The ISCST3 model is also used in the *SO*il *F*umigant *E*xposure *A*ssessment (SOFEA) modeling system to simulate PDFs of 1,3-D concentrations in air within townships in California to estimate both acute and chronic bystander exposure.[4,6]

Due to the US Environmental Protection Agency's (EPA) adoption of AERMOD as the official regulatory air dispersion model, the EPA's Office of Pesticide Programs (OPP) requested that SOFEA be upgraded to include AERMOD, so that it could be used to model 1,3-D concentrations in ambient air for the purpose of human exposure and risk assessment, as part of the registration review of 1,3-D. SOFEA4 was also modified to include a GUI that replaces the Excel Visual Basic for Applications (VBA)-based user interface in SOFEA2. The development and functionality of SOFEA4 is described in detail by Cryer and van Wesenbeeck.[9]

Zou et al.[10] studied the sensitivity of AERMOD-simulated SO_2 concentrations to variations in dispersion coefficients, meteorological data, and terrain data at 3 locations in Texas, and found that while variations in meteorology had the most significant effect on simulated concentrations, the dispersion coefficients and terrain data had very limited influence. Long[11] examined the sensitivity of AERMOD-simulated concentrations of SO_2 to variations in 8 model input parameters, including albedo, Bowen ratio, surface roughness, cloud cover, solar radiation, and height at which ambient temperature is measured using meteorological data from the San Francisco Bay Area. Long found that AERMOD-modeled SO_2 concentrations were the most sensitive to variations in surface roughness

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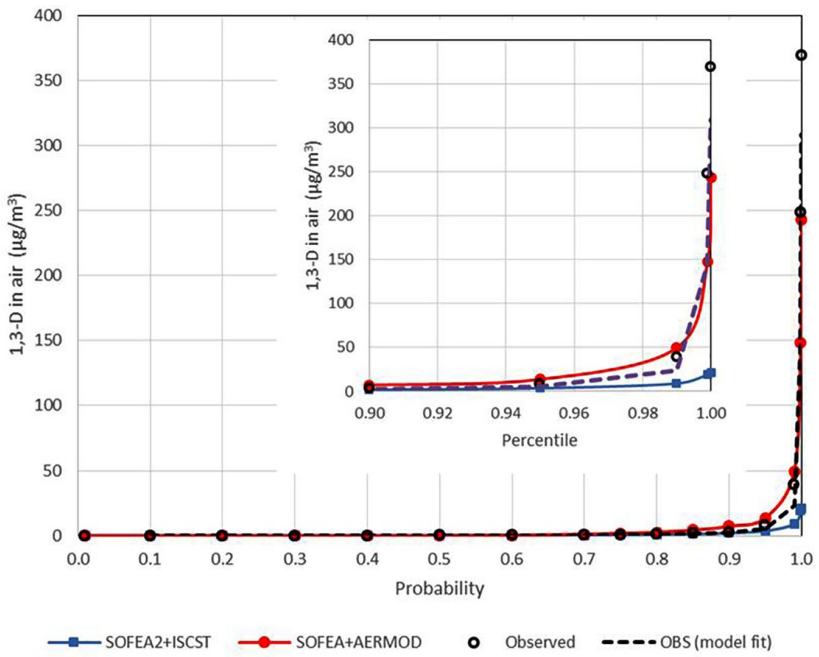


Figure 1. SOFEA2 (with ISCST3) and SOFEA4 (with AERMOD) modeled 72-hour 1,3-D concentrations in air for the 9-receptor grid in Merced County, CA. SOFEA indicates *SO*il *F*umigant *E*xposure *A*ssessment

(–67% to +104%), albedo (–33% to +6%), and solar radiation (–53% to +50%), when those parameters were varied from 0.25× to 4× the base case. Faulkner et al[12] compared the sensitivity of AERMOD and ISCST simulations of particulate matter (PM) concentrations from a ground-level area source with input parameter selection. That study showed that concentrations predicted using ISCST3 were sensitive to changes in wind speed, temperature, solar radiation, mixing height (MH), and surface roughness, while AERMOD was sensitive to changes in surface roughness, albedo, wind speed, temperature, and cloud cover.

The objectives of this study were to compare SOFEA version 4 (with AERMOD) predictions with SOFEA version 2 (with ISCST3) predictions of 1,3-D concentrations in ambient air measured in the air monitoring study conducted in Merced County, CA.[13] The second objective is to use SOFEA4 to simulate output PDFs of 1,3-D in ambient air in 3 additional high 1,3-D use areas of the United States representing the Pacific Northwest (WA/OR), the mid-Atlantic states (NC/SC/VA), and the Southeast USA (GA/FL), for the purpose of assessing human exposure and risk to 1,3-D in ambient air. As monitoring data only represent potential exposure at the location and time period that sampling occurs, and given the logistical issues associated with obtaining many representative ambient air samples, the potential exposure to 1,3-D in ambient air is best characterized with the use of a validated model such as SOFEA. Detailed 1,3-D product use data and local weather were used to parameterize SOFEA for each of the WA, NC, and FL study areas for 2 complete calendar years. SOFEA4 (v.4.2.1) was used to simulate 24-hour, 28-day, 90-day, and annual average concentrations of 1,3-D in ambient air for assessing human exposure and risk.

Incorporation of AERMOD into SOFEA

The SOFEA was upgraded from an Excel-based interface to a GUI, programmed with modern software engineering standards (by Exponent, INC, Alexandria, VA) and renamed to SOFEA4. SOFEA4 (v.4.2.1) with AERMOD (v.18081) was used to perform all simulations of 1,3-D for WA, NC, and FL. The differences and similarities between SOFEA2 and SOFEA4 are further discussed in this article.

SOFEA2 and SOFEA4 comparison with Merced County monitoring data

The SOFEA2-simulated 1,3-D concentrations in air were compared with over 1300 ambient air samples, collected continuously for a 14½-month period at 9 receptor locations in a high 1,3-D use area in Merced County, CA. 1,3-D (482 605 kg) were applied in the study area during the monitoring period.[13] Detailed 1,3-D product use information (date, mass, and depth applied; treated area; field location) for all 478 applications made during the study period were collected and used to parameterize SOFEA2. In summary, SOFEA2 under-predicted the annual average 1,3-D concentration by 4.7-fold, primarily due to the under estimation of the daily MH by the PCRAMMET weather preprocessor required by ISCST3.[13] An over-predicted MH will result in an under-prediction in air concentration, because the MH dictates the volume of air that an airborne contaminant can be diluted into (eg, MH and concentration are inversely correlated). The over-prediction of the MH by PCRAMMET is well documented and is addressed in AERMOD via a formulation of the processes that use hourly data to more accurately predict diurnal MH changes.[14] The effect of the MH over-prediction can be seen

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Table 1. Average concentration and standard deviation for each receptor over 14.5-month monitoring period in Merced County, CA, showing measured and SOFEA2- and SOFEA4-simulated results.

RECEPTOR #	MEASURED		SOFEA2 (ISCST3)		SOFEA4 (AERMOD)	
	MEAN	SD	MEAN	SD	MEAN	SD
1	0.88	1.97	0.4	0.77	1.33	3.23
2	4.85	24.8	0.79	1.56	2.82	6.30
3	0.79	1.69	0.54	0.87	2.55	5.20
4	1.28	2.79	0.6	1.61	5.12	25.33
5	8.74	38.04	1.16	2.54	5.38	13.36
6	3.55	8.92	1.34	2.33	6.15	3.55
7	0.44	0.97	0.3	0.53	0.85	2.32
8	1.3	3.27	0.66	1.23	1.72	3.54
9	0.6	0.93	0.61	0.87	1.86	3.04
Global mean	2.49	9.26	0.71	1.37	3.09	7.32

Abbreviations: SD, standard deviation; SOFEA, *SO*il *F*umigant *E*xposure *A*ssessment.

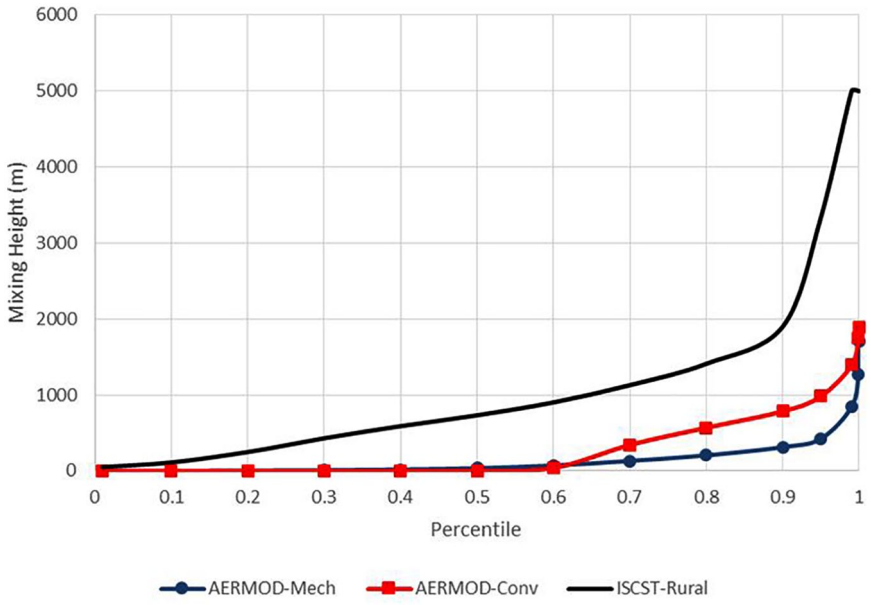


Figure 2. Comparison of mixing height calculated for SOFEA2 (ISCST-Rural) and SOFEA4 (AERMOD-Conv/Mech). SOFEA indicates *SO*il *F*umigant *E*xposure *A*ssessment.

in Figure 1, which shows that SOFEA2 underestimates 1,3-D concentrations at the higher (>95th) percentiles, whereas SOFEA4-simulated concentrations of 1,3-D are visually closer to the measured distribution.

Table 1 shows that the SOFEA4-predicted 1,3-D concentrations result in the measured global mean annual average concentration being overestimated by approximately 1.2-fold (eg, 3.09/2.49), without adjusting the MHs in the preprocessed weather data as was required for SOFEA2. Table 1 also shows that the global mean standard deviation of the SOFEA4 simulations matches the measured standard deviation more closely with a 1.3-fold under-prediction compared with a 6.6-fold under-prediction by SOFEA2, suggesting that SOFEA4 more closely represents the variability in monitored concentrations of 1,3-D in air.

The MHs calculated by the PCRAMMET and AERMET weather preprocessors are shown in Figure 2 and highlight the difference in MH predictions. This is a result of the refined algorithms in AERMOD for predicting atmospheric MH during calm conditions, based on understanding of Planetary Boundary Layer (PBL) 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 $L > 0$).

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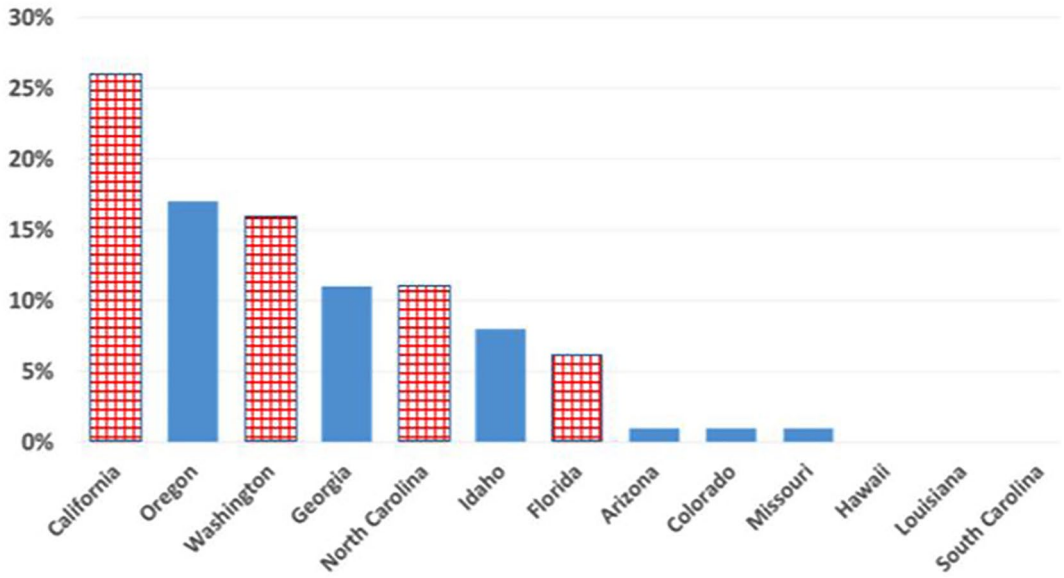


Figure 3. Relative 1,3-D use by state. Hash-marked bars indicate regions modeled in this study.

Future versions of AERMOD will also have plume meander from area sources built into the model[15] which could further improve SOFEA model predictions in agricultural scenarios.

Methods

Model

The SOFEA4 GUI manages inputs and outputs for the AERMOD model and enables large airsheds (100-km scale) to be modeled. SOFEA4 can be used in "prospective" mode or "retrospective" mode. The prospective mode allows the user to specify actual or hypothetical PDFs for product use via parameters, including field size, application rate, and total mass of fumigant applied, and to simulate short-, medium-, and long-term concentrations of 1,3-D in ambient air for periods as short as a few hours to as long as several decades. The receptor density and specific locations where 1,3-D concentrations in ambient air are simulated can also be varied, one of the major advantages of modeling over monitoring. Modeling corroborates the spatial and temporal variability associated with 1,3-D concentrations in the California Department of Pesticide Regulation (CDPR) Air Monitoring Network (AMN) data[16] and underscores the importance of using a model for estimating lifetime exposure. The uncertainties in estimating exposure associated with spatially and temporally sporadic air measurements, such as those collected in the AMN program, is easily overcome with the use of a validated air dispersion model that considers spatial and temporal variability in product use patterns as well as weather variability.

For this modeling study, SOFEA was used in "retrospective mode" because the exact field locations and 1,3-D application parameters were known. The model was then run for 2 consecutive 1-year simulations using equally spaced receptors (500 m) in the study area, where hourly 1,3-D concentrations in ambient air were predicted. The full distribution of annual average, as well as 24-hour, 28-day, and 90-day moving average (MA) 1,3-D air concentrations that could be used for acute, short-term, sub-chronic, and chronic human exposure and risk assessment for 1,3-D are summarized.

Study regions

The Southwest (SW), Pacific Northwest, (PNW) mid-Atlantic States, and GA/FL Coastal Plain were selected to represent the highest 1,3-D use areas in the United States. National sales data show that these areas account for approximately 95% of the mass of 1,3-D applied annually in the United States (Figure 3).

Approximately 25% of the 1,3-D sold in the United States is applied annually in CA (Figure 3). Crops grown in the SW United States that typically require fumigation include tree and vine crops (almonds, walnuts, wine, and table grapes), strawberries, sweet potatoes, and vegetables (peppers, tomatoes). Monitoring and modeling data from the Merced monitoring study are sufficient to characterize exposure and risk to 1,3-D in the SW, and the reader is referred elsewhere for results.[13]

Figure 3 shows that approximately 15% of 1,3-D sold in the United States is applied annually in WA. Primary crops in the WA area are potatoes and onions, with some tree and vine and vegetable crop uses. A study area spanning approximately 4900 km^2, to the southeast of the town of Quincy, WA (Figure 4), contains a significant amount of agricultural land planted in potato and onion that is regularly fumigated with 1,3-D, and is considered representative of the PNW region.

Figure 3 shows that approximately 10% of 1,3-D sold in the United States is applied annually in North Carolina, primarily to annual crops such as tobacco and market vegetables, including sweet potatoes. A study area spanning approximately

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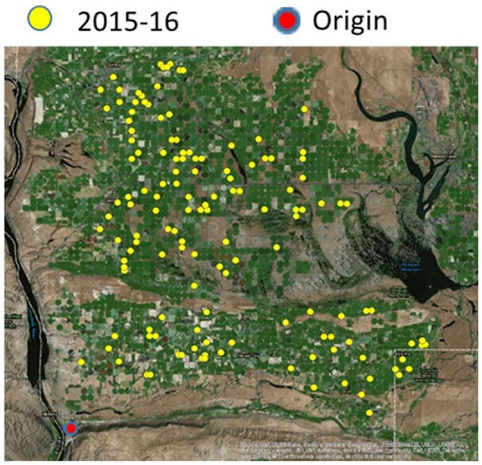


Figure 4. Google Earth image of the WA study area with origin and treated field locations for 2015-2016.

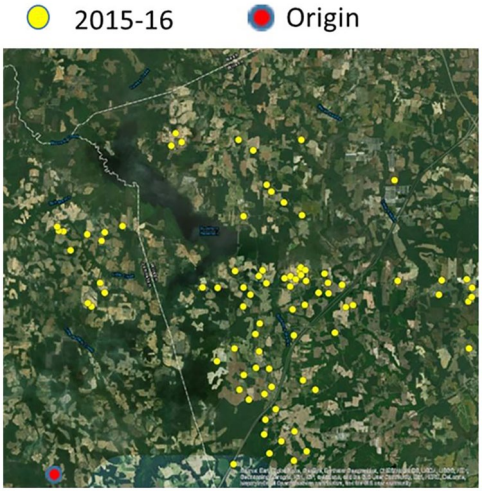


Figure 5. Google Earth image of the NC study area with origin and treated field locations for 2015-2016.

415 km^2 in Wilson County, NC, that contains a significant amount of fumigated land and 1,3-D use was selected as representative of the mid-Atlantic states (Figure 5).

Figure 3 shows that approximately 20% of 1,3-D sold in the United States is applied annually in Georgia and Florida, primarily to soil being prepared for annual crops such as potatoes, peppers, and tomatoes, and with some tree and vine use. A study area spanning approximately 700 km^2 of intensively cultivated land in northern FL, bounded by the town of St. Johns to the north and Palatka to the south, contains a significant amount of fumigated land and was selected for modeling as an area typical of agricultural production in GA/FL, where 1,3-D is heavily used (Figure 6).

Documentation of 1,3-D use and application parameters

The mass of 1,3-D used and the conditions under which it was applied (eg, shank vs drip, application depth, time of year) are

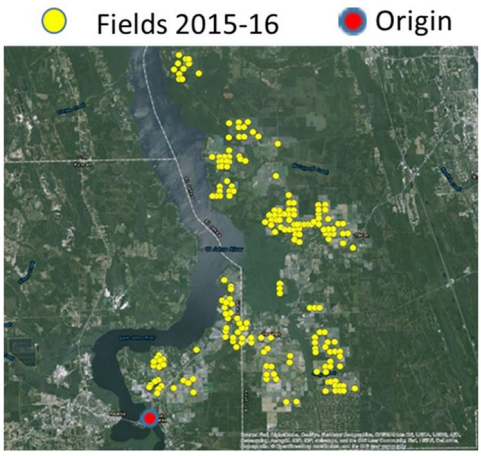


Figure 6. Google Earth image of the FL study area with origin and treated field locations in 2015-2016.

critical inputs for determining the source strength and concomitant concentrations of 1,3-D in ambient air. The use of products containing 1,3-D (eg, Telone II, Telone EC, and Telone C-17) is used in different ways depending on the local market dynamics and label requirements. In California, all pesticide use is reported to the state and documented in the Pesticide Use Reporting (PUR) database, making it very straightforward to obtain accurate, high-quality information necessary to parameterize the model. Other states, however, do not have mandatory PUR systems, and therefore other methods of obtaining those data were used as described below.

Product use information in WA was obtained from growers directly via an incentive program that rewards growers for product stewardship activities such as application timing of 1,3-D to improve product efficacy against certain pests and to help manage the supply of 1,3-D at critical times of the year. Growers were required to submit a "Fumigation Report" to the Corteva Telone specialist that documents critical application parameters, including type of 1,3-D product applied, application date/time, application depth, mass of 1,3-D applied, and area of the treated field, before receiving an incentive. This program has operated successfully for several years and has proven extremely useful for obtaining the necessary 1,3-D product use information needed for this modeling study. Year 1 of the present ambient air modeling study in WA started on August 1, 2015, and ended on July 31, 2016, while Year 2 started on August 1, 2016, and continued until July 31, 2017.

Product use information for the North Carolina and Florida areas was obtained via a special program specifically designed to engage growers in high use areas to provide the necessary 1,3-D application information required for modeling. Growers were given a booklet unique to their study area that included large-scale maps of their study area and detailed instructions, so growers could locate and identify the fields treated with 1,3-D. The fields were identified by a grower code that linked the 1,3-D application information to the field marked on the map. At the end of each year of the study, the grower application

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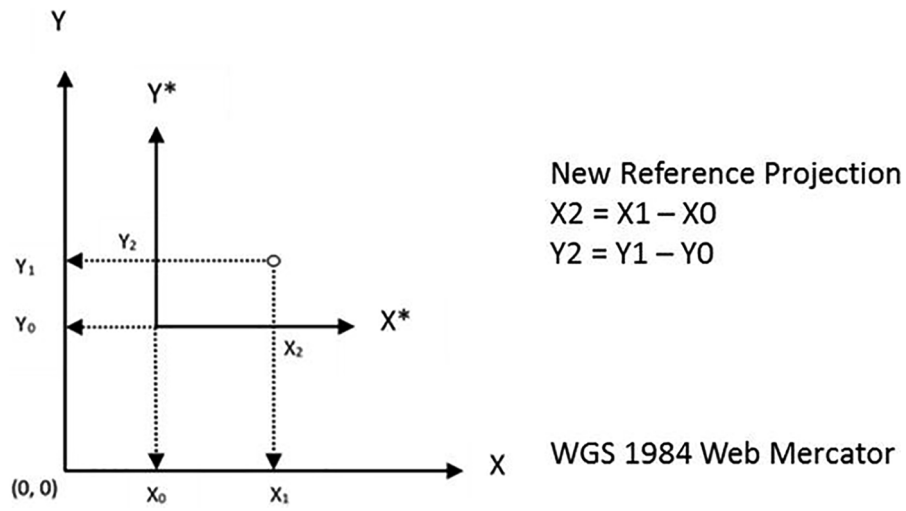


Figure 7. Geo-referencing field locations from the Web Mercator grid to the SOFEA coordinate system for the WA study area. SOFEA indicates *SO*il *F*umigant *E*xposure *A*ssessment.

information was sent to a third-party consultant (Paragon Research Inc, Indianapolis, Indiana) where the data were quality checked (QC'd) and collated for use in SOFEA4. Each field was given a unique identification code to ensure confidentiality of grower information.

Geo-referencing and exporting grower data into SOFEA4

The treated field locations provided by the growers on Google Maps, for each of the respective study areas, were geo-referenced to be consistent with the coordinate system used by SOFEA4. The treated field information was directly transferred to an ArcMap 10.3 (ESRI 1999-2014) Project, using ESRI, HERE, DeLorme, MapmyIndia, OpenStreetMap contributors, and the GIS user community as a satellite imagery basemap. The WGS 1984 Web Mercator (auxiliary sphere) was used as a Projected Coordinate System. Web Mercator is a slight variant of the Mercator projection that is used primarily in Web-based mapping programs; however, it uses the same formulas as the standard Mercator projection, for small-scale maps. The coordinate values (units of measure) are in meters from the origin point of the projection. To accommodate the SOFEA model, field locations were re-referenced with the origin (X_0, Y_0) located in the SW corner of each study area as shown in Figures 4 to 6. To get the new reference values (X_2, Y_2) and considering that the measured units are in meters, we subtracted both X_0 and Y_0 coordinates from the origin (in the WGS 1984 Web Mercator) to each field point (X_1, Y_1) as shown in Figure 7. Figures 4, 5, and 6 show the SW corner of fields treated with 1,3-D in WA, NC, and FL, respectively, in the 2015/2016 use season, as yellow dots.

Product use information for each treated field was entered into an attribute table and linked with each field location. All treated fields were assumed to be square, and the location was designated by the *x* and *y* coordinates of the SW corner of the field. The attribute table contained the following information: Site ID, Application Date, Applied Area, Application Rate, Application Depth, Crop Type, and *X* and *Y* Coordinates of the SW corner of the treated field. To export the field and application information for use by software like Google Earth, the "Layer to KML" tool was used to convert a feature (or raster layer) into a KML file containing a translation of ESRI geometries and symbology. This file was compressed using ZIP compression and given a .kmz extension so that it could be read by any KML client, including ArcGIS Explorer, ArcGlobe, and Google Earth, and accessed for modeling.

1,3-D flux files

Flux files characterize the rate of 1,3-D emission ($g/m^2/h$) from the soil as a function of time from field volatility studies. A field volatility study conducted by Knuteson and Petty[17] near Salinas, CA, showed 25% emission of 1,3-D and was used to parameterize the flux from shank injection applications (Figure 8), whereas a study conducted near Valdosta, GA, by van Wesenbeeck et al,[18] using drip applied 1,3-D showing 29% emission was used to parameterize the flux from drip applications (Figure 9).

The use of these flux profiles forms a conservative basis for the flux because improved application techniques, new formulations, and flux emission mitigation technologies such as low permeability agricultural films result in significantly lower emissions of 1,3-D and other fumigants.[19,20] For example, a significant portion of the 1,3-D applied by coastal strawberry producers is applied as PicClor60 (nominally 40% 1,3-D and 60% chloropicrin) and has "Totally Impermeable Film" (TIF) placed over the field after the 1,3-D is broadcast shank-applied.

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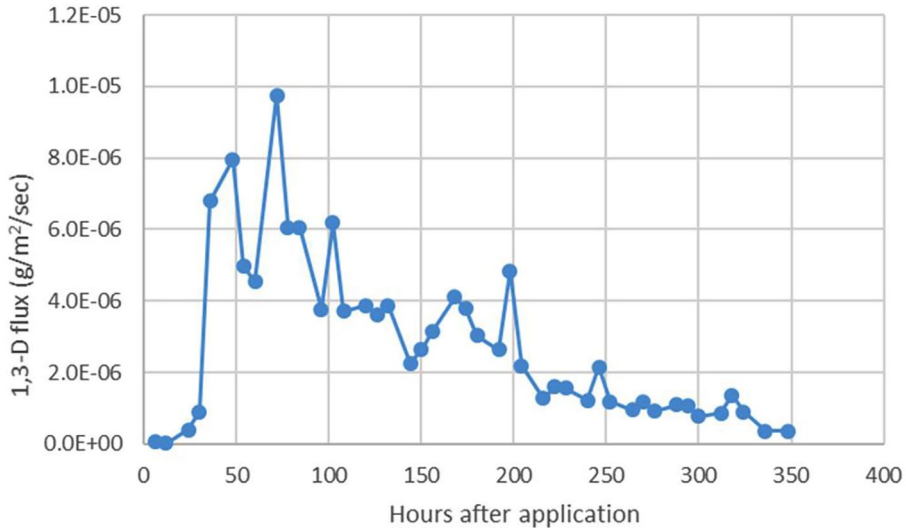


Figure 8. 1,3-D flux from a volatility study with a shank application near Salinas, CA.[17]

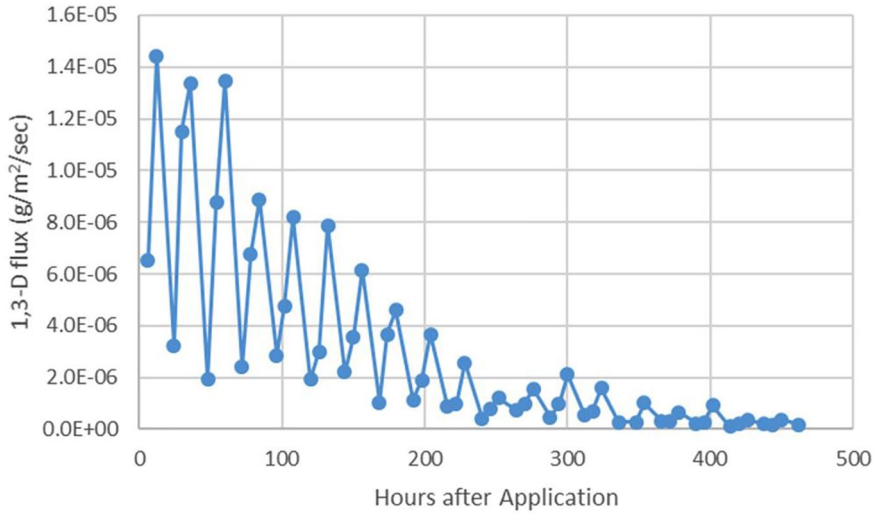


Figure 9. 1,3-D flux from a volatility study with a drip application near Valdosta, GA.[18]

This has been shown in field studies to reduce total 1,3-D emissions by 43%, and the peak emission reduced by 78% if the TIF tarp is left in place for 10 days.[21] As new application technologies and flux mitigation technologies enter the market, emissions will be further reduced, and therefore the use of the flux profiles from Knuteson and Petty[17] and Van Wesenbeeck et al[18] conservatively estimate ambient air concentrations.

Weather files

Weather data required by SOFEA (air temperature, wind speed, and direction) were obtained from a weather station near the study site in each region. The weather files were processed using the AERMET preprocessor (v. 15181). The AERMET surface file with PBL parameters and profile weather files for each study area are shown in the table below.

STUDY AREA	WASHINGTON	NORTH CAROLINA	FLORIDA
Met station	Ephrata	Raleigh	Jacksonville
Latitude/Longitude	47.308N, 119.515W	35.892N, 78.782W	30.459N, 81.694W
Upper Air file ID	04106	13723	13723
Surface file ID	727900	13722	13880
Surface file (*.SFC)	Ephrata.SFC	Raleigh.SFC	Jackson.SFC
Profile file (*.PFL)	Ephrata.PFL	Raleigh.PFL	Jackson.PFL

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Receptors

A uniform receptor grid was specified in SOFEA4 for each of the study regions as shown below.

REGION	DIMENSIONS OF SIMULATION DOMAIN	RECEPTOR SPACING (M)	TOTAL # RECEPTORS
WA	70 km × 70 km	500	19881
NC	18 km × 20 km	500	1656
FL	20 km × 35 km	500	2911

The SOFEA simulates hourly concentrations at each receptor which are then averaged (arithmetic mean) into daily 1,3-D concentrations that are used to calculate the annual average and other MA concentrations required for exposure and risk assessment.

Annual average, 24-hour, 28-day, and 90-day MA calculation

The annual average concentration was calculated by averaging the hourly concentrations for an entire year. The 24-hour MA was calculated by averaging sequential series of 24-hourly 1,3-D concentrations at each receptor, for the entire year. The 28-day MA was calculated by averaging 28 sequential days of hourly values (ie, 672 hourly concentrations). The 90-day MA was calculated by averaging 90 sequential days of hourly values (ie, 2160 hourly concentrations).

Results

Product use

The number of 1,3-D applications, the total land area receiving 1,3-D, and the total mass of 1,3-D applied in the WA, NC, and FL study areas for the 2015/2016 and the 2016/2017 growing seasons are summarized in Table 2. The mass of 1,3-D applied, land area treated, date and time applied, and the field location details obtained from the growers for each treated field were used to parameterize SOFEA4 for each study area.

Washington. The average treated field area and 1,3-D application rate were approximately 44 and 45 ha and approximately 184 and 178 kg ha^{-1}, respectively, for the 2015/2016 and 2016/2017 use seasons. The 1,3-D use by month during the 2015/2016 and 2016/2017 study seasons is shown in Figure 10 and is consistent with historical use patterns in Washington, with major use in the fall (October/November) and the spring (March), and no use between April and July.

North Carolina. The average treated field area was approximately 9.6 and 9.2 ha, and the average 1,3-D application rate was approximately 90 and 95 kg ha^{-1}, for the 2015/2016 and 2016/2017 use seasons, respectively. This is consistent with the smaller field sizes and application rates typical of tobacco and market vegetable crops. The 1,3-D use by month during both study years is shown in Figure 11 and is consistent with historical use patterns in NC, with extensive use of 1,3-D for fumigating tobacco fields in March and April.

Florida. The average treated field area was approximately 24.5 and 21.4 ha, and the average 1,3-D application rate was approximately 64 and 58 kg ha^{-1}, for the 2015/2016 and 2016/2017 use seasons, respectively. The 1,3-D use by month during both study years is shown in Figure 12 and indicates that most of the 1,3-D is applied in December, which is consistent with the extensive potato production in that area.

SOFEA simulation results

The probability distributions of 24-hour, 28-day, 90-day MA, and annual average 1,3-D concentrations for the WA, NC, and FL study areas, for 2015/2016 and 2016/2017, are summarized in Tables 3 to 5, respectively. All simulations spanned 1 year (June 1, 2015, through May 31, 2016 and June 1, 2016, through May 31, 2017), resulting in 2 simulations for each region.

Washington. The arithmetic means of the annual average concentration simulated by SOFEA at each receptor location (ie, the global mean) were 0.086 and 0.063 µg/m^3 for 2015/2016 and 2016/2017, respectively, which corresponds approximately to the 70th percentile of the PDF of annual average concentrations (Table 3). The maximum 24-hour concentration was 17.7 and 13.3 µg/m^3 for 2015/2016 and 2016/2017, respectively.

North Carolina. The arithmetic means of the annual average concentrations simulated by SOFEA at each receptor location in NC were 1.39 and 1.71 µg/m^3 for 2015/2016 and 2016/2017, respectively, which corresponds approximately to the 70th percentile of the PDF of annual average concentrations (Table 4). The maximum 24-hour concentration was 277 and 473 µg/m^3 for 2015/2016 and 2016/2017, respectively.

Florida. The arithmetic means of the annual average concentrations simulated by SOFEA at each receptor location in FL were 29.1 and 25.6 µg/m^3 for 2015/2016 and 2016/2017, respectively, which is close to the 70th percentile of the PDF of annual average concentrations (Table 5). The maximum 24-hour concentration was 2474 and 1710 µg/m^3 for 2015/2016 and 2016/2017, respectively. The higher 24-hour concentrations in the FL and NC regions compared with the WA region are likely due to the greater density of farms in those study areas, which increases the probability that a receptor is located in close proximity to a treated field and thus potentially higher 1,3-D concentrations. The higher concentrations could also be due to meteorological effects such as stable air or calm periods occurring at those sites.

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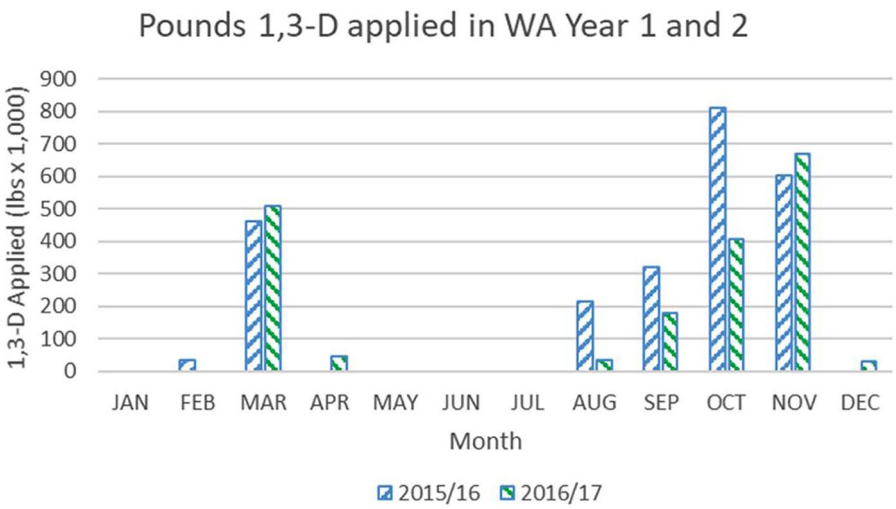


Figure 10. Pounds 1,3-D applied by month in the WA study area in 2015/2016 and 2016/2017 use seasons.

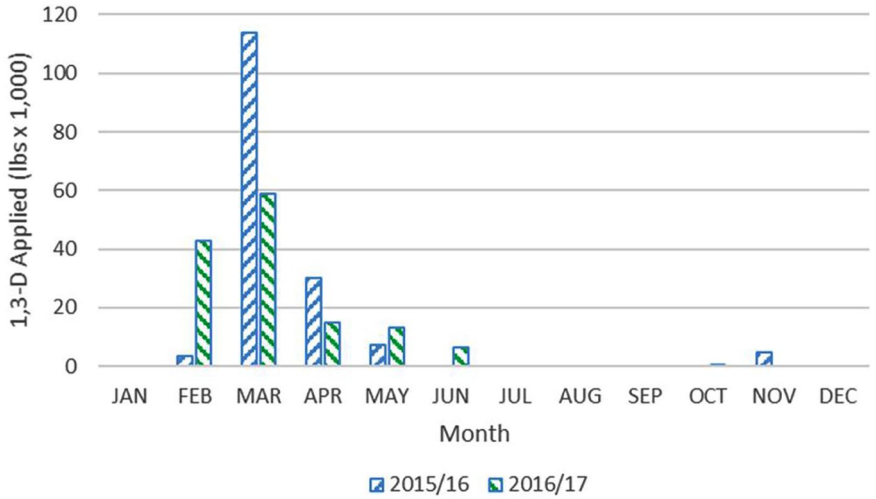


Figure 11. Pounds 1,3-D applied by month in the NC study area in 2015/2016 and 2016/2017 use seasons.

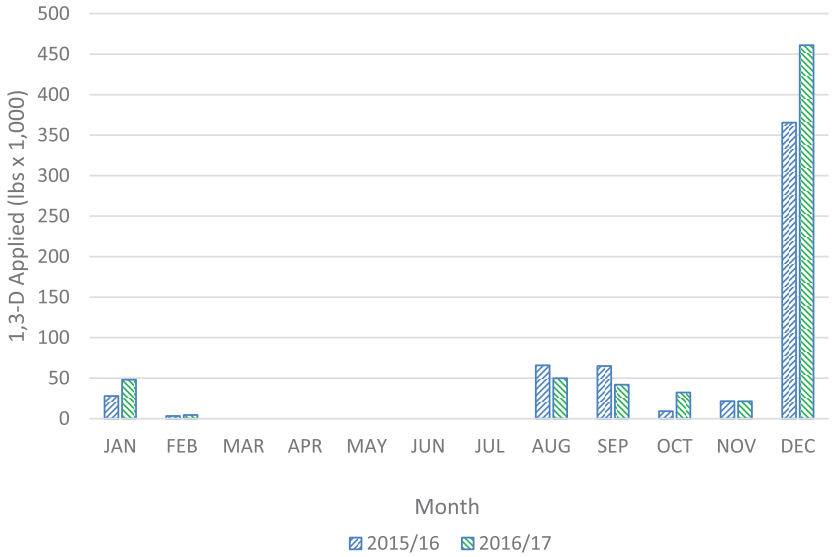


Figure 12. Pounds 1,3-D applied by month in the FL study area in 2015/2016 and 2016/2017 use seasons.

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Table 2. Mass of 1,3-D applied and land area treated in the WA, NC, and FL study areas.

REGION	YEAR	NUMBER OF 1,3-D APPLICATIONS	TREATED AREA (HA)	1,3-D APPLIED (KG)
WA	2015-2016	138	6039	1 113 083
	2016-2017	107	4784	851 367
NC	2015-2016	84	809	72 894
	2016-2017	71	657	62 186
FL	2015-2016	206	5044	324 707
	2016-2017	205	4380	252 532

Table 3. Summary of 24-hour, 28-day, 90-day MA, and annual average 1,3-D concentrations in WA for 2015/2016 and 2016/2017 application seasons.

2015/2016	1,3-D CONCENTRATION ($\mu G\,M^{-3}$)			
PERCENTILE	24-HOUR MA	28-DAY MA	90-DAY MA	ANNUAL AVERAGE
10	0.16	0.04	0.03	0.02
20	0.23	0.05	0.04	0.02
30	0.30	0.07	0.06	0.03
40	0.38	0.10	0.08	0.04
50	0.47	0.12	0.09	0.06
60	0.56	0.15	0.12	0.07
70	0.67	0.18	0.14	0.08
80	0.83	0.23	0.18	0.10
90	1.21	0.33	0.25	0.15
95	1.82	0.48	0.37	0.21
99	5.22	1.97	1.52	0.84
99.5	6.70	2.77	2.21	1.26
100	17.68	6.74	5.35	3.38
2016/2017	1,3-D CONCENTRATION ($\mu G\,M^{-3}$)			
PERCENTILE	24-HOUR MA	28-DAY MA	90-DAY MA	ANNUAL AVERAGE
10	0.16	0.03	0.02	0.01
20	0.20	0.05	0.03	0.02
30	0.24	0.06	0.04	0.03
40	0.29	0.07	0.05	0.03
50	0.33	0.08	0.06	0.04
60	0.40	0.10	0.08	0.05
70	0.48	0.12	0.09	0.05
80	0.62	0.15	0.11	0.07
90	0.93	0.22	0.17	0.10
95	1.43	0.34	0.26	0.15
99	4.17	1.38	1.10	0.56
99.5	6.12	2.31	1.92	1.09
100	13.33	6.04	5.05	3.52

Abbreviation: MA, moving average.

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Table 4. Summary of 24-hour, 28-day, 90-day MA, and annual average 1,3-D concentrations in NC for 2015/2016 and 2016/2017 application seasons.

2015/2016	1,3-D CONCENTRATION ($\mu G M^{-3}$)			
PERCENTILE	24-HOUR MA	28-DAY MA	90-DAY MA	ANNUAL AVERAGE
10	10.58	1.87	1.24	0.31
20	14.62	2.62	1.77	0.44
30	17.98	3.34	2.21	0.54
40	21.84	3.90	2.69	0.66
50	26.93	4.90	3.23	0.80
60	33.12	6.23	4.13	1.02
70	41.04	8.16	5.47	1.36
80	54.45	11.05	7.50	1.85
90	84.61	17.17	11.52	2.84
95	125.09	27.38	18.64	4.60
99	211.28	56.98	34.34	9.25
99.5	236.72	79.31	50.67	12.87
100	276.98	116.43	95.01	126.68
2016/2017	1,3-D CONCENTRATION ($\mu G M^{-3}$)			
PERCENTILE	24-HOUR MA	28-DAY MA	90-DAY MA	ANNUAL AVERAGE
10	14.35	2.19	1.55	0.40
20	17.68	2.96	1.99	0.51
30	21.10	3.77	2.46	0.63
40	24.70	4.65	3.02	0.77
50	28.49	5.59	3.66	0.94
60	34.15	6.90	4.39	1.13
70	43.76	8.66	5.78	1.49
80	56.99	11.97	8.13	2.08
90	86.71	19.30	12.81	3.30
95	127.38	28.95	18.80	4.93
99	279.88	90.95	54.49	14.96
99.5	309.69	104.55	80.73	22.32
100	472.85	173.35	137.19	130.67

Abbreviation: MA, moving average.

Discussion

None of the maximum 24-hour, 28-day, 90-day, or annual-average-modeled concentrations of 1,3-D exceeded the applicable acute, short-term, sub-chronic, or chronic Human Equivalent Concentration (HEC) for 1,3-D at any of the sites (Table 6).

The results also indicate that the receptor location with the maximum annual average concentration varies from year to year, depending on the proximity of a 1,3-D application and local weather conditions. This is consistent with previous 1,3-D modeling[13] and results from CDPR's AMN in CA,[22] which shows that the annual average concentration at a given receptor location varies widely from year to year, and that the maximum occurs at different locations, depending on the proximity to 1,3-D applications, the mass of 1,3-D applied, and local weather conditions. Figure 13(A) to (C) shows the daily modeled 1,3-D concentrations at the receptor where the maximum *annual*

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Table 5. Summary of 24-hour, 28-day, 90-day MA, and annual average 1,3-D concentrations in FL for 2015/2016 and 2016/2017 application seasons.

2015/2016	1,3-D CONCENTRATION ($\mu G M^{-3}$)			
PERCENTILE	24-HOUR MA	28-DAY MA	90-DAY MA	ANNUAL AVERAGE
10	108.3	19.8	14.8	6.5
20	133.5	25.9	19.0	8.6
30	154.4	31.7	23.7	11.0
40	176.6	38.4	29.0	13.6
50	205.2	46.5	35.5	17.0
60	239.6	57.6	45.2	21.9
70	286.9	70.2	55.4	27.4
80	367.4	92.0	73.2	36.0
90	548.9	157.0	121.1	58.5
95	738.2	241.3	198.8	97.9
99	1296.9	445.4	377.0	198.0
99.5	1564.9	564.9	489.2	299.1
100	2473.6	946.1	784.4	563.2
2016/2017	1,3-D CONCENTRATION ($\mu G M^{-3}$)			
PERCENTILE	24-HOUR MA	28-DAY MA	90-DAY MA	ANNUAL AVERAGE
10	79.4	17.5	12.4	5.7
20	102.0	22.4	15.7	7.3
30	123.3	27.3	19.1	9.0
940	142.5	33.9	23.7	11.3
50	165.8	40.6	29.4	14.2
60	196.3	49.9	37.8	18.2
70	234.4	62.9	49.2	24.1
80	306.2	81.7	63.2	32.6
90	461.1	135.8	103.4	52.4
95	639.7	217.5	182.5	86.4
99	1123.2	409.3	328.9	198.3
99.5	1297.8	480.3	406.5	266.4
100	1709.8	743.1	670.4	445.5

Abbreviation: MA, moving average.

average concentration occurred in the first and second year of the study for each region and that it occurred at different receptor locations each year.

Figure 13(A) to (C) also shows that the daily concentrations that occurred at the location of the maximum annual average do not exceed the acute HEC for 1,3-D. This demonstrates the value of modeling to capture the spatial-temporal variability in 1,3-D concentrations in ambient air, compared with the use of a single concentration on the space-time continuum obtained by monitoring, to assess human exposure and risk.

Uncertainties

Various model inputs have uncertainty, for example, the exact starting time of an application was missing in some cases. Applications with missing start times were assumed to start at 8:00 a.m. The single flux profile obtained from a field volatility

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Table 6. Comparison of 24-hour, 28-day, and 90-day moving average and annual average with acute, short-term, sub-chronic, and chronic HECs for WA, NC, and FL study areas.

EXPOSURE SCENARIO	HEC (PPM)	EXPOSURE (PPM)[A]	
		2015/2016	2016/2017
WA study area			
Acute (24-hour)[b]	42	3.93E−03	2.96E−03
Short term (28-day)[c]	4.5	1.07E−04	7.52E−05
Sub-chronic (90-day)[c]	2.6	8.21E−05	5.85E−05
Chronic (1-year)[d]	0.99	1.91E−05	1.39E−05
NC study area			
Acute (24-hour)[b]	42	6.11E−02	1.04E−01
Short term (28-day)[c]	4.5	6.07E−03	6.41E−03
Sub-chronic (90-day)[c]	2.6	4.13E−03	4.16E−03
Chronic (1-year)[d]	0.99	3.09E−04	3.80E−04
FL study area			
Acute (24-hour)[b]	42	5.49E−01	3.80E−01
Short term (28-day)[c]	4.5	5.36E−02	4.83E−02
Sub-chronic (90-day)[c]	2.6	4.41E−02	4.05E−02
Chronic (1-year)[d]	0.99	6.46E−03	5.69E−03

Abbreviation: HECs, human equivalent concentrations.
[a]Modeled 1,3-D concentrations in $\mu g\,m^{-3}$ were converted to "ppm," where $1\,\mu g\,m^{-3}$ of 1,3-D = 0.00022 ppm.
[b]Maximum 24-hour concentration.
[c]95th percentile 28-day and 90-day moving average, respectively.
[d]Arithmetic mean of annual average concentrations for all receptors.

study using a shank application in a loamy sand soil is assumed to represent all shank applications, whereas a single flux profile from a volatility study using a drip application is assumed to represent all drip applications. These flux profiles were used to validate SOFEA and suggest that on average these flux estimates describe reality. Future refinements, however, could include estimating the flux for different soil types and for different weather conditions. There are also numerous additional field volatility studies conducted on different soils and in different parts of the country, and using new application techniques, that could be used to describe the mandatory flux profiles in future assessments. For example, the use of low permeability tarp (eg, TIF) has been shown to reduce 1,3-D emissions and flux rates compared with the flux profiles used in this study, and therefore, the results of this modeling project can be conservative.

Conclusions

SOFEA4, using AERMOD in lieu of ISCST3, was compared with the ambient air monitoring data collected in an intensive 1,3-D fumigation area in Merced County, CA, and was shown to improve the prediction of high concentrations (and thus the annual average concentration) compared with SOFEA2 (using ISCST3). This is due to the improved characterization of the PBL during calm period (low wind) conditions and more realistic MH calculations that are employed by AERMOD compared with ISCST3. This validated SOFEA4 model was used to simulate 1,3-D concentrations in 3 study areas with significant use of 1,3-D as a preplant soil fumigant: Quincy, WA (representing the Pacific Northwest), Wilson, NC (representing the Atlantic coastal plain), and St. John's, FL (representing GA/FL). These 3 regions, along with Merced County, CA, represent agricultural land areas that account for approximately 95% of the 1,3-D sold in the United States. Actual field locations and 1,3-D application parameters for 2 annual product use cycles (2015-2016 and 2016-2017) were documented by local growers in each study area and were used to parameterize the model.

SOFEA4 simulations of 1,3-D concentration in ambient air in WA, NC, and FL are consistent with concentrations observed in other monitoring programs (eg, DPR's AMN), with the advantage of being an uncensored dataset with no missing data. Modeled concentrations of 1,3-D in ambient air are used to assess acute, short-term, sub-chronic, and chronic bystander exposure and risk to 1,3-D. SOFEA4 has been shown to yield accurate levels of air concentrations for the soil fumigant 1,3-D in CA, and now has been used to assess exposure to 1,3-D by

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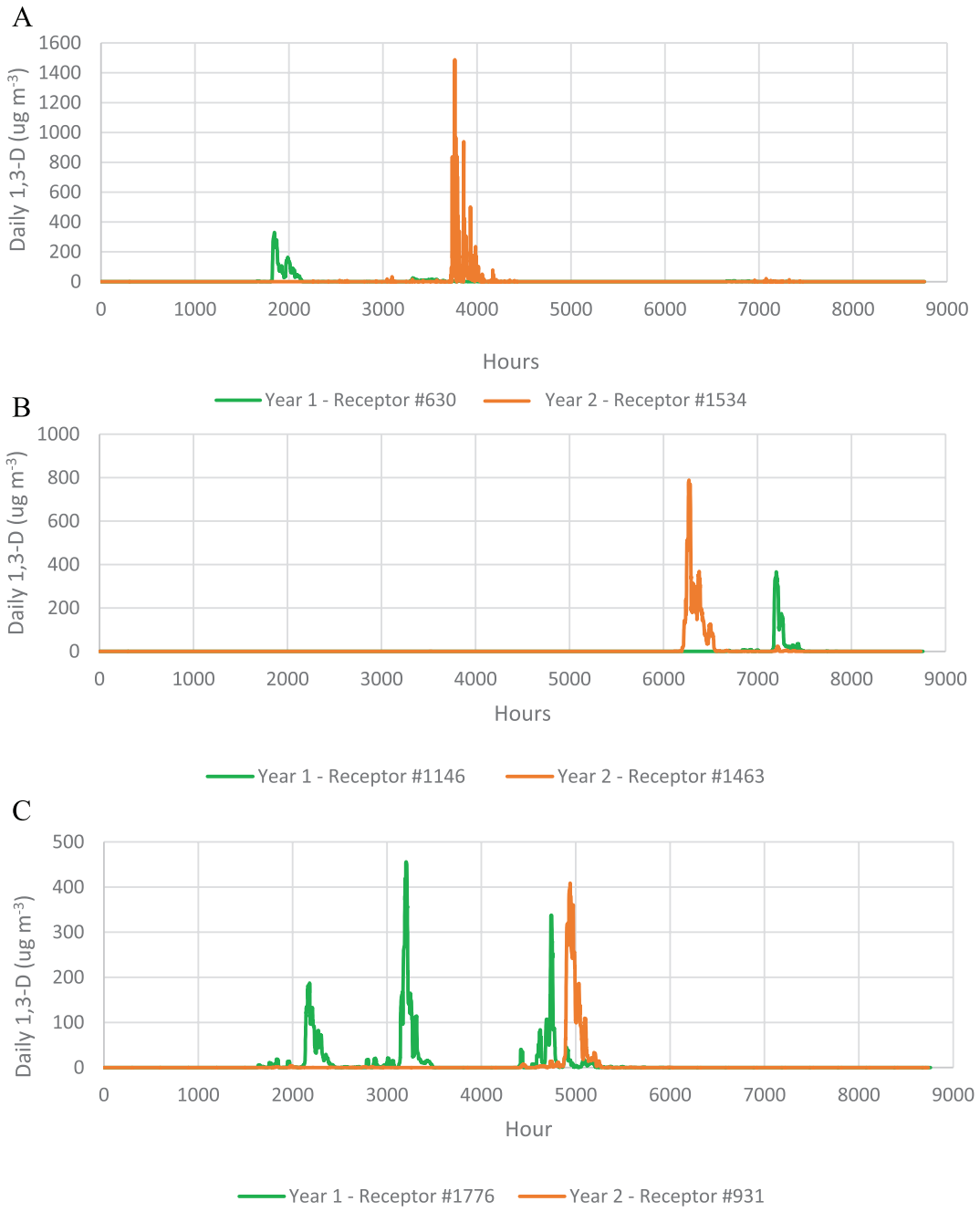


Figure 13. (A) Hourly 1,3-D concentration for the entire simulation year at the receptor with the highest annual average concentration for both years, in the WA study area. (B) Hourly 1,3-D concentration for the entire simulation year at the receptor with the highest annual average concentration for both years, in the NC study area. (C) Hourly 1,3-D concentration for the entire simulation year at the receptor with the highest annual average concentration for both years, in the FL study area.

humans residing in and around high use areas of the United States. None of the maximum 24-hour, 28-day, 90-day, or annual-average-modeled concentrations of 1,3-D exceeded the applicable acute, short-term, sub-chronic, or chronic HEC for 1,3-D, in any of the US study areas. SOFEA4 can also be used to predict concentrations of volatile or semi-volatile pesticides in ambient air across large airsheds for assessing exposure to humans or non-target animal or plant receptors.

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Author Contributions

IV designed study methodology, conducted SOFEA modeling and data analysis. SC developed and programmed original SOFEA air dispersion model. OD georeferenced 1,3-D treated field locations for SOFEA input, prepared GIS maps of fields. ZY derived acute, short-term, sub-chronic, and chronic HECs for 1,3-D from toxicology studies. JD provided guidance on HEC derivation, risk assessment and study conclusions.

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