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Modeling for the township cap of 1,3-Dichloropropene applications, modeling approach #2

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1 Modeling overview

The Department of Pesticide Regulation (DPR) has been proposing mitigation measures to reduce acute and chronic exposure from 1,3-Dichloropropene (1,3-D) to nonoccupational bystanders. Air dispersion modeling is used to determine the applications factors, setback settings, and township caps of 1,3-D. Various modeling approaches have been tested, and two of them are recommended for further evaluations. Table 1 summarizes the modeling approaches, configurations, and their associated documents.

Table 1. Modeling approaches for mitigating 1,3-D exposures non-occupational bystanders

Mitigation measures	Description
Approach #1:	
[1.1] Application factors	Seasonal factors: winter (Jan-Feb) and nonwinter (Mar-Nov); applications are prohibited during December
[1.2] Setbacks	Year-round setbacks for 11 months (Jan-Nov); applications are prohibited during December
[1.3] Township cap	170,750 ATP calculated based on [1.1] and [1.2]
Approach #2:	
[2.1] Application factors	Seasonal factors: winter (Nov-Feb) and nonwinter (Mar-Oct); applications are allowed during December
[2.2] Setbacks	Seasonal setbacks: winter (Nov-Feb) and nonwinter (Mar-Oct); applications are allowed during December
[2.3] Township cap (**this report**)	204,200 ATP calculated based on [2.1] and [2.2]

List of documents:

- [1.1] “Modeling for application factors of 1,3-Dichloropropene, modeling approach #1”
- [1.2] “Modeling for mitigation measures to reduce acute exposure from 1,3-Dichloropropene, modeling approach #1”

- [1.3] "Modeling for the township cap of 1,3-Dichloropropene applications, modeling approach #1"
- [2.1] "Modeling for application factors of 1,3-Dichloropropene, modeling approach #2"
- [2.2] "Modeling for mitigation measures to reduce acute exposure from 1,3-Dichloropropene, modeling approach #1"
- [2.3] "Modeling for the township cap of 1,3-Dichloropropene applications, modeling approach #2"

2 Introduction

1,3-Dichloropropene (1,3-D) is a fumigant used to control nematodes, insects, and disease organisms in the soil. It is commonly used as a pre-plant treatment that is injected into soil. It may also be applied through drip irrigation. Regardless of the application method, the possibility of offsite transport of this fumigant due to volatilization may subsequently result in human exposure through inhalation. To mitigate its potential cancer risk, the Department of Pesticide Regulation (DPR) limits the use of 1,3-D on a regional basis (township cap). The current township cap is 136,000 "adjusted" total pounds (ATP) during a calendar year in any township[1] . Adjusted pound refers to the amount of 1,3-D active ingredient multiplied by an application factor (AF) to account for differences in air concentrations due to application method, region, and season of application.

The current township cap of 136,000 ATP was determined by DPR based on an analysis of annual 1,3-D use and ambient air concentrations detected from year-round air monitoring during 2011-2015 at multiple locations (plus data for 2006 at one location) (Tao, 2016). Consistent with DPR's 2016 risk management directive (Marks, 2016), this township cap amount equates to a 95% probability of achieving a regulatory target concentration of no more than 0.56 ppb as a 70-year average to control lifetime cancer risk.

To address acute exposures to non-occupational bystanders from 1,3-D, DPR established a regulatory target concentration of 55 ppb averaged over a 72-hour period (Henderson, 2021). In the updated 1,3-D regulation, new requirements for 1,3-D field fumigation have been developed to mitigate the acute, non-occupational bystander exposure from 1,3-D. The new requirements include minimum requirements for all applications and additional restrictions for individual fumigation methods.

This report updates the township cap according to the new requirements for 1,3-D field fumigation. In this study, the mitigation effects of the new requirements are evaluated by air dispersion modeling, and the modeling results are used to estimate the township cap for 1,3-D applications in California with the regulatory target concentration and associated exposure

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[1] A township is a 6×6 mi^2 area as defined by the Public Land Survey System (PLSS). Each PLSS township is identified by its "meridian" (Humboldt, Mount Diablo, or San Bernardino), "township" (sequential number north or south of the meridian), and "range" (sequential number east or west of the meridian), and is referred to as MTR. Each township contains 36 1×1 mi^2 "sections," identified by number and is referred to as MTRS. Example: For MTR M15S22E, "M" refers the Mount Diablo Meridian, "15S" refers to 15th township south of the meridian, and "22E" refers to the 22nd range east of the meridian. For MTRS M15S22E03, "03" refers to the 3rd section within the township.

scenarios. This modeling approach includes two major components: concentration simulation and exposure simulation. Similar methods were previously used by DPR to evaluate the potential risks from proposed values of township cap (Barry and Kwok, 2016; Johnson and Powell, 2005; Johnson, 2007a, b). The previous modeling studies first converted concentrations to doses (which are further compared to the reference risk goal), while this study estimates the exposure directly from the model-predicted concentrations (by comparing with the regulatory target of 0.56 ppb). Therefore, the dose calculations by stochastic simulations over age- and gender-specific parameters are not appropriate for this study. A new method is proposed by following the assumptions and requirements in DPR's 2016 risk management directive (Marks, 2016). The reported historical 1,3-D uses and associated meteorological conditions in California during a 5-year period of 2013-2017 are used as the base input data. The reported uses are adjusted according to the new requirements, mathematically representing the future uses of 1,3-D after the implementation of the mitigation practices. The adjusted use data are used to determine (1) the ATPs with the AFs based on the same fumigation requirements (Luo and Brown, 2022), and (2) ambient concentrations at a township scale from air dispersion modeling. Finally, the township cap is determined based on the relationship between the ATPs and model-predicted concentrations at the reference concentration of 0.56 ppb. With the mitigation practices in the new fumigation requirements, the ambient concentrations of 1,3-D are expected to be decreased and thus the new township cap will be increased from the previous value of 136,000 ATP.

3 Methods and Materials

3.1 Overview of modeling approach

This section reviews DPR's previous modeling studies on township caps and introduces the methods updated in this study. Similar approaches were used in the previous modeling efforts and in this study to evaluate or estimate the township cap of 1,3-D, by establishing the relationship between ATP and exposure (measured as exposure dose, µg/kg/day, or exposure concentration, ppb) (Figure 1). Both exposure dose and exposure concentration are calculated from air concentrations of 1,3-D by following the assumptions in the exposure scenario. The general requirement for concentration simulation is to include a range of ATPs representing the realistic conditions in the high-use areas of California, so there are sufficient data points (Figure 1) to establish a reliable relationship between use and exposure.

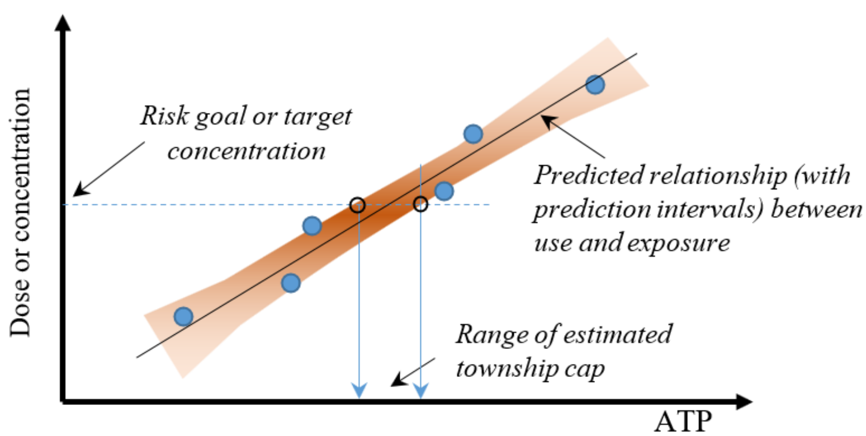

Figure 1. Conceptual model to evaluate or estimate the township cap of 1,3-D

In the previous studies (Barry and Kwok, 2016; Johnson and Powell, 2005; Johnson, 2007a, b), air concentrations were predicted by the ISCST3 (Industrial Source Complex – Short Term version 3) model. Model simulations were managed by SOFEA (Soil Fumigant Exposure Assessment) model system developed by Dow AgroSciences (Cryer, 2005; van Wesenbeeck et al., 2013) for regional modeling of 1,3-D over 3×3 or 5×5 townships with the center township of M07S11E (Merced County) or S01N21W (Ventura County). With a proposed value of township cap, hypothetical application data were randomly generated by SOFEA based on the probability distributions of application rate, acreage, and timing reported in past years. In order to introduce the variation of ATPs (so, more data points in Figure 1), multiple ATP values were usually tested (e.g., 0.1X, 1.0X, 1.5X of the proposed cap). For the same purpose, multi-station meteorological data might be used regardless of the simulated areas (e.g., meteorological data from Merced used for simulations in Ventura).

In this study, AERMOD (American Meteorological Society/ Environmental Protection Agency Regulatory Model) is used for concentration simulation. Modeling performance of AERMOD has been recently evaluated by DPR (Luo, 2019a), and the results suggest that AERMOD with regulatory default settings (without the ADJ_U* option) satisfactorily predicts annual average concentrations of 1,3-D in high-use areas of California. Model simulations are managed by AERFUM, an integrated air dispersion modeling system for soil fumigants developed by DPR (Luo, 2019b). AERFUM enables regional modeling for anywhere in California, so simulations are conducted for multiple locations with various use patterns and field mitigation methods of 1,3-D. In addition, the reported 1,3-D use data and meteorological data specific to the simulated areas are used in modeling.

Results of air dispersion modeling (by ISCST3 in the previous studies or AERMOD in this study) are summarized as annual average concentrations of 1,3-D at multiple receptors in a township for each year of the study period. The next step is to estimate the exposures based on the predicted concentrations. In the previous studies, exposures were evaluated by two variables: annual average daily dose (ADD) by age and gender, and its accumulated value as lifetime average daily dose (LADD). The residency mobility (e.g., "low mobility" or "intermediate mobility") was incorporated in ADD, and the exposure period (e.g., 70-year or 30-year) was considered in LADD. Specifically, ADD was calculated from the joint probability distribution between the predicted annual air concentrations of 1,3-D and age- and gender- specific parameters (breathing rate, body weight, and time spent in different locations). Stochastic simulation was utilized for this purpose, and implemented in computer programs: HEE5CB (the High End Exposure Version 5 Crystal Ball) (Johnson and Powell, 2005; Sanborn and Powell, 1994), or MCABLE (Monte Carlo Annual Based estimate of Lifetime Exposure) (Driver et al., 2015). Finally, the resulting LADD was converted to risk by multiplying the human cancer potency factor (e.g., 5.5×10^{-5} kg×day/μg for portal-of-entry effect), and compared to the "risk goal" of 1.0×10^{-5} to evaluate the proposed township caps.

In 2016, DPR established the regulatory target concentration (0.56 ppb) and exposure scenario (i.e., "*low-mobility scenario and 70-year lifetime exposure*") for 1,3-D cancer risk mitigation (Marks, 2016). The residency mobility determines the spatial coverage of air concentrations used in risk assessment. Under the low-mobility assumption, concentrations are only predicted for one township (the center township). This setting is used in this study and is equivalent to stating that individuals spend their entire lives in the corresponding township. More details on the selection of townships for modeling are provided in the next section.

The exposure period of 70 years was only used in the previous studies for summarizing ADD values to LADD. In this study, mitigation is based on the target concentration, so the variables ADD and LADD are not calculated. Therefore, the target concentration defined as the 70-year average (Marks, 2016) cannot be directly evaluated. In the recent township cap estimation (Tao, 2016), risks were evaluated based on the annual (i.e., 1-year) averages of monitoring data. In this study, both the 1-year and 5-year averages of model-predicted concentrations are considered.

Finally, the 95% probability of protection is represented in this study by calculating the exposure concentration as the 95th percentile of the annual average concentrations over the township of modeling. This method is comparable to the previous studies with low-mobility assumption, where the 95th percentile of LADDs in a township was used for deriving the use-exposure relationship (Figure 1). Minitab version 19 is utilized for regression and other statistical tests in this study. Table 2 summarizes the components of the modeling approaches for evaluating or estimating township caps.

Table 2. Modeling approaches previously used (risk-goal based risk assessment) and proposed in this study (target concentration based)

	Previous studies	This study
Risk management	Risk goal at 1×10^{-5} (Gosselin, 2001)	Target concentration at 0.56 ppb (Marks, 2016)
Simulation of concentration		
Simulation engine	ISCST3	AERMOD
Modeling system	SOFEA	AERFUM
Study area	One location	Multiple locations
Use data and ATP ("x-axis" in Figure 1)	Based on hypothetical use data and the current AFs	Reported use data, both the current and modeled AFs
Meteorological data	5-year	5-year
Simulation of exposure		
Residency mobility	Low (using air concentrations in one township), or intermediate (in 3×3 townships)	Low (using air concentrations in one township)
70-year average dose	Based on age-specific parameters for ages 0-70	Not applicable
70-year average concentration	Not applicable	Based on 1-year and 5-year average concentrations
Probability of protection	95%	95%
Exposure measure ("y-axis" in Figure 1)	The 95th percentile of predicted doses (LADDs)	The 95th percentile of predicted air concentrations

3.2 Study period and areas

This study determines township caps based on the reported 1,3-D uses and meteorological data in California between 2013-2017. The U.S. Environmental Protection Agency (USEPA) Guideline on Air Quality Models recommends that five years of consecutive meteorological data should be used for air quality modeling studies (USEPA, 2015). The Office of Environmental Health Hazard Assessment (OEHHA) Air Toxics Hot Spots Program Guidance Manual for the Preparation of Risk Assessments also recommends that five years of consecutive meteorological data should be used for risk assessment analysis (OEHHA, 2015). Similarly, 5-year meteorological data were used in DPR's previous modeling effort to evaluate township caps (Barry and Kwok, 2016; Johnson and Powell, 2005; Johnson, 2007a, b). The same sets of 5-year (2013-2017) meteorological data are also used in other modeling studies for 1,3-D (Table 1).

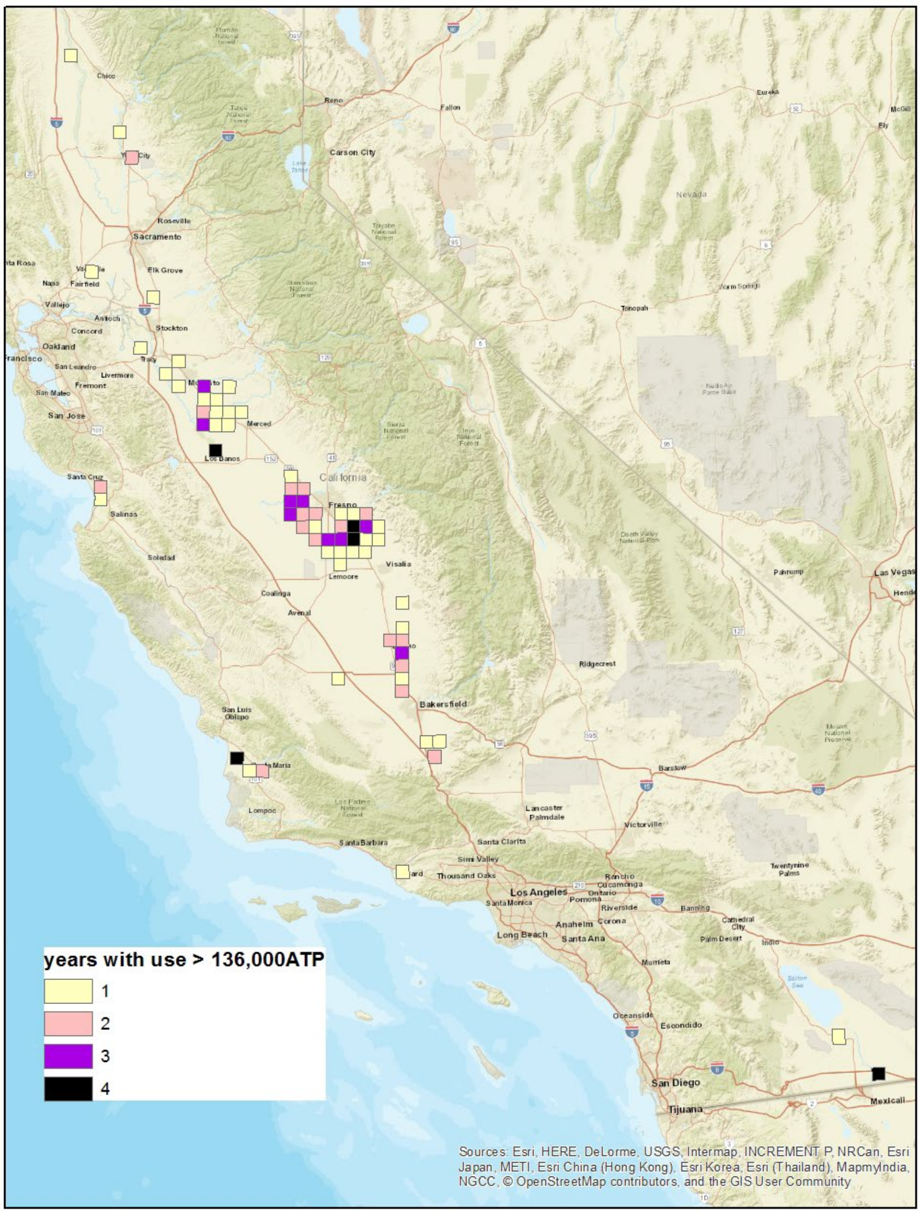

Figure 2. Townships with uses above 136,000 ATP (based on the current AFs) during 2013-2016. No townships exceeded this level in 2017.

Based on the ATPs calculated with the current AFs, the locations with high uses of 1,3-D during 2013-2017 are selected for modeling. There were 507 townships with reported 1,3-D uses during the study period: 69 of them were observed with uses greater than the current township cap (115,000 ATP for M07S11E in 2017, or 136,000 ATP for all other townships and years)[2] for at least one year (Figure 2). The center townships for modeling are selected by the following steps:

- High-use areas are observed from Sacramento Valley to Imperial Valley. For the consistency with the previous cap estimation (Tao, 2016), the townships for modeling are selected in the areas monitored by DPR's Air Monitoring Network for 1,3-D (DPR, 2022), including Ripon, Watsonville, Parlier, Shafter, Santa Maria, and Oxnard.
- Top townships by 1,3-D uses in the above areas are considered for modeling. High-use townships are usually adjacent to each other. In this case, only one of them is modeled to reduce the bias from shared townships in the simulation domain of 3×3 townships. For example, M15S22E is selected to represent a cluster of 5 connected high-use townships in the area of Parlier (M15S22E, M15S23E, M16S20E, M16S21E, and M16S22E). Finally, eight townships with high uses of 1,3-D are selected for modeling (Table 3).

Table 3. Modeling areas and weather stations

Area	Center township(s)	Surface station	Upper air station
Ripon	M02S08E	23237	OAK
Watsonville	M12S02E	23277	OAK
Parlier	M14S18E, M15S22E	93193	OAK
Shafter	M24S26E, M31S27E	23155	VBG
Santa Maria	S11N35W	23273	VBG
Oxnard	S02N22W	93110	VBG

Notes: WBAN = Weather-Bureau-Army-Navy, a five-digit identifier for weather stations operated by National Weather Service. OAK = Oakland International Airport (WBAN=23230) and VBG = Vandenberg (93214).

3.3 Modeling representation of the new fumigation requirements

This study uses the reported historical applications of 1,3-D during 2013-2017 as the base data for air dispersion modeling. The application data were taken from the database processed by DPR. The new field fumigation requirements to mitigate the acute, non-occupational bystander exposure from 1,3-D are incorporated in the model simulations. According to the updated 1,3-D regulation, 18 field fumigation methods (FFMs) are allowed in California (Appendix I), including 13 FFMs currently registered and 5 FFMs newly proposed (24-inch injection and 50% TIF methods). Some of the field fumigation requirements, including soil moisture requirements, tarp cut-times, and new fumigation methods with lower emissions, have been reflected in the generation of flux time series by HYDRUS modeling (Brown, 2022) as emission input data for

[2] Prior to 2017, the township cap was a two-tier program that allowed up to 180,500 ATP in some townships.

air dispersion modeling. Additional restrictions in the fumigation requirements are established as setback tables (Luo, 2022), showing the relationship among fumigation method, setback distance, application rate, and application block size. The required setback distances (100, 200, or 500 ft) and duration (7 days) are simulated by excluding the model-predicted hourly concentrations for 7 days after an application from the calculation of annual average concentrations for the receptors located within the setback distance. The setbacks are required to reduce the acute concentrations to below the reference of 55 ppb over a 72-hour period. By excluding the hours over the setback duration, therefore, this approach actually evaluates the effects of the acute mitigation practices on the annual average concentrations.

According to the new requirements, some of the historical uses of 1,3-D may not be allowed in the future. For example, an 18-inch method (FFM1206) with a rate of 200 lb/ac over a 20-ac field is no longer allowed during the winter season (November to February). A lower-emission method such as 24-inch injection (FFM1224) can be used with the same rate and acreage. Alternatively, the treated field could be separated for multiple applications with smaller acreages for each one according to the provided setback tables.

For computational implementation, each record of the reported 1,3-D uses in the simulation domain is first compared with the maximum allowed application block size in the setback table for the corresponding FFM and rate under a 100-ft setback distance (i.e., the minimum requirement). If the reported acreage is equal to or less than the maximum allowed block size, the record of report 1,3-D use is directly used in modeling without any change. Otherwise, if the reported acreage is larger than the maximum allowed block size, the required application is not allowed in the future and should be modified for the compliance with the new field fumigation requirements. The following scenarios will be modeled:

1) Remain the reported FFM and rate, but use multiple applications with smaller treated acreages to meet the requirements on the maximum block size. This scenario does not change the total emission from the proposed 1,3-D application. Therefore, it's not expected to result in significant reduction on the annual average concentrations in addition to that from the minimum requirements (e.g., higher soil moisture). To simplify the model simulations, the minimum requirements, including the flux time series with new soil moisture requirements and the setback of 100 ft for 7 days, are incorporated in the air dispersion modeling to represent the worst-case condition by separating a reported 1,3-D use into multiple applications.
2) Remain the reported rate and acreage, but change the FFM to a lower-emission method, so that the reported application rate and treated acreage comply with the new requirements. The sequence of FFM search is ordered by the relative values of maximum allowed block sizes in the setback tables: non-tarp 18-inch methods, 50% TIF with 18-inch method (FFM1250), 24-inch methods, 50% TIF with 24-inch method (FFM1264), then the TIF methods of FFMs 1242, 1247, or 1249 (for which no additional restriction is required). Note that the sequence of FFM selection is used for conservative estimation of 1,3-D uses by following the new requirements. In field conditions, there might be other considerations for adopting an alternative FFM, which would generate ATPs and concentrations not higher than those based on the above sequence of FFM selection.

The above two modeling scenarios (smaller application blocks and lower-emission methods) establish the upper and lower bounds of the projected field conditions for 1,3-D applications after the implementation of the new fumigation requirements. The selected townships (Table 3) are modeled with the two scenarios for determining the township cap.

3.4 Simulation of concentration

For each selected township for modeling (Table 3), the simulation area is generally set as 3×3 townships with the township of interest located in the center, called the "*center township*" or "*township #5*" following the terminology in DPR's previous studies (Barry and Kwok, 2016; CDPR, 2015; Johnson, 2007a, b). The only exception is the township S11N35W at Santa Maria, which is located close to the shoreline, and some of its adjacent townships are not in a regular shape (see Appendix II for more information). Meteorological data are retrieved from nearby weather stations operated by the National Weather Service with Automated Surface Observing System (Table 3). The MetProc program is used to prepare input meteorological data in the AERMOD required format (Luo, 2017).

With the "low mobility" assumption, air concentrations are only predicted within the center township for modeling. A receptor grid is developed at an interval of 268 m, following the previous modeling settings (Barry and Kwok, 2016; Johnson and Powell, 2005; Johnson, 2007a, b). In the center township, there are 1369 receptors in total (1369=37×37, where 37 = 1mi/268m + 1). Receptor height for the receptors is 1.5 m above the ground surface to mimic the breathing height of an adult. AERFUM retrieves hourly concentrations at each receptor from AERMOD predictions, and calculates the annual average concentrations by considering the required setback distance and duration for 1,3-D applications. Mathematically, hourly concentrations predicted within the setback distance and duration are set to a missing value, and thus not used in the calculation of annual averages.

All 1,3-D applications within the simulation area during 2013-2017 are considered for modeling. The application data, in terms of FFM, application rate, and treated acreage, are pre-processed to reflect the proposed mitigation practices as the new fumigation requirements in the updated 1,3-D regulation. See the previous section for more information.

Application events are reported at the spatial resolution of section, but the location and dimensions of a treated field are not specified. AERFUM assumes each treated field (i.e., a source) is a square, and randomly locates it within the reporting section. To account for the variations on model predictions by this randomization, each township and scenario is modeled by 10 model runs and their averages are used in the subsequent simulation of exposure. In each model run, sources are re-randomized with the system clock as a random seed (a number used to initialize a pseudorandom number generator). Although the predicted hourly concentrations of 1,3-D at individual receptors may significantly vary with source locations, the 95th percentile of annua average concentrations over all receptors in a section, which is used in this study to determine the township cap, is relatively stable and not sensitive to the spatial placement of sources. When the GIS data for field boundaries become available, the actual coordinates of treated fields can be modeled by AERFUM and the results for township cap modeling are expected to be similar to these with source randomization. Finally, AERFUM reports

1369×8×5×2 values of annual concentrations for the 8 selected townships (Table 3) and the two modeling scenarios (Section 3.3) during the 5-year study period (2013-2017).

3.5 Simulation of exposure

The predicted annual concentrations for each township, scenario, and year are used as the input data for exposure simulation. For each township-year set, the 95th percentile is calculated over the corresponding 1369 values, resulting in 80 values (8 townships, 5 years, and 2 scenarios). The resulting 95th percentile value, referred to as the "exposure concentration", is the key variable for risk assessment in this study. The exposure concentrations are paired with the associated ATPs, as in the conceptual model illustrated in Figure 1.

The use-exposure relationship for the center township is determined by linear regression, and the township cap is estimated at the critical value of 0.56 ppb (i.e., the regulatory target concentration). Predicted concentrations from the air dispersion modeling are reported in the unit of $\mu g/m^3$. By assuming a temperature of 25 degrees Celsius, 0.56 ppb = 2.54 $\mu g/m^3$. The township cap is calculated based on the upper 90% prediction interval of the regression (Figure 1). The 90% prediction intervals of the regression equation are conceptually different from the 95th percentile of the air concentrations in a township. The 95th percentile is calculated to achieve the 95% probability of protection required by DPR's 2016 risk management directive (Marks, 2016). The prediction interval accounts for the observed variances not captured by the regression analysis.

The calculation of the township cap is based on the annual averages of predicted air concentrations of 1,3-D. However, the township cap is designed to address cancer risks based on a 70-year average air concentration of 0.56 ppb. Based on the available data during 2013-2017, this study also tests 5-year averages using the same method to evaluate whether the calculated township cap achieves this goal. In this case, the modeled values of annual air concentrations are combined into 1369 values of 5-year averages, and the 95th percentile of those values is assigned to each township and scenario.

4 Results and discussion

4.1 Estimation of the township cap

The linear relationships (Figure 3) between the ATP and exposure concentration (as the 95th percentile of the predicted annual average concentrations over a township) are significantly established ($p<0.001$), with the coefficients of determination (R^2) of 79.6%. The assumptions for linear regression are tested with the method recommended by Peña and Slate (2006). The regression passes all tests; see Appendix IV for the test results. The township cap is determined as 204,200 ATP based on the upper 90% prediction interval at the target concentration of 0.56 ppb.

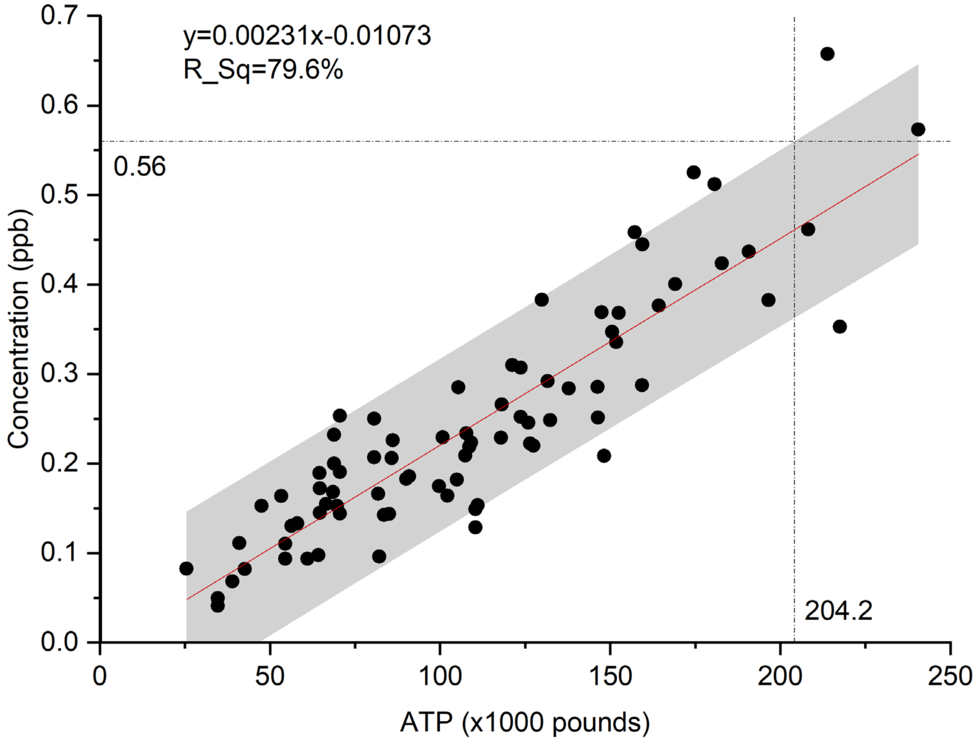

Figure 3. The ATPs and exposure concentrations (as the 95th percentile of the predicted 1-year average concentrations over a township). Results of data analysis are shown as the regression line (solid), the 90% prediction intervals (shaded), regression equation, and coefficient of determination ("R-Sq" for R^2). The township cap is determined based on the upper 90% prediction interval.

Some data points are located above or on the upper interval. These data points are not predicted for one location or one year, but distributed over multiple modeled regions (Parlier, Ripon, Santa Maria, and Shafter) and years (2013-2017). Long-term average of these locations, evaluated as 5-year average concentrations and ATPs in the next section, are all below the upper 90% prediction interval.

The township cap (204,200 ATP) predicted with the new field fumigation requirements in the updated 1,3-D regulation is higher than the current value (136,000 ATP) derived in the previous study with monitoring data analysis (Tao, 2016). Compared to the previous study, the township cap in this study is determined based on different years of PUR and meteorological data, different fumigation methods and associated flux time series, application factors, and modeling/statistical approach. Therefore, there is no simple comparison between the current and new township caps. Generally, the new field fumigation requirements introduce low-emission methods and mandate the use of mitigation practices including high soil moisture and setback distances. Those practices are expected to reduce the ambient concentrations of 1,3-D, thus allow more use of 1,3-D in terms of ATP values. Another component that could significantly affect the final result is the mathematical representation of the 95% probability of protection as required in the DPR's risk management directive (Marks, 2016). The modeling approach considers the protection "within" a township-year set by taking the 95th percentile of concentrations predicted over the township in a year (i.e., exposure concentration). The data analysis of monitoring data compared "between" township-year sets and the 95th percentiles of "concentration/ATP" ratios over all sets were used to estimate the township cap.

In addition to the approaches and results presented above, other model configurations and post-processing methods to determine the township cap are also evaluated, including extended simulation domain of 5×5 township area (Appendix V), region-specific township caps (Appendix VI), and logistic regression with receptor-year data (Appendix VII). By investigating the alternative approaches and their results, we conclude that the linear regression with township-year data presented in this section is the most appropriate approach to determine the township cap of 1,3-D for statewide mitigation purpose.

4.2 Evaluation of the estimated township caps using 5-year average concentrations

The township cap is designed to address cancer risks based on a 70-year average air concentration of 0.56 ppb. As the annual air concentrations used to estimate the township cap have greater variability than a longer-period average, the township caps are compared with the 5-year average concentrations predicted during 2013-2017 for the modeled townships and scenarios to evaluate their potential efficacy (Figure 4).

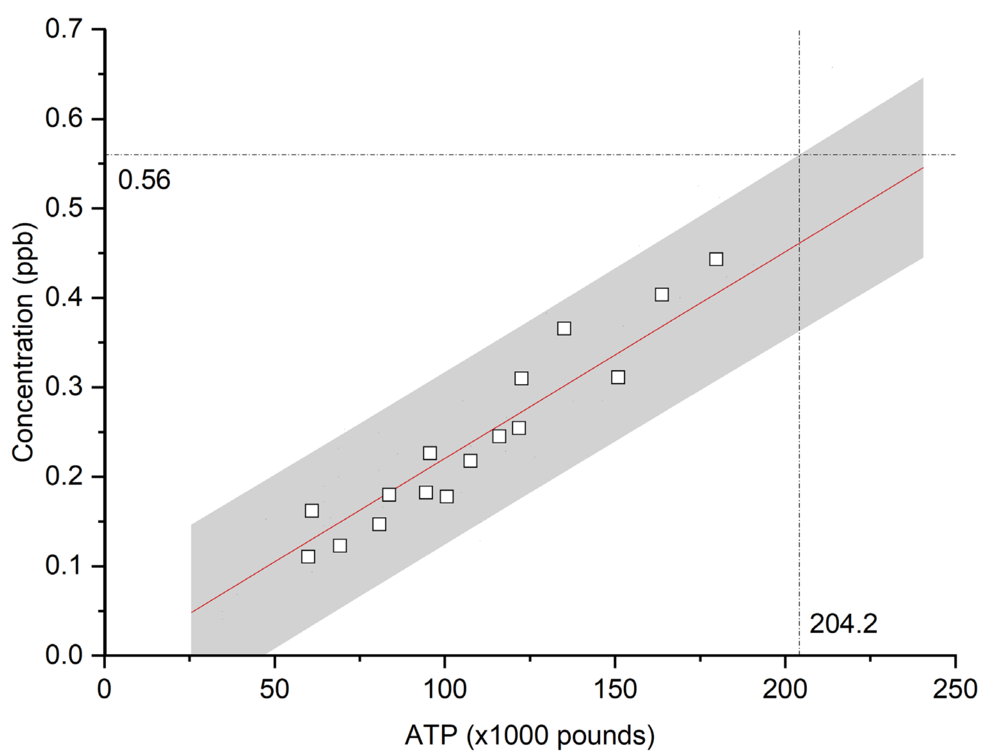

Figure 4. The ATPs and exposure concentrations (as the 95th percentile of the predicted 5-year average concentrations over a township) for the modeled townships and scenarios (squares). The regression line (solid) and the 90% prediction intervals (shaded) are taken from Figure 3.

The township cap is determined based on the upper 90% prediction interval, which is considered as the critical curve for validation. Graphically, a data point (i.e., a township) below (i.e., to the lower right of) the critical curve suggests that the 5-year average concentration of 1,3-D will be lower than the regulatory target concentration if the township complies with the corresponding township cap. All data points are below the upper 90% prediction interval (Figure 4). If the township cap is determined from the regression line, about 40% (6 out of 16 data points above the regression line, Figure 4) of modeled township-scenarios may not be sufficiently protected when the ATP would have been increased to the corresponding township cap.

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Appendix I. 1,3-Dichloropropene field fumigation methods

Method Name	Field Fumigation Method (FFM) Code
Nontarp/shallow/broadcast or bed	1201
Tarp/shallow/broadcast	1202
Nontarp/18 inches deep/broadcast or bed	1206
Tarp/18 inches deep/broadcast	1207
Chemigation (drip system)/tarp	1209
Nontarp/18 inches deep/strip	1210
Nontarp/18 inches deep/GPS targeted	1211
Nontarp/24 inches deep/broadcast	1224
Tarp/24 inches deep/broadcast	1225
Nontarp/24 inches deep/strip	1226
Totally Impermeable Film (TIF) tarp/shallow/broadcast	1242
TIF tarp/shallow/bed	1243
TIF tarp/shallow/bed/3 water treatments	1245
TIF tarp/deep/broadcast	1247
TIF tarp/deep/strip	1249
50% TIF tarp/18 inches deep/broadcast	1250
Chemigation (drip)/ TIF tarp	1259
50% TIF tarp/24 inches deep/broadcast	1264

Appendix II. Simulation domains
II.1 Sources

The simulation domain for each of the 18 selected townships includes 9 adjacent townships. Generally, the domain is defined by 3×3 townships with the township of interest in the center where air concentrations are reported. For Santa Maria, the domain is defined based on the township arrangement and reported 1,3-D uses in the surrounding areas (Figure 5).

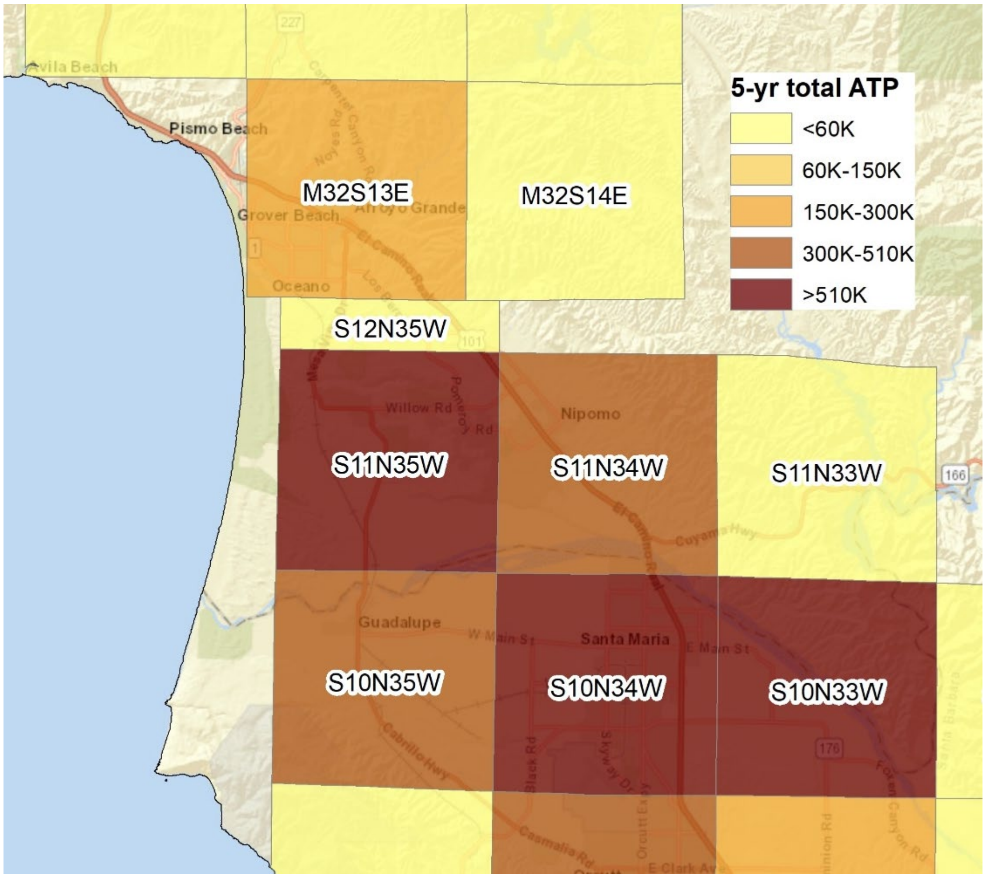

Figure 5. The 9 townships selected for model simulations on S11N35W (Santa Maria). Townships without 1,3-D use are not shown. Range classification is based on the "Natural Breaks (Jenks)" algorithm in ArcGIS

II.2 Receptors

AERMOD simulations consider all 1,3-D applications in the 9-township area, but only predict air concentrations in the center township. See Figure 6 for a graphic description of model configurations.

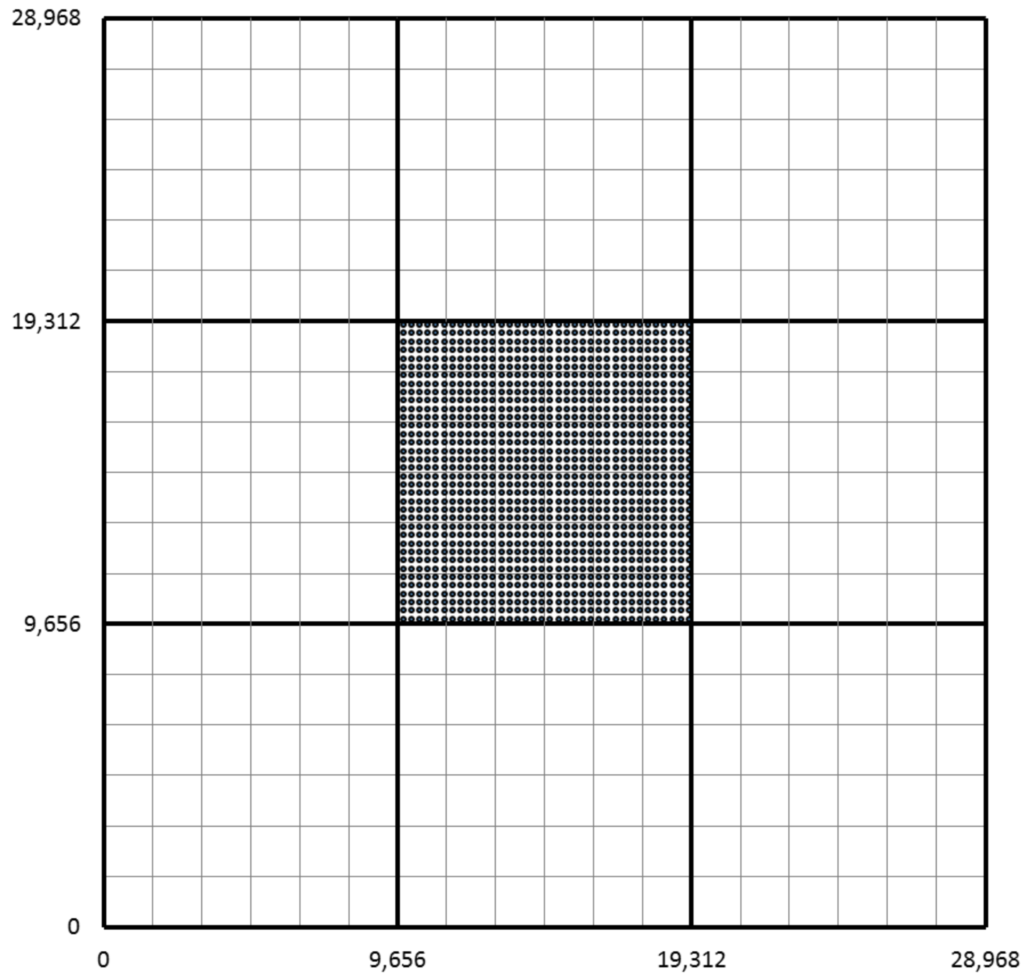

Figure 6. Model configurations with 9 townships and the receptor grid over the center township. All distances are in meters, 9656 m is about 6 miles. The small squares represent sections (1×1 mi^2)

Appendix III. Application factors used in this study

Table 4. Application factors used in this study.

(a) Current application factors, used to rank and identify high-use areas of 1,3-D in California (Figure 2)

Field Fumigation Methods (FFMs) and FFM codes	Within SJV		Outside SJV	
	Dec-Jan	Feb-Nov	Dec-Jan	Feb-Nov
Standard nontarped and non-TIF tarp shallow (12 inch) methods (1201, 1202)	-	1.9	2.3	1.9
Standard nontarped and non-TIF tarp deep (18 inch) methods (1206, 1207, 1210, 1211)	1.9	1.0	1.2	1.0
Chemigation (drip) (1209, 1259)	1.16	1.16	1.16	1.16
TIF tarp broadcast/bed (1242, 1243, 1245, 1247)	0.6	0.3	0.6	0.3
TIP tarp strip (1249)	1.2	0.6	1.2	0.6
Other label method for 1,3-D (1290)	2.3	1.9	2.3	1.9

SJV = San Joaquin Valley. Within SJV = Counties of Fresno, Kern, Kings, Madera, Merced, San Joaquin, Stanislaus, and Tulare. Outside SJV = All other counties in California.

Note that, in the current regulation of 1,3-D, all applications have been prohibited during December since 2017. The factors for December are only used to calculate ATPs for the reported 1,3-D applications during the first 4 years (2013-2016) of the simulation period.

(b) Modeled application factors for the updated 1,3-D regulation, used to estimate the new township cap

Field Fumigation Methods (FFMs) and FFM codes	Inland		Coastal	
	Dec-Feb	Mar-Nov	Dec-Feb	Mar-Nov
Standard nontarped and non-TIF tarp shallow (12 inch) methods (1201, 1202)	2.56	1.41	2.18	1.68
Standard nontarped and non-TIF tarp deep (18 inch) methods (1206, 1207, 1210, 1211)	1.50	0.83	1.28	0.98
Chemigation (drip)/non-TIF tarp method (1209)	1.87	1.03	1.56	1.15
24-inch injection methods (1224, 1225, 1226)	0.87	0.49	0.74	0.57
TIF methods (broadcast: 1242, 1247, 1249)	0.39	0.21	0.33	0.23
TIF methods (bed: 1243, 1245, 1259)	0.66	0.36	0.55	0.42
50% TIF with 18-inch injection depth method (1250)	0.90	0.50	0.76	0.59
50% TIF with 24-inch injection depth method (1264)	0.56	0.31	0.47	0.37

Notes: The coastal region includes counties of Del Norte, Humboldt, Los Angeles, Marin, Mendocino, Monterey, Orange, San Diego, San Francisco, San Luis Obispo, San Mateo, Santa Barbara, Santa Cruz, Sonoma, Ventura. All other counties are the inland region.

Appendix IV. Validation of linear model assumptions

The data used in linear regressions are validated by the methods proposed by Peña and Slate (2006) and implemented in a package "gvlma" (https://cran.r-project.org/web/packages/gvlma/gvlma.pdf). All assumptions for a linear model are acceptable for the input data in this study (Figure 3 and Table 5).

Table 5. Statistical tests on linear model assumptions for the data points used in this study. Test results are directly copied from the "gvlma" outputs.

	Value	p-value	Decision
Global Stat	8.1420	0.08651	Assumptions acceptable.
Skewness	0.8188	0.36554	Assumptions acceptable.
Kurtosis	1.1526	0.28301	Assumptions acceptable.
Link Function	2.7369	0.09805	Assumptions acceptable.
Heteroscedasticity	3.4338	0.06387	Assumptions acceptable.

Appendix V. Modeling with an extended simulation domain

In air dispersion modeling, the consideration of more sources will generally increase the predicted concentrations. In addition, the near-receptor sources have higher relative contributions to the predictions compared to the sources far away from the receptors. For example, a previous study modeled a 1,3-D measurement in the DPR's monitoring site at Parlier with three groups of sources located in a similar direction but different distances (at approximately 0.1, 0.6, and 1.1 mi) from the monitoring site. Modeling results suggested that 74% of the total predicted concentration value was contributed by the sources at 0.1 mi, 25% by the sources at 0.6 mi, and 1% at 1.1 mi (Tao, 2019).

According to DPR's previous modeling studies for evaluation the township cap of 1,3-D (Barry and Kwok, 2016; CDPR, 2015; Johnson, 2007a, b), the configuration of simulation domain is related to the assumed mobility scenarios. Specifically, a 3×3 township area is recommended for the "low mobility" scenario (person spends entire life within the center township), while a 5×5 township area is more appropriate for the "intermediate mobility" scenario (person's home in the center township, but travels around throughout the other 3×3 township area). According to the risk management directive (Marks, 2016), DPR concluded that a low-mobility scenario would be health protective to address chronic risk of 1,3-D. Therefore, this study models all sources in the simulation domain of a 3×3 township area. The configuration suggests a domain size of about 41 km (the diagonal of a 3×3 township area).

In this appendix, model simulations are conducted to investigate the effects on the predicted 1,3-D concentrations by considering additional sources out of the 3×3 township area. The domain is extended from 3×3 to 5×5 township area, and other model configurations are not changed (meteorological data and receptor grids). Note that a 5×5 township area has a domain size of 68 km, larger than the recommended size of up to 50 km for AERMOD (USEPA, 2017).

Two center townships are selected for modeling: M15S22E in Parlier and M12S02E in Watsonville. Modeling results are reported as the relative changes of the total uses of 1,3-D in the simulation domain and prediction exposure concentrations in the center township (). As the 5-year averages in the tested center township of M15S22E in Parlier, the modeled use of 1,3-D is increased by about 78.8% and the predicted exposure concentration is increased by 4.5%. In the township of M12S02E in Watsonville, the 5-year average increases of use and concentration are 32.2% and 1.5%. As annual data, the increases of use and concentration are significantly correlated ($p < 0.001$).

Table 6. Relative changes of the modeled 1,3-D uses and predicted exposure concentrations in the center township by extending the simulation domain from 3×3 to 5×5 township areas at M15S22E in Parlier and M12S02E in Watsonville

Year	Use increase (Parlier)	Conc. increase (Parlier)	Use increase (Watsonville)	Conc. increase (Watsonville)
2013	82.8%	5.7%	37.6%	1.7%
2014	76.5%	5.0%	32.5%	1.2%
2015	95.2%	7.1%	28.8%	1.6%
2016	64.0%	3.5%	28.8%	1.8%
2017	75.8%	3.4%	32.1%	1.6%
5-year Average	78.8%	4.5%	32.2%	1.5%

Appendix VI. Spatial variability of township cap estimates

The same statistical approach as described in Section 4.1 is applied to estimate the township cap for each region (Table 7). In this case, only the data points for the corresponding region are used in regression, e.g., 10 data points for the area of Ripon (with one center township modeled) and 20 points for Parlier (two center townships). The regional cap values range from 181,021 ATP (Santa Maria) to 259,581 ATP (Oxnard). The median over the regional results is similar to the township cap estimated with all data points (204,200 ATP, Figure 3).

Table 7. The township cap values estimated by modeling areas

Area	N	Township cap (ATP)
Ripon	10	236,382
Watsonville	10	211,053
Parlier	20	189,355
Shafter	20	198,288
Santa Maria	10	181,021
Oxnard	10	259,581

Appendix VII. Township cap estimation based on logistic regression

The township cap in this study is determined by linear regression with township-year data points (Figure 3), which reflects the low-mobility scenario as specified in DPR's 1,3-D risk management directive (RMD) (Marks, 2016). In this appendix, an alternative method is tested with receptor-year data. There are 109,520 data points in total, including 80 ATP values and associated 1,369 (i.e., the number of receptors in each center township) annual average concentrations predicted for each ATP.

According to the input data structure, logistic regression is used by assigning "0" for the annual average concentration less than or equal to the target concentration of 0.56 ppb and "1" for those above the target. With "0" as the response event, the resulting regression equation is:

$$-\ln\left(\frac{1}{P}-1\right)=8.289-2.405\times10^{-5}X$$

where X is the ATP and P is the level of protection (i.e., the probability to have an annual concentration not exceeding 0.56 ppb). Both regression coefficients are significant, although the R^2 value is only 12.8%. At the required 95% protection (P=95%), the township cap (X) is calculated as 222,230 ATP.

The logistic regression with receptor-year data determines the 95% protection over all modeled center townships and scenarios. This is not consistent with the low-mobility scenario in the 1,3-D RMD, but reflects a higher mobility for which a larger township cap is usually expected.