Department of Pesticide Regulation
Environmental Monitoring Branch
1001 I Street, P.O. Box 4015
Sacramento, CA 95812-4015

Modeling for mitigation measures to reduce acute exposure from 1,3-Dichloropropene, modeling approach #1

Yuzhou Luo, Ph.D.

Research Scientist IV

9/12/2022

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 (**this report**)	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	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 lifetime cancer risk, Department of Pesticide Regulation (DPR) limits the use of 1,3-D on a regional basis (township cap) (Marks, 2016). To address acute exposures to non-occupational bystanders from 1,3-D, DPR recently established a regulatory target concentration of 55 ppb averaged over a 72-hour period (Henderson, 2021).

This study evaluates various options to mitigate acute exposure from 1,3-D applications. Mitigation options are implemented by introducing setbacks from occupied structures and reducing application rates and block sizes. The mitigation effects are evaluated by air dispersion modeling. A hypothetical set of 1,3-D applications is simulated for ambient concentrations according to the application conditions in terms of setback settings, application rate, block size, and month of application. The predicted concentrations, summarized as the 95^{th} percentile of 72-hour moving averages over a 5-year simulation period, are compared with the regulatory target concentration to determine the critical conditions.

A two-stage evaluation on the proposed mitigation options is conducted in this study. For a single application event, first, the required setback distances are determined as a function of application rate and block size. The modeling results are tabulated for the maximum allowed application block sizes for various application rates (100 – 332 lb/ac) and setback distances (100, 200, and 500ft). Second, multiple applications of 1,3-D are modeled for their combined effects on the acute exposure. Based on the modeling results, multiple applications may be subject to additional restrictions according to the distance and interval of applications. Additional restrictions are proposed by limiting the combined acreage of the involved applications and re-evaluating their setback distances.

3 Modeling approach for single applications

3.1 Field fumigation methods and flux time series

According to the updated 1,3-D regulation, 23 field fumigation methods (FFMs) are allowed in California (Appendix I), including 18 FFMs currently registered and 5 FFMs newly proposed (24-inch injection and 50% TIF methods). The FFMs are categorized into 8 groups according to injection depth, tarpaulin type, and emission ratio (Table 2). For each group of FFMs, the method with the highest 72-hour peak flux is selected as the representative FFMs and modeled for conservative estimation of setback distances (Table 2).

Table 2. Groups of field fumigation methods (FFMs) and the representative method

Group of FFMs	FFMs in the group
1-Standard nontarped and non-TIF tarp shallow (12 inch) methods	**1201**, 1202, 1203, 1204, 1205
2-Standard nontarped and non-TIF tarp deep (18 inch) methods	**1206**, 1207, 1208, 1210, 1211
3-Chemigation (drip)/non-TIF tarp method	**1209**
4-24-inch injection methods	**1224**, 1225, 1226
5-TIF methods – broadcast and drip	**1242**, 1247, 1249
6-TIF methods – bed and strip	**1243**, 1245, 1248, 1259
7-50% TIF with 18-inch injection depth method	**1250**
8-50% TIF with 24-inch injection depth method	**1264**

Notes: TIF = Totally Impermeable Film. Highlighted is the representative FFM for the group

For the representative FFMs, their flux time series with hourly flux rates ($\mu g/m^2/s$) were generated by HYDRUS model (Brown, 2022). The field conditions and management practices following the minimum requirements of 1,3-D field fumigations in the updated 1,3-D regulation, such as soil moisture and tarp cutting time (if applicable), have been reflected in the modeling of flux time series. The variability in soil properties is represented by the use of 21 soil datasets describing agricultural soils collected in fields prepared for fumigation. In summary, there are 168 flux time series (8 representative methods and 21 soils) used for air dispersion modeling in this study.

The flux time series are generated with a reference application rate of 100 lb/ac over a 500-hour period after application, by which time volatilization is effectively complete (Figure 1). A 100 lb/ac application rate was chosen as the reference rate primarily with respect to DPR conventions for the reporting of simulation results. Although the assumed 100 lb/ac application rate falls below the maximum allowed rate of 332 lbs/ac, HYDRUS-estimated flux varies linearly with application rate and the chosen rate therefore has no bearing on the outcome of a relative comparison such as the one performed here, provided application rates are identical across simulations.

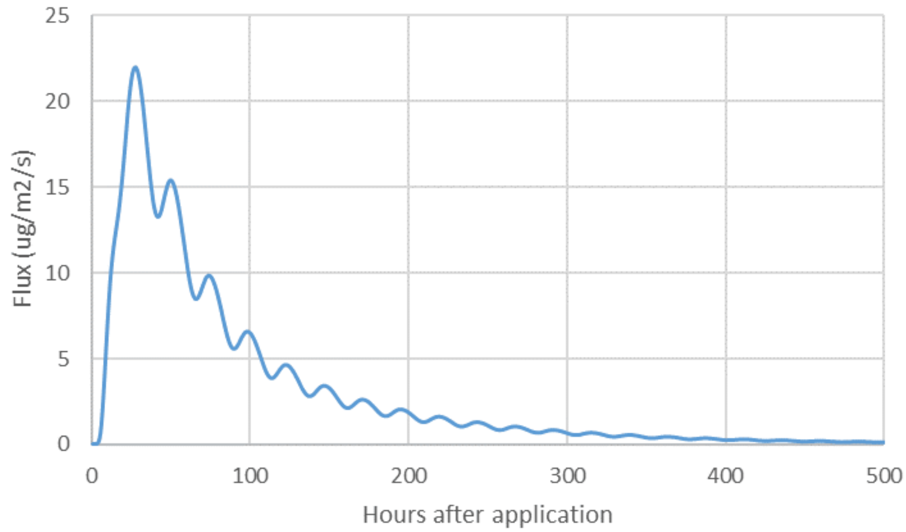


Figure 1. Example of the flux time series generated by HYDRUS, shown as one of the time series for FFM 1206

The flux time series were generated based on warm weather conditions. In order to investigate the effects of temperature on 1,3-D emissions, flux time series for cool-weather soil conditions were also generated with meteorological data representing multiple locations in California, using FFM 1206 as an example (Brown, 2019). Cool weather conditions result in lower air/water partitioning and slower degradation of 1,3-D. HYDRUS modeling results suggest that temperature effects on cumulative flux are likely to be minor compared to regional or seasonal variation in soil properties. Therefore, the effects are not considered in the estimation of setbacks.

3.2 Air dispersion modeling

Air concentrations of 1,3-D are simulated by AERFUM, an integrated air dispersion modeling system for soil fumigants developed by DPR (Luo, 2019a). The current version of AERFUM uses 64-bit AERMOD v21112 (USEPA, 2021) as the simulation engine for predicting hourly concentrations of 1,3-D in the air. AERFUM includes two modeling approaches: “unit simulation” which simulates a hypothetical pesticide application event on one field for air concentrations around the treated area, and “regional simulation” which simulates reported pesticide uses for concentration distribution at a regional scale (usually a 3×3 township area). This study is based on the unit simulation of AERFUM. The similar modeling approach has been used to determine the application factors of 1,3-D (Luo and Brown, 2022).

In addition to flux time series, the unit simulation of AERFUM is also driven by meteorological data. The effects of meteorological inputs on predicted acute exposure of 1,3-D have been preliminarily evaluated over the weather stations in high-use areas of 1,3-D of California. The tested stations and meteorological data have been used in the modeling efforts for application factors (Luo and Brown, 2022) and township caps (Luo, 2022) of 1,3-D. The evaluated high-use areas are located in the Counties of Fresno, Kern, Tulare, Stanislaus, San Joaquin, Imperial, Madera, Monterey, Santa Barbara, San Luis Obispo, Kings, Santa Cruz, and Ventura, accounting for 92% of statewide uses of 1,3-D by adjusted total pounds (ATPs) during 2013-2017. In these areas, meteorological data are retrieved from the Automated Surface Observing Systems (ASOS) program. In the 10 evaluated weather stations, 6 of them are located in the inland areas of California (Imperial, Madera, Merced, Parlier, Shafter, and Stockton) and 4 in the coastal areas (Salinas, Santa Maria, Oxnard, and Watsonville). Results showed that, with the same amount of 1,3-D emissions, meteorological data at Watsonville in Santa Cruz County generates the highest exposure potential, followed by Parlier in San Joaquin Valley. The predicted exposure potentials at other coastal stations (Salinas, Santa Maria, and Oxnard) are generally lower than the inland stations, and the average over all coastal stations is lower than that over the inland stations. In addition, the inland areas are associated with higher reported uses and higher observed air concentrations of 1,3-D than the coastal regions. For the statewide mitigation purpose, the selection of meteorological data is not just based on the results of individual stations, but also considers the regional comparison (inland vs. coastal areas) for the predicted exposure potentials and reported use amounts/patterns of 1,3-D. Therefore, the meteorological conditions in the inland areas, which are conservatively represented by Parlier data, are used for acute mitigation modeling in this study.

A 5-year simulation period during 2013-2017 is used in this study. Meteorological data are taken from the station at Parlier operated by National Weather Service (NWS), WBAN 93193 (WBAN = Weather-Bureau-Army-Navy, a five-digit identifier for NWS weather stations). The MetProc program (Luo, 2017) is utilized to generate meteorological input data during the simulation period in the AERMOD required format.

3.3 Simulation design

Setbacks around occupied structures (zones where no 1,3-D applications are allowed) are modeled as the mitigation practice to reduce acute exposure from 1,3-D applications. Setback settings include two components: setback distance and setback duration. Setback duration is the time period that the setback is in effect after application. At the end of setback duration, air concentration of 1,3-D should be lower than the regulatory target concentration of 55 ppb averaged over 72-hour period at the setback distance from the treated field.

In previous studies, buffer zone has been used by DPR to mitigate exposure from soil fumigants (DPR, 2017). Buffer distance and setback distance are associated with different physical meaning and field implementation. But they share the same value based on modeling approach where a critical distance from the edge of treated field is determined with the statistics of predicted air concentrations at the regulatory target concentration. For field implementation, setback distance is only applied to some of the directions from the treated field where occupied structures are located. For modeling purpose, however, it's reasonable to assume that an occupied structure could be located in any direction of the field. With this assumption, the setback distance around a structure mathematically establishes an equivalent "setback zone" (conceptually similar to a buffer zone) around the field where no structure is allowed to be occupied within the period of setback duration (Figure 2). Therefore, the modeling approach for determining buffer distance is used in this study for setback distance. In this report, "setback distance to a field" or "setback zone around a field" are used to describe modeling approach and results, by following the same terminology for buffer distance or buffer zone.

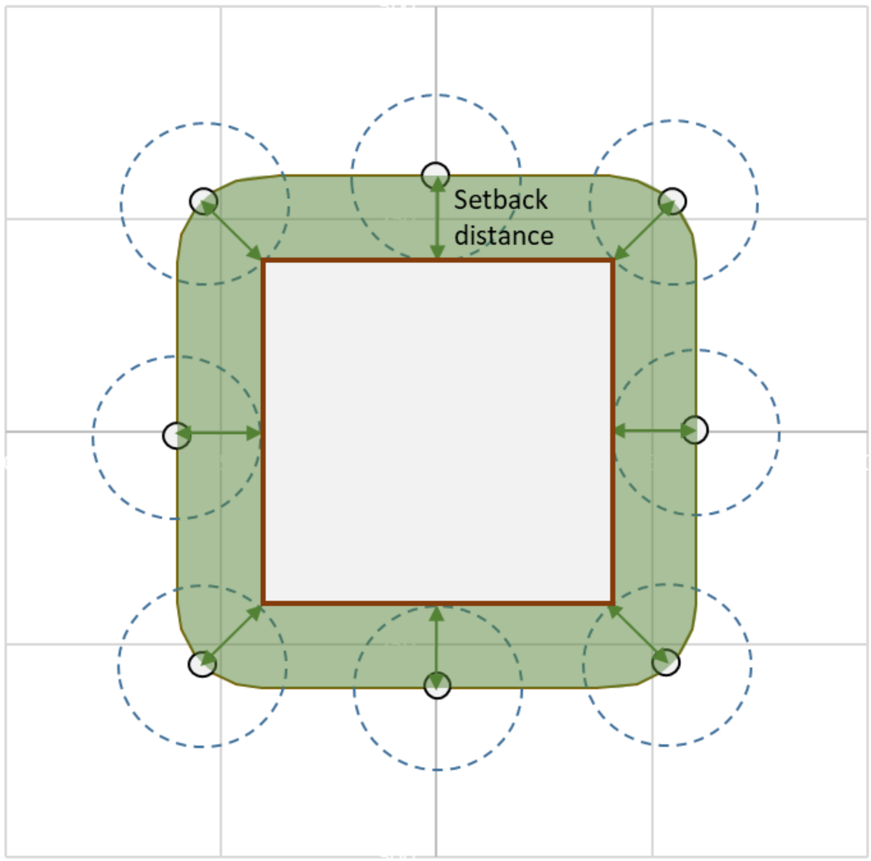


Figure 2. The setback distance around an occupied structure (open circle) near to a treated field mathematically establish an equivalent "setback zone" (shaded area) around the field, by modeling the structure at all potential directions from the field. Eight directions are shown in the figure for demonstration purpose.

AERFUM implements the modeling approach proposed by Johnson (2001) for buffer distances. The predicted air concentrations of 1,3-D are processed by following the "maximum direction" method to construct the probability distribution of buffer distances (Barry and Johnson, 2007). The probability distribution of buffer distances is established based on individual application on each day during the simulation period. (Barry, 2006; Johnson, 2001; Segawa et al., 2000). Thus, the resulting distribution reflects the variations in period-to-period meteorology. The 95th percentiles of the predicted daily results are calculated as the required buffer distance for the given flux time series, application rate, and application block size. This approach was incorporated in PERFUM (Reiss and Griffin, 2006), and has been used by DPR for evaluating the effectiveness of buffer zones for various fumigants, including 1,3-D, chloropicrin, methyl bromide, and methyl isothiocyanate (MITC)-generating pesticides (metam-sodium, dazomet, and metam-potassium).

AERFUM assumes the source area (i.e., treated field) as a square, and creates a grid of receptors around the source (Figure 3). Receptors are defined by the intersection of rings (rounded rectangles surrounding the field) and spokes (lines originated from the edges or corners of the field). More details on the receptor configuration are documented in the technique report for AERFUM (Luo, 2019a). This configuration is consistent with USEPA's definition on buffer distances for soil fumigants (USEPA, 2012).

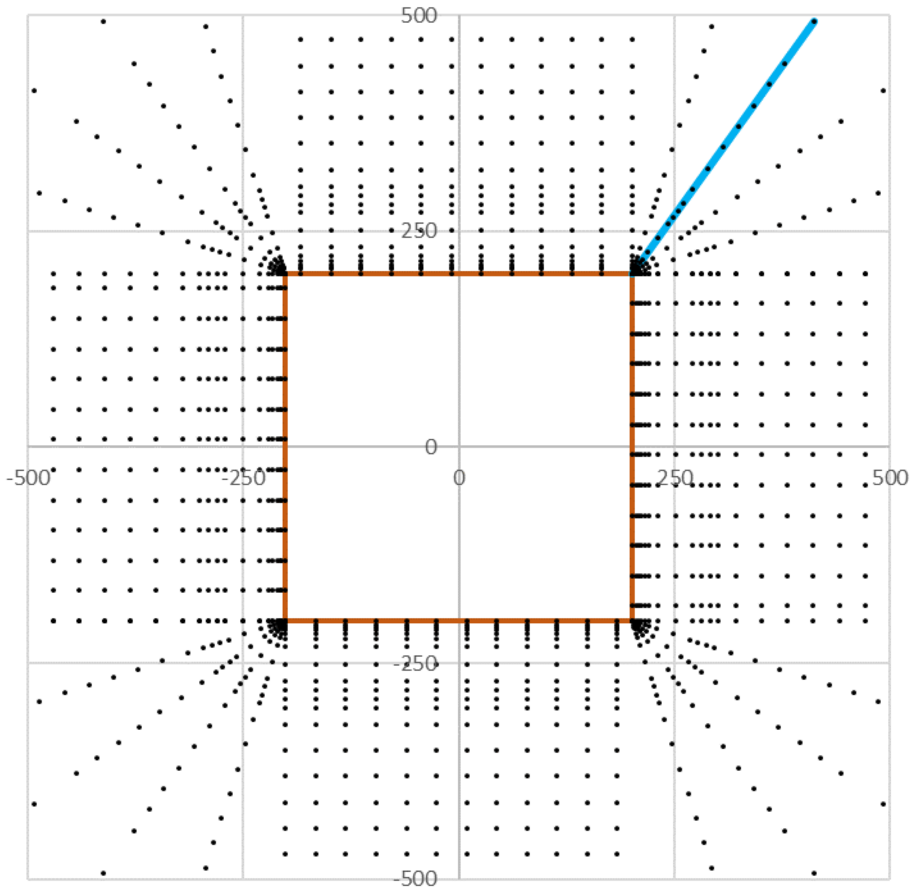


Figure 3. Receptor grids for a 40-ac field used in AERFUM for setback modeling, only showing receptors within about 500 meters from the field. Blue line is an example of a spoke. Distances are in meter.

The duration for setback or buffer zone has not been modeled in previous studies. In AERFUM, the setback duration is set as the critical time (after application) since when the 72-hour average concentrations *at the setback distance* are equal to or less than the regulatory target concentration. Modeling for buffer duration is also developed in AERFUM but not used in this study. It's worth noting that, although the distances for setback and buffer have the same value for a given set of inputs, the durations of setback and buffer are different. Buffer duration is longer than setback duration; additional time is needed for all receptors *in the simulation domain* having average concentrations equal to or less than the regulatory target concentration.

Table 3. Input data and parameters for model simulations

Inputs	Description	N
Field fumigation methods	Representative methods (Table 2)	8
Flux time series	21 time series (soils) for each method	21
Application rates (lb/ac)	100, 110, 125, 150, 200, 250, 300, and 332	8
Application block size (ac)	1, 5, 10, 20, 40, 60, and 80	7

AERFUM simulations are conducted for various flux time series, application rate, and application block sizes (Table 3). For each set of model inputs, the following model configurations and modeling procedures are implemented in AERFUM to determine the required setback distance and duration:

- Setup the source area and receptor grid according to the input application block size. Figure 3 shows an example for a 40-ac field.
- Start on 1/1/2013, a 1,3-D application event on the source area is assumed to be completed at 8AM. The hourly flux rates from the flux time series are adjusted by the specified application rate and assigned to the subsequent hours after application.
- At each receptor, predict hourly concentrations over the duration of flux time series (500 hours in this study).
- For each spoke of the receptor grid and each 72-hour averaging period, estimate the distance where the 72-hour average concentration is equal to the critical concentration (55ppb). Cubic spline interpolation is used to estimate the distance between receptors (Press et al., 2007).
- The maximum value of the resulting distances (from the edge of field) and associated time (hours after application) are reported as the setback distance and duration, respectively, for the first day of simulation (1/1/2013).
- Move to the next day in the simulation period (2013-2017), and repeat above processes. (Note: according to the 500-hour duration of flux time series, applications on the last 21 days of 2017 will not be modeled, i.e., 12/11/2017-12/31/2017).
- AERFUM generates 1805 pairs (1805 = total days 2013-2017 minus the flux duration) of daily setback distances and duration, indexed by date.
- Report the 95th percentile of daily setback distances and the 95th percentile of daily setback durations as the final results of setback settings required for the input dataset of flux time series, application rate, and block size.

All percentile results are calculated with the percentile function in NumPy (https://numpy.org/). The same function has been used in the previous study for summarizing monitoring data of 1,3-D (Luo, 2019b). AERFUM continuously models all days and months during the simulation period. Since 1,3-D applications are prohibited in December (Marks, 2016), however, all daily results (setback distances and setback durations) simulated from applications in December are excluded before the percentile calculation.

Modeling results show that a setback duration of 7 days is sufficient for any FFM even at the worst-case condition (i.e., application rate of 332 lb/ac and application block size of 80 ac. See Section 4.1 for more information). Therefore, 7-d setback duration is set as the minimum requirement, while the post-processing of modeling results is focused on setback distances. For each FFM, its 21 flux time series result in 21 values of setback distances for each season by following the above modeling procedures. The median value of the distances for each season is reported for the corresponding set of FFM, application rate, and application block size. In total, 448 (=8 FFMs × 8 rates × 7 block sizes, Table 3) setback distances are derived as a function of season, FFM, application rate, and application block size. The modeling results are further interpolated to determine the maximum application rate and maximum application block size for each FFM and season at 3 predefined setback distances of 100, 200, and 500 ft.

4 Modeling results for single applications

4.1 Setback settings under the worst-case condition

Setback distances and durations are first modeled by AERFUM for the worst-case condition with the maximum application rate of 332 lb/ac and the maximum application block size of 80 ac. The median values of model predictions over the 21 soils are reported for each FFM and season (Table 4).

Table 4. Setback settings required for 1,3-D application under the worst-case condition (application rate of 332lb/ac and application block size of 80ac)

FFM	Setback distance (ft)	Setback duration (day)
1201	4615	2
1206	1932	4
1209	3200	1
1224	741	4
1242	0	0
1243	594	3
1250	890	3
1264	183	4

The currently registered non-tarp and non-TIF tarp methods (FFMs 1201-1211, represented by FFMs 1201, 1206, and 1209 in this study) require setback distances significantly larger than the TIF methods and newly proposed methods (24-inch injection and 50%TIF) ($p < 0.001$). Setback distances also vary with soils. For FFM1206 as an example, the predicted buffer distances range from 54.5 to 4393.4 ft. Soil #5 is generally predicted with largest buffer distances over the modeled soils. This soil was measured with lowest moisture level in fields prepared for fumigation (Brown, 2022).

For FFM1242, the predicted setback distance and duration of zero indicate that no setback is needed for the method even under the worst-case condition. Therefore, no additional restrictions are needed for applications with FFM1242.

Predicted setback durations are less than 7 days for all FFMs even under the worst-case condition. Therefore, the label requirement for a setback duration of 7 days is adequate. The following modeling efforts will only focus on setback distances.

4.2 Restrictions on application rate and block size

Table 4 shows an example of modeling results of buffer distances under the worst-case condition (application rate of 332 lb/ac and block size of 80 ac). The same modeling procedures are conducted for other combinations of application rates and block sizes (Table 3). The modeling results are combined for the setback distance as a function of application rate and block size for each FFM:

[distance] = f (rate, block size), for an FFM

At a given setback distance (one of the 3 predefined distances of 100, 200, or 500 ft) and application rate (one of the 8 predefined rates from 100 to 332 lb/ac, Table 2), the above function is interpolated for the maximum application block size. The results are tabulated for each group of FFMs represented by the modeled FFM (Table 5). The predicted maximum application block sizes are rounded down the nearest 5 (or down to the nearest integer if the prediction is less than 5). For example, a predicted value of 7.5 ac is reported as 5 ac in the table. Two special conditions are considered:

1) If the estimated application block size is less than 1 ac, the corresponding application (by FFM, application rate, and setback distance) is “Not Allowed”.
2) If the estimated application block size is larger than 80 ac, “no restriction” (NR) is required for the corresponding application in addition to the minimum requirements (i.e., setback distance = 100 ft).

Table 5. Maximum application block sizes

(a) Standard nontarped and non-TIF tarp shallow (12-inch) methods

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size (ac) and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	4	5	20
110 lbs/ac	3	5	20
125 lbs/ac	2	5	15
150 lbs/ac	1	3	10
200 lbs/ac	Not allowed	2	5
250 lbs/ac	Not allowed	1	5
300 lbs/ac	Not allowed	Not allowed	3
332 lbs/ac	Not allowed	Not allowed	3

(b) Standard nontarped and non-TIF tarp deep (18 inch) methods

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size (ac) and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	40	55	NR
110 lbs/ac	30	45	NR
125 lbs/ac	20	35	75

150 lbs/ac	15	25	55
200 lbs/ac	5	10	30
250 lbs/ac	4	5	20
300 lbs/ac	2	5	15
332 lbs/ac	2	4	10

(c) Chemigation (drip)/non-TIF tarp method

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size (ac) and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	10	20	45
110 lbs/ac	5	15	40
125 lbs/ac	5	10	30
150 lbs/ac	4	5	20
200 lbs/ac	2	4	15
250 lbs/ac	1	2	10
300 lbs/ac	Not allowed	2	5
332 lbs/ac	Not allowed	1	5

(d) 24-inch injection methods

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size (ac) and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	NR	NR	NR
110 lbs/ac	NR	NR	NR
125 lbs/ac	NR	NR	NR
150 lbs/ac	NR	NR	NR
200 lbs/ac	40	60	NR
250 lbs/ac	25	35	75
300 lbs/ac	15	25	55
332 lbs/ac	10	20	45

(e) Totally Impermeable Film (TIF) methods – broadcast and drip (FFMs 1242, 1247, and 1249)

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size (ac) and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	NR	NR	NR
110 lbs/ac	NR	NR	NR
125 lbs/ac	NR	NR	NR
150 lbs/ac	NR	NR	NR
200 lbs/ac	NR	NR	NR
250 lbs/ac	NR	NR	NR
300 lbs/ac	NR	NR	NR
332 lbs/ac	NR	NR	NR

(f) Totally Impermeable Film (TIF) methods – bed and strip (FFMs 1243, 1245, and 1259)

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	NR	NR	NR
110 lbs/ac	NR	NR	NR
125 lbs/ac	NR	NR	NR
150 lbs/ac	NR	NR	NR
200 lbs/ac	55	NR	NR
250 lbs/ac	30	50	NR
300 lbs/ac	20	30	70
332 lbs/ac	15	25	55

(g) 50% TIF with 18-inch injection depth method

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	NR	NR	NR
110 lbs/ac	NR	NR	NR
125 lbs/ac	NR	NR	NR
150 lbs/ac	60	NR	NR
200 lbs/ac	30	45	NR
250 lbs/ac	15	30	65
300 lbs/ac	10	20	45
332 lbs/ac	5	15	40

(h) 50% TIF with 24-inch injection depth method

Broadcast Equivalent a.i. App Rate	Maximum Application Block Size and Occupied Structure Distance		
	100 ft	200 ft	500 ft
100 lbs/ac	NR	NR	NR
110 lbs/ac	NR	NR	NR
125 lbs/ac	NR	NR	NR
150 lbs/ac	NR	NR	NR
200 lbs/ac	NR	NR	NR
250 lbs/ac	NR	NR	NR
300 lbs/ac	65	NR	NR
332 lbs/ac	50	70	NR

With the proposed restrictions in Table 5, some of the historical uses of 1,3-D may not be allowed in the future. For example, an 18-inch method (FFM1206, Table 5b) with a rate of 332 lb/ac over a 15-ac field is no longer allowed. A lower-emission method such as 24-inch injection (FFM1224), TIF methods, or 50% TIF methods, can be used for the same rate and acreage by following the required setback distances (Table 5d to Table 5e). Alternatively, the treated field could be divided as multiple applications with smaller acreages according to the provided setback tables. In addition to the minimum requirements and setback distances for single applications of 1,3-D, those multiple applications are also subject to additional restrictions as described in the next sections.

5 Modeling approach for multiple applications

5.1 Conceptual model

In this study, multiple applications are defined as two or more field fumigations of 1,3-D close to each other by time (interval between applications) and space (distance between treated areas). For example, 1,3-D application events were reported for three adjacent fields in Shafter (sections of M28S25E01 and M28S26E06) on three consecutive days of October 15 to 17, 2020, with a total treated area of 78.4 ac and total applied mass of 6230.5 lb (Table 6). Based on the reported FFM, application rate, and block size, each individual application meets the requirements for field fumigation with a setback distance of 100 ft (Table 5b). However, the multiple applications on adjacent fields could result in additional exposure which may not be sufficiently mitigated by the field fumigation requirements derived for single applications.

Table 6. Example of multiple applications of 1,3-D on adjacent fields

Section	Date	FFM	Application rate (lb/ac)	Application block size (ac)	Required setback distance (ft)
M28S25E01	10/15/2020	1206	79.5	19.0	100
M28S26E06	10/16/2020	1206	79.5	19.1	100
M28S26E06	10/17/2020	1206	79.5	40.3	100

Note: the required setback distance for each individual application is determined from Table 5b.

Previous regulations on buffer zone proximity (DPR, 2017) suggested that multiple applications of soil fumigants would be restricted by the combined acreage and the worst-case condition among the involved applications. For conservative estimation, therefore, multiple applications of 1,3-D are modeled in this study with two applications with the maximum application rate and maximum application block size according to the mitigation measures for single applications (Table 5). The two treated areas for modeling are labelled as "Field1" (the earlier application) and "Field2" (the later application), respectively, and their spatiotemporal relationship is defined based on two parameters:

- Distance (ΔL) between the edges of the two treated fields (Figure 4).
- Time interval (ΔT) between the two application events.

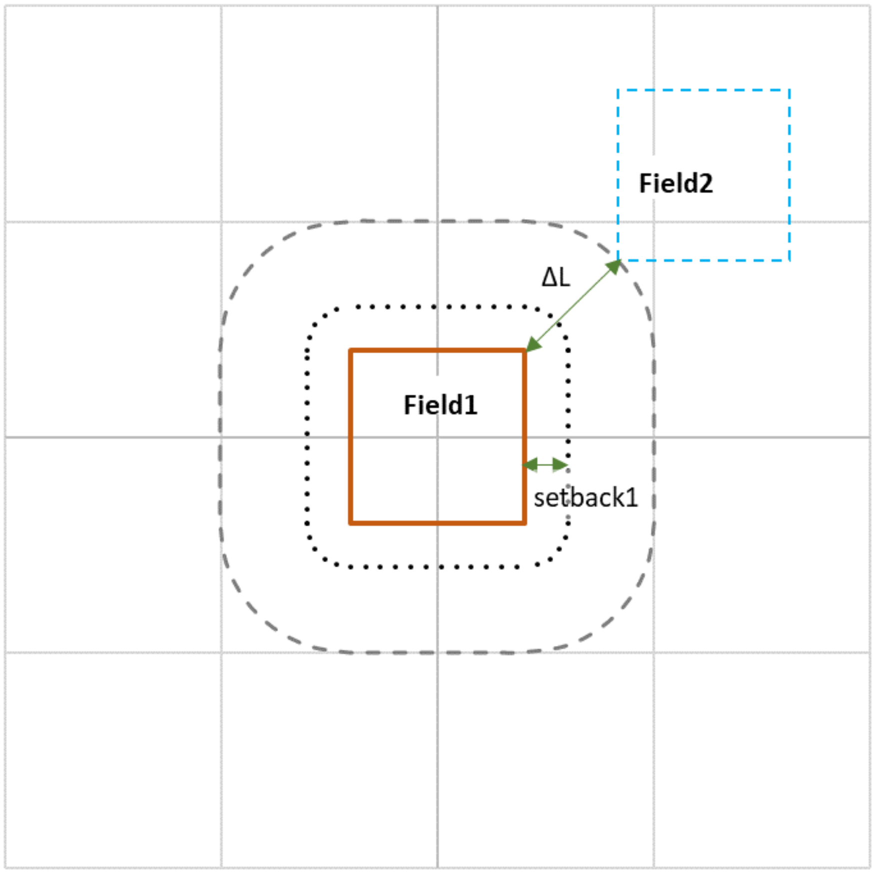


Figure 4. Definition of the distance between two fields. The dashed line delineates a perimeter with the same distance ΔL. Black dots represent receptors at the required setback distance for "Field1".

For example, the three adjacent applications on consecutive days in Table 6 could be characterized as ΔL=0 and ΔT= 1 or 2 days. ΔL is defined as the same way as in the modeling for setback distance (Figure 4). Note that "Field2" represents an ensemble of all potential locations of the second field with a distance of ΔL to the "Field1", while Figure 4 only shows one of the locations for demonstration purpose. To reflect the temporal variation of wind direction, multiple locations of "Field2" would be considered in model simulations. More details on the model simulation design are provided in the next section. To be consistent with HYDRUS modeling on flux time series (Brown, 2022), ΔT is counted by the completion time of applications. For example, if the earlier application is started at 8AM on day 1 and the later one at 8AM on day 3, the application interval is 48 hours. In addition to the application interval used for modeling (ΔT), multiple applications are also characterized by a separation time in field fumigations, defined as the time period "from the time the earlier application is complete until the start of the later application" (DPR, 2017). By assuming that it takes 12 hours to complete a fumigation, the required separation time can be estimated from the corresponding application interval as [separation time] = ΔT-12. For example, a 36-hour separation time is equivalent to a ΔT of 48 hours.

To facilitate the evaluation, an "*exposure concentration*" (i.e., concentration for exposure assessment) is defined in this study to summarize the predicted concentrations of 1,3-D on the perimeter of the setback distance from "Field1" (dots in Figure 4) with the averaging period (72 hours) and probability (95% over a 5-year simulation period excluding December). The setback distance for "Field1" is determined from Table 5 according to its application method, rate, and block size. By definition, if "Field1" is the only source in the simulation domain, the predicted exposure concentration at the setback distance from "Field1" is equal to or lower than the target concentration of 55 ppb. With the introduction of "Field2", the exposure concentration could be increased, and thus should be re-modeled to determine the "dependence" between the two applications:

- Dependent applications. After the introduction of "Field2", if the exposure concentration predicted along the setback distance from "Field1" *exceeds the target concentration*, the two applications are considered to be "dependent" under the corresponding settings (ΔT and ΔL). For example, two simultaneous applications ($\Delta T=0$) on adjacent fields ($\Delta L=0$) are probably dependent applications. Setback distances for dependent applications would be re-evaluated by combining all application as one hypothetical application. Section 6 provides detailed information on the additional restrictions and associated critical conditions of ΔL and ΔT.
- Independent applications. After the introduction of "Field2", if the exposure concentration predicted along the setback distance from "Field1" is still *equal to or lower than the targe concentration*, the two applications are "independent" under the corresponding settings (ΔT and ΔL). In this case, additional restrictions are not required for either application. Applications with large values of ΔL and ΔT are likely to be independent.

Similar approach has been used in DPR's mitigation efforts on chloropicrin, where applications are considered dependent if their buffer distances overlap within 36-hour separation time between the earlier and later applications (DPR, 2017). Commonly used mitigation measure for dependent multiple applications is to increase setback distances (in addition to the distance required for single, independent applications). For chloropicrin, the buffer distance should be updated based on the combined acreages of all dependent applications (DPR, 2017).

The modeling approach for single-field assessment (Section 3) is extended for applications to multiple fields. Modeling capability is developed in AERFUM by evaluating the effects of ΔL and ΔT on the acute exposure from multiple applications of 1,3-D. The objectives of modeling are to (1) determine the critical conditions for multiple applications to be dependent, and (2) propose additional restrictions for multiple dependent applications.

5.2 AERFUM development and simulation design

In the model configuration for multiple applications, the main source "Field1" is located at the center of the simulation domain. The second source "Field2" is located around "Field1" with a given distance ΔL. To reflect the variations in period-to-period meteorology, potential locations of "Field2" are considered in eight directions from "Field1": E, NE, N, NW, W, SW, S, SE

(Figure 5). In summary, there are 9 model runs ("Field1" and the eight locations of "Field2") in AERFUM; each will be modeled with the same 5-year meteorological data.

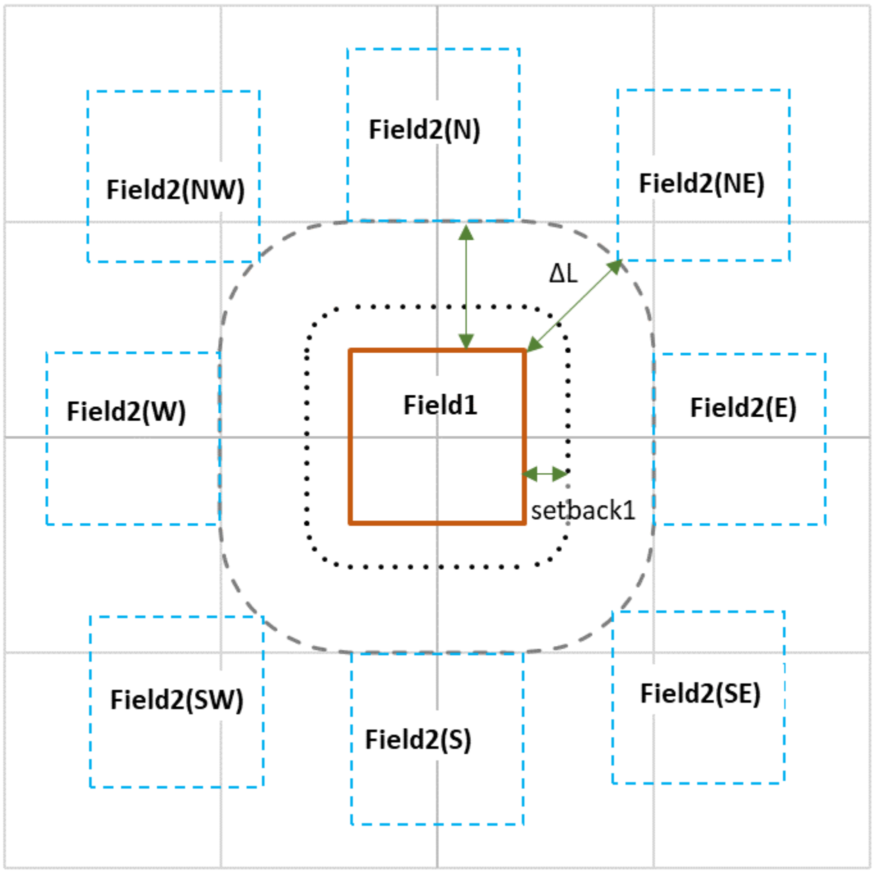


Figure 5. Simulation domain for multiple applications, showing the main source "Field1" and the eight potential locations of the 2nd source "Field2" with a distance of ΔL from "Field1". Black dots represent receptors at the required setback distance for "Field1".

A grid of receptors is generated around "Field1" by following the configurations for setback modeling (Figure 3), but only at the given setback distance "setback1" (Figure 5). AERFUM manages model simulations for the 9 fields/locations ("Field1" and the 8 locations of "Field2") to generate hourly concentrations at each receptor. It's assumed that the 8 locations of "Field2" have equal chance (1/8) for the second application. Therefore, the total concentration (C) with contributions from all fields/locations for each hour and each receptor is aggregated as,

$$C = C_0 + \frac{1}{8}\sum_{i=1}^{8} C_i \quad (1)$$

where C_0 is the concentration from the application in "Field1" and C_1 to C_8 are the contributions from applications in the 8 locations of "Field2" (Figure 5). The total concentrations predicted along the perimeter of ΔL are used to calculate the exposure concentration, which is further compared with the target concentration (55 ppb over a 72-hour period) to evaluate the combined exposure from the modeled multiple applications.

According to the placement of the receptors, two special conditions are considered in the modeling:

- Receptors located within "Field2" (ΔL < [setback1]). In this case, all concentrations predicted at these receptors will be excluded from the calculation of moving average concentrations for the corresponding "Field2".
- Receptors located within the setback distance of "Field2" ([setback1] < ΔL < [setback1] + [setback2]). Modeling results for these receptors during the setback duration of 7 days are excluded from the calculation of moving average concentrations for the corresponding "Field2".

To simplify the model simulations and capture the worst-case conditions, the following assumptions are incorporated in the model configurations for multiple applications:

- The two applications on "Field1" and "Field2" are assumed to have the same method, rate, and block size. Therefore, they have the same setback distance as retrieved from Table 5 for single applications, i.e., [setback1] = [setback2].
- For each FFM and each distance of setbacks (100, 200, or 500ft), the worst-case condition for modeling multiple applications is defined based on the maximum allowed mass of 1,3-D for each single application. The allowed mass is calculated as the product of application rate and block size paired in Table 5. The allowed mass increases with the application block size. For FFM1206 with a 100-ft setback as an example (Table 5b), the maximum mass applied is increased from 664 lb for a 2-ac field (with the maximum allowed application rate of 332 lb/ac) to 4000 lb for a 40-ac field (100 lb/ac).
- Since the setback distances (Table 5) are developed for each application block size, the predicted exposure concentrations for multiple applications are insensitive to the modeled block size. In this study, the maximum size of 80 ac is used to model multiple applications.
- For the application block size of 80 ac, the maximum allowed single application rate ("rate limit") is determined by interpolating the setback modeling results, same as that used in the generation of setback tables (Table 5). Note that the rate limits for 80 ac are calculated for all FFMs and setbacks, but some of them are not reported in Table 5 if they are below 100 lb/ac.
- For each FFM and each season, there are 3 rate limits (for the 3 setback distances of 100, 200, and 500ft) used in model simulations. Results show that the rate limits with the 100-ft setback generate the highest exposure concentrations in most cases compared to the other two setback distances (200 and 500 ft). Therefore, results for rate limits at 100 ft are presented in the main text of the report and used for the evaluation of multiple applications. Results for rate limits at 500 ft are provided in Appendix II for comparison.
- Similar to the previous mitigation on multiple applications (DPR, 2017), the applications with "overlapping setbacks" are modeled in this study. Two critical model configurations are considered: "adjacent fields" (ΔL=0) and [2] "adjacent setbacks" (ΔL = [setback1] + [setback2]) where [setback1] and [setback2] are the setback distances for single

applications of "Field1" and "Field2", respectively. According to the above assumptions and discussions, [setback1] = [setback2] =100 ft.

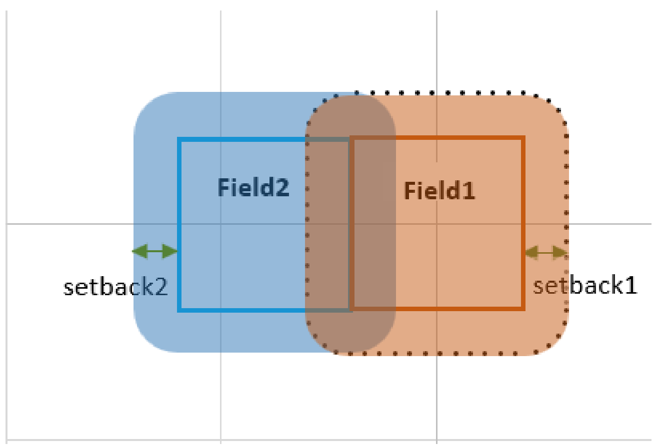
- Various time intervals (ΔT = 0, 24, 48, 72, and 96 hours) between the two applications are modeled. To be consistent with the predefined completion time in the 1,3-D flux time series, this study assumes that all applications are completed at 8AM, and thus ΔT increases by 24 hours. For example, applications scheduled on the same day are conservatively modeled as simultaneous applications (i.e., ΔT = 0), and applications scheduled on two consecutive days are modeled with ΔT = 24 hours.

6 Modeling results for multiple applications

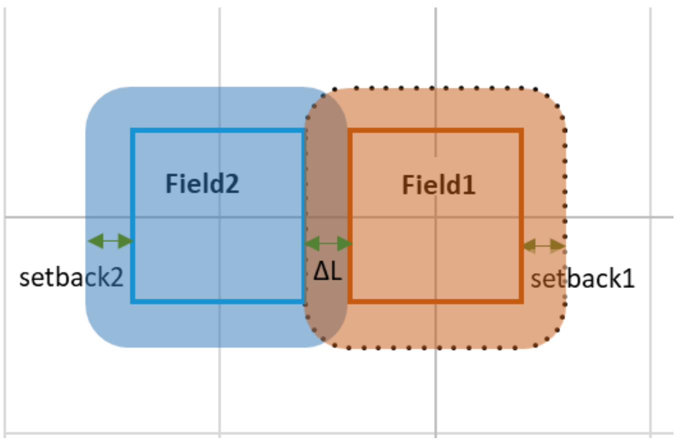
6.1 Predicted concentrations from multiple applications with setbacks overlapping

AERFUM simulations are conducted for two identical applications with overlapping setbacks. According to the discussions in Section 5.2, the fields are modeled with application block size of 80 ac, setback distance of 100 ft, and corresponding maximum application rate determined from the setback modeling for single applications. Three critical model configurations are considered: ΔL = 0 ("adjacent fields", Figure 6a), ΔL = 100 ft (Figure 6b), and ΔL = 200 ft ("adjacent setbacks", Figure 6c).

(a)



(b)



(c)

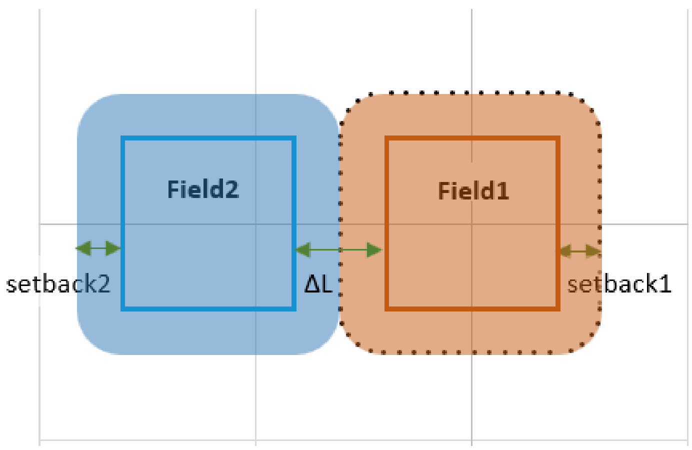


Figure 6. Model configurations for (a) ΔL=0 (adjacent fields), (b) ΔL=[setback] (setback adjacent to field), and (c) ΔL= 2×[setback] (adjacent setbacks). Two identical fields are modeled in this study, so [setback1]=[setback2]. Eight locations are modeled for "Field2" (Figure 5), here showing only one of them for demonstration.

Modeling results show that the configuration of "adjacent setbacks" (Figure 6c) generates higher concentrations than the other two conditions. For the fields adjacent to each other (Figure 6a) or one field adjacent to the setback perimeter of the other field (Figure 6b), some receptors for air dispersion modeling are located within the treated area or within the setback zone. In AERFUM simulations, these receptors will be fully or partially excluded from the calculation of exposure concentrations. Specifically, the receptors within a treated field (where an occupied structure is unlikely located) will be excluded for all hours of simulation, while the receptors within the setback zone (but not in the treated field) will be excluded for the setback duration of 7 days. These receptors are usually associated with high concentrations due to their proximity to both treated fields. By excluding them, the resulting exposure concentrations are less than those with the model configuration of "adjacent setbacks" (Figure 6b) where all receptors are used for determining the exposure concentration. Therefore, "adjacent setbacks" (ΔL=200 ft modeled here) represent the worst-case condition for the spatial placement of the two applications with overlapping setbacks.

The modeling results for "adjacent setbacks" are presented as the exposure concentrations (Table 7), which are compared to the target concentration of 55 ppb for exposure analysis. Model predictions exceeding the target concentration are highlighted in the table. There is a general decreasing trend for the predicted concentrations with the interval between the two applications (ΔT). With ΔT≤48 hours, most of the application methods are associated with concentrations above the regulatory target. The exceptions are FFM1242. No restrictions are proposed for this method even with the highest application rate and block size, indicated by "NR" in Table 5e. With the interval increased to 72 or 96 hours, only some of the application methods and seasons are predicted with exposure concentration above 55 ppb. With ΔT>96 hours (modeled as 120 hours), predictions for all methods and seasons are equal to or less than 55 ppb (the last column in Table 7).

Table 7. Predicted exposure concentrations (ppb) from two applications of 1,3-D with adjacent setbacks (ΔL=200 ft) with application interval (ΔT) from 0 to 120 hours (shaded are concentrations above 55ppb)

FFM	ΔT=0	ΔT=24 hr	ΔT=48 hr	ΔT=72 hr	ΔT=96 hr	ΔT=120 hr
1201	58.5	58.1	56.2	≤55	≤55	≤55
1206	59.1	58.5	56.7	≤55	≤55	≤55
1209	59.2	58.8	57.0	≤55	≤55	≤55
1224	59.9	59.6	58.1	56.6	55.2	≤55
1242	≤55	≤55	≤55	≤55	≤55	≤55
1243	60.2	59.4	58.3	56.4	55.1	≤55
1250	59.9	58.5	56.8	55.4	≤55	≤55
1264	60.4	59.8	58.7	57.3	55.9	≤55

In addition to the setback distance of 100 ft, this study also models applications with a 500-ft setback. Results are provided in Appendix II. As mentioned before, predicted concentrations for applications with a 500-ft setback are generally lower than these with 100-ft setback (Table 7).

6.2 Predicted protection levels with an application interval of 48 hours

To be consistent with the 36-hour separation required for overlapping buffer zones of chloropicrin applications (DPR, 2017), the application interval of 48 hours modeled for 1,3-D is further investigated. For most of the application methods, the predicted concentrations at ΔT=48 hours exceed the target concentration of 55 ppb (Table 7), suggesting a protection level below 95%. Additional model simulations are conducted to estimate the acute protection level with the given application interval of 48 hours (Table 8). Modeling results show that multiple applications with a 48-hour interval could provide at least 93.2% protection over the 5-year simulation period. Except for the methods of FFM1242, the predicted protection levels (93.2% - 94.3%) are slightly lower than the expected level of 95%. With the conservative configurations used in the modeling, the protection could be underestimated compared to that in the field conditions. In addition, multiple applications with overlapping setbacks are less frequently observed relative to single, independent applications. Therefore, a 48-hour interval (i.e., 36-hour separation) is accepted in this study as the criteria for multiple applications of 1,3-D requiring additional restrictions.

Table 8. Predicted protection levels with a 48-hour interval (i.e., 36-hour separation) between applications

FFM	Jan-Nov
1201	93.9%
1206	94.3%
1209	93.8%
1224	93.8%
1242	≥95%
1243	93.6%
1250	93.9%
1264	93.2%

6.3 Additional restrictions for multiple applications

Based on the modeling results, the following criteria are proposed to identify multiple applications which are dependent to other each:

- Setbacks for two or more applications overlap within 36 hours from the time the earlier application is complete until the start of the later application.

Dependent multiple applications should be conservatively considered as one application, and subject to additional restrictions, including:

- Combined acreage of all blocks shall not exceed 80 acres, and
- Setback distance shall be re-evaluated from Table 5 based on the combined acreage of all overlapping blocks, the highest application rate, and the application method with the highest setback distance.

If all blocks are treated by the same method, the above restrictions can be simplified as:

- Combined acreage of all blocks shall not exceed 80 acres, and
- Setback distance shall be re-evaluated based on the combined acreage and the highest application rate of all overlapping blocks.

Taking the multiple applications in Table 6 as an example, the applications to three blocks are dependent because they are adjacent to each other and treated on consecutive days. Input data for the re-evaluation of required setback distance include: [1] application method = FFM1206 for all blocks, [2] the combined acreage = 78.4, and [3] the maximum application rate = 79.5 lb/ac. A new distance of setback is determined from Table 5b as 500 ft, compared to 100 ft for individual applications (Table 6). The new distance should be applied to all of the three blocks.

Alternative, the multiple applications could be rescheduled with a time interval larger than 36 hours from the time the earlier application is complete until the start of the later application, so that they are considered to be independent to each other. Independent applications are not subject to restrictions in addition to the mitigation measures for single applications.

Acknowledgments

The author acknowledges Colin Brown, Jing Tao, Jazmin Gonzalez, Aniela Burant, Maziar Kandelous, Minh Pham, Edgar Vidrio, Pam Wofford, Randy Segawa, and Karen Morrison for valuable discussions and critical reviews in the initialization and development of this study.

References

Barry, T. (2006). Development of methyl isothiocyanate buffer zones using the probabilistic exposure and risk model for fumigants version 2 (PERFUM2). California Department of Pesticide Regulation, Sacramento, CA.

Barry, T. and B. Johnson (2007). Analysis of the relationship between percentiles of the whole field buffer zone distribution and the maximum direction buffer zone. California Department of Pesticide Regulation, Sacramento, CA.

Brown, C. (2019). HYDRUS-simulated flux estimates of 1,3-Dichlorpropene max period-averaged flux and emission ratio for approved application methods. California Department of Pesticide Regulation, Sacramento, CA.

Brown, C. (2022). Updates to HYDRUS-simulated flux estimates of 1,3-dichloropropene maximum period-averaged flux and emission ratios. California Department of Pesticide Regulation, Sacramento, CA.

DPR (2017). Additional Labeling Requirements for Use of All Products Containing Chloropicrin as an Active Ingredient in California. California Department of Pesticide Regulation, Sacramento, CA.

Henderson, J. (2021). Risk management directive and mitigation guidance for acute, non-occupational bystander exposure from 1,3-dichlorpropene (1,3-D). California Department of Pesticide Regulation, Sacramento, CA.

Johnson, B. (2001). Evaluating the Effectiveness of Methyl Bromide Soil Buffer Zones in Maintaining Acute Exposures Below a Reference Air Concentration. California Department of Pesticide Regulation, Sacramento, CA.

Luo, Y. (2017). Meteorological data processing for ISCST3 and AERMOD. California Department of Pesticide Regulation, Sacramento, CA.

Luo, Y. (2019a). AERFUM: an integrated air dispersion modeling system for soil fumigants. California Department of Pesticide Regulation, Sacramento, CA.

Luo, Y. (2019b). Evaluating AERMOD for simulating ambient concentrations of 1,3-Dichloropropene. California Department of Pesticide Regulation, Sacramento, CA.

Luo, Y. and C. Brown (2022). Modeling for application factors of 1,3-Dichloropropene, modeling approach #1 (under review). California Department of Pesticide Regulation, Sacramento, CA.

Luo, Y. (2022). Modeling for the township cap of 1,3-Dichloropropene applications, modeling approach #1 (under review). California Department of Pesticide Regulation, Sacramento, CA.

Marks, T. (2016). Risk management directive and mitigation guidance for cancer risk from 1,3-Dichlorpropene (1,3-D). California Department of Pesticide Regulation, Sacramento, CA.
Press, W. H., S. A. Teukolsky, W. T. Vetterling and B. P. Flannery (2007). Numerical Recipes 3rd Edition: The Art of Scientific Computing, Cambridge University Press.
Reiss, R. and J. Griffin (2006). A probabilistic model for acute bystander exposure and risk assessment for soil fumigants. Atmospheric Environment 40(19): 3548-3560.
Segawa, R., T. Barry and B. Johnson (2000). Recommendations for methyl bromide buffer zones for field fumigations. California Department of Pesticide Regulation, Sacramento, CA.
USEPA (2012). Calculating Buffer Zones: A Guide for Applicators. U.S. Environmental Protection Agency, Office of Pesticide Program, Washington, DC.
USEPA (2021). User's Guide for the AMS/EPA Regulatory Model (AERMOD), version 21112 (EPA-454/B-21-001). U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC.

Appendix I. 1,3-Dichloropropene field fumigation methods

Method Group	Method Name	Field Fumigation Method (FFM) Code
1	Nontarp/shallow/broadcast or bed	1201
1	Tarp/shallow/broadcast	1202
1	Tarp/shallow/bed	1203
1	Nontarp/shallow/broadcast or bed/3 water treatments	1204
1	Tarp/shallow/bed/3 water treatments	1205
2	Nontarp/18 inches deep/broadcast or bed	1206
2	Tarp/18 inches deep/broadcast	1207
2	Tarp/18 inches deep/bed	1208
3	Chemigation (drip system)/tarp	1209
2	Nontarp/18 inches deep/strip	1210
2	Nontarp/18 inches deep/GPS targeted	1211
4	Nontarp/24 inches deep/broadcast	1224
4	Tarp/24 inches deep/broadcast	1225
4	Nontarp/24 inches deep/strip	1226
5	Totally Impermeable Film (TIF) tarp/shallow/broadcast	1242
6	TIF tarp/shallow/bed	1243
6	TIF tarp/shallow/bed/3 water treatments	1245
5	TIF tarp/deep/broadcast	1247
6	TIF tarp/deep/bed	1248
5	TIF tarp/deep/strip	1249
7	50% TIF tarp/18 inches deep/broadcast	1250
6	Chemigation (drip)/ TIF tarp	1259
8	50% TIF tarp/24 inches deep/broadcast	1264

Appendix II. Modeling results for two applications with adjacent 500-ft setbacks

FFM	ΔT=0	ΔT=24 hr	ΔT=48 hr	ΔT=72 hr	ΔT=96 hr	ΔT=120 hr
1201	59.0	58.9	56.7	≤55	≤55	
1206	59.3	58.4	56.8	55.1	≤55	
1209	59.0	58.4	56.6	≤55	≤55	
1224	59.3	58.2	57.1	55.8	≤55	
1242	≤55	≤55	≤55	≤55	≤55	
1243	59.8	58.9	58.1	56.5	≤55	
1250	59.7	59.6	58.0	56.4	≤55	
1264	≤55	≤55	≤55	≤55	≤55	

Notes: ΔL=1000 (adjacent setbacks). Application block size = 80 ac, and application rate = the rate limit for the corresponding method, block size, and month of application.