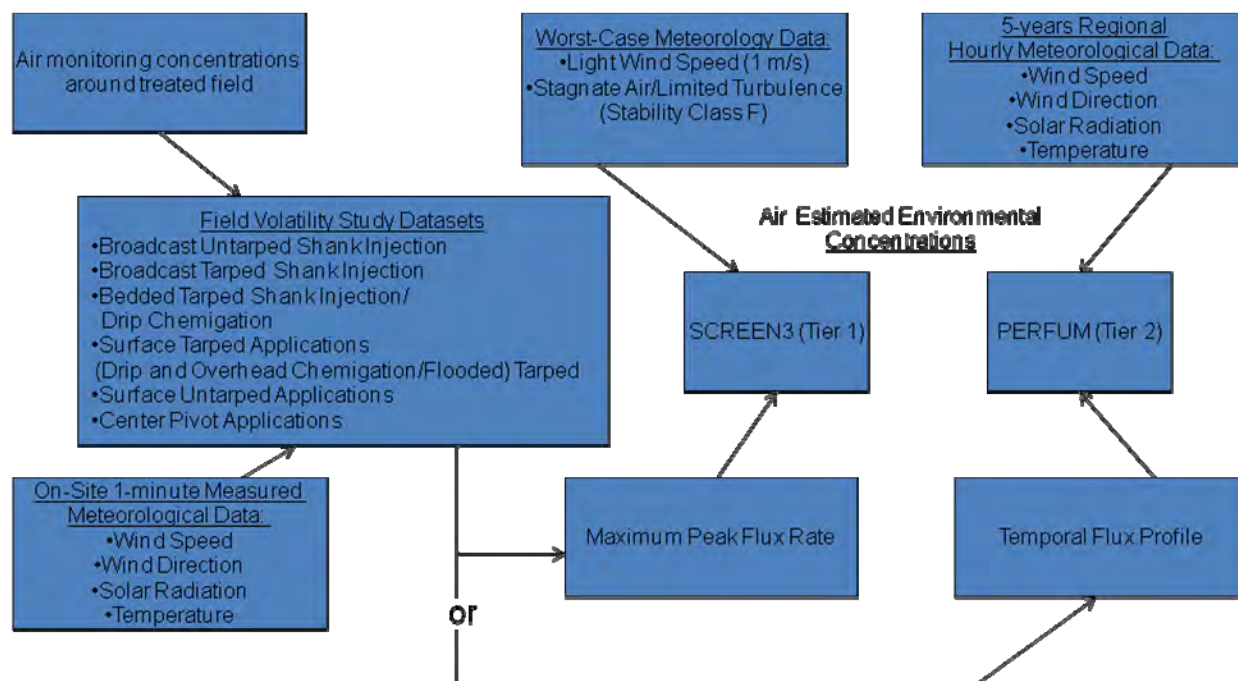


Appendix M –SCREEN3 and PERFUM Model Descriptions and Sample Model Outputs

ATMOSPHERIC DISPERSION MODEL APPLICATION FOR SOIL FUMIGANTS

The purpose of atmospheric dispersion modeling is to arrive at an upper-bound EEC based on a temporal profile of flux rates coupled with a range of meteorological conditions. Dispersion models have the ability to integrate individual plume elements emitted from the treated field to an accumulated mass (that may not be captured by stationary on-field air monitors alone) and couple the on-field vapor flux to varying meteorological conditions to arrive at an estimated exposure concentration in air. **Figure M-1** below shows the process and related input parameters used to develop flux rates from the field volatility study and how these are used in screening and refined air dispersion models used to estimate air EECs. Typically, two sets of estimated exposure values are determined for the various surface and incorporated application techniques described in Appendix 1. The maximum flux rate from each application method should be extracted and input into air dispersion models.

Figure M-1. Process and related throughput entailed in the assessing air exposure.

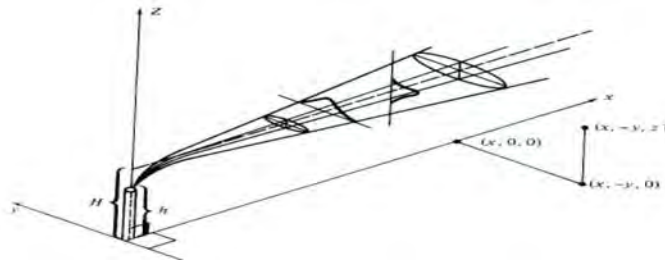


Both the screening and refined dispersion models that have been used deterministically in EFED's ecological risk assessments are calculated using various forms of the ISCST3 (Industrial Source Complex Short-Term) Gaussian Plume Model. The ISCST3 model was developed by the Office of Air Quality Planning and Standards (OAQPS)

(http://www.epa.gov/ttn/scram/dispersion_alt.htm, Accessed 8/17/2011). The ISCST3 Gaussian Plume Model builds the plume structure for each modeled time step based on meteorological information and corresponding Pasquill-Gifford turbulence stability class which governs the degree of mixing inside and width of the plume (A = Unstable, B = Unstable, C = Unstable, D = Neutral, E = Stable, F = Stable), where unstable refers to turbulent conditions with a lot of mixing and stable refers to stagnant conditions with limited mixing. **Figure M-2** illustrates the plume structure at one time step of the ISCST3 model. The plume structure assumes a Gaussian

distribution in the contaminant concentrations which is determined by mixing within the plume. It is assumed that the pollutant does not undergo any chemical reactions, and that no other removal processes, such as wet or dry deposition, act on the plume during its transport from the source. The Gaussian model equations and the interactions of the source-related and meteorological factors are described in Volume II of the ISC User's Guide (USEPA, 1995), and in the Workbook of Atmospheric Dispersion Estimates (Turner, 1970). ISCST3 estimates concentrations within and adjacent to the field. The size of the plume and plume rise is determined by the degree of turbulence in the atmosphere, which is parameterized according to stability class. The stability classes are determined by incorporating wind speed and insolation (or cloud cover) data using empirical methods (Turner, 1970). The 10-meter wind speed governing the transport of the plume is adjusted to the plume height according to the Log Law relationships of the neutral boundary layer (USEPA, 1995).

Figure M-2. Gaussian plume structure in the ISCST3 model.

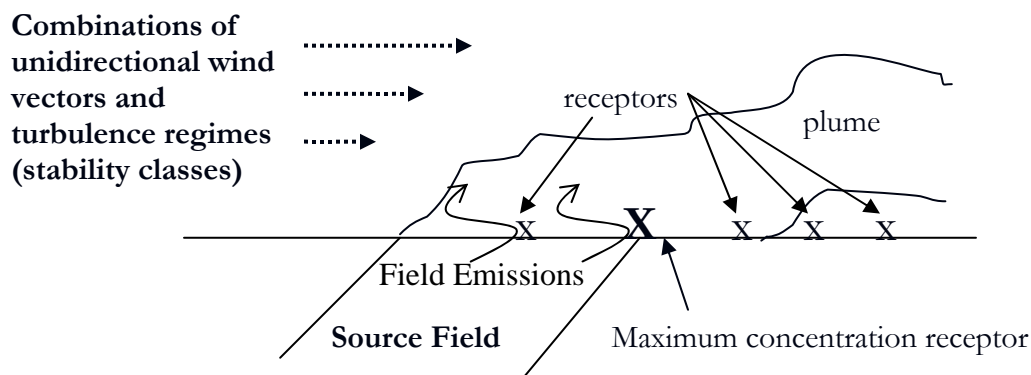


The various forms of the ISCST3 model are ran in screening and refined modes based on the appropriate tier of the fumigant risk assessment. These screening and refined models are described below.

Screening Dispersion Models

EFED currently uses the SCREEN3 dispersion model, developed at the Office of Air Quality Planning and Standards (OAQPS) in the Office of Air (http://www.epa.gov/ttn/scram/dispersion_screening.htm, Accessed 8/17/2011) to estimate tier 1 air EECs. The SCREEN3 model is the screening mode of the ISCST3 model. The SCREEN3 model was vetted for analysis on case studies related to semi-volatile pesticide treatments at the recent Science Advisory Panel meeting, “Field Volatilization of Conventional Pesticides”, held December 2009. **Figure M-3** illustrates that the SCREEN3 model predicts the peak upper-bound ground-level EEC directly downwind along the edge of a treated field. Typically, worst case meteorological conditions (light wind speeds and stagnate air) coupled with a peak flux rate obtained for surface and incorporated application methods are used to calculate the air EECs.

Figure M-3. Schematic of field representation input factors and concentration output configuration for screening dispersion models.



In the tier 1 approach, the treated field of specified size is used to determine upper-bound air concentrations. In the absence of label stipulation, an 80-acre field size is chosen as the upper-limit field size. This is the case since this is often the upper limit field size that can be treated in one day. Since the SCREEN3 model assumes an open system, the upper limit field size is chosen since air EECs are directly related to the size of the field over which the wind blows the entire plume unidirectionally towards the field edge. The field size contrasts with the 10 ha field size in the Georgia Farm Pond scenario of the PRZM/EXAMS model based on . However, this field size is more appropriate for aquatic exposure where a 10 to 1 field-to-pond size ratio is defined for the Georgia Farm Pond scenario based on typical water shed contributions to pollutant loadings in water bodies.

The sample output file for SCREEN3 used in this risk assessment is included in **Attachment M-1**. The results are shown for air concentrations normalized to a flux rate of $1 \mu\text{g}/\text{m}^2\text{s}$. These results are then scaled to the appropriate flux rate for a given application rate for each pre-plant crop use. The resulting EEC are compared to the appropriate inhalation toxicological endpoint to determine RQs.

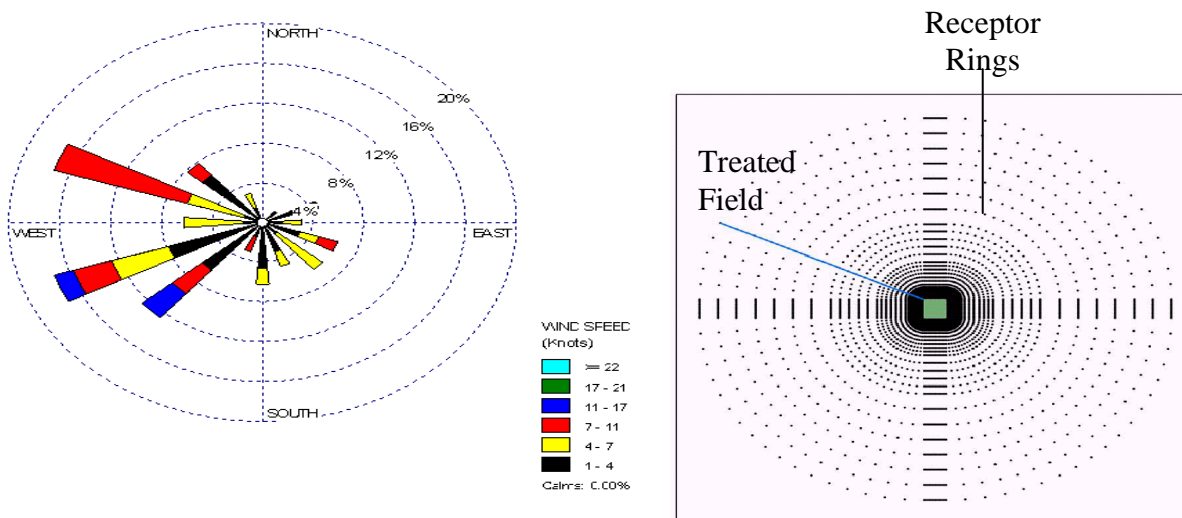
Refined Dispersion Models

As mentioned in Chapter 1, there have been several FIFRA Science Advisory Panel Meetings in 2004 to consider different refinement schemes for the use of dispersion models. These meetings were driven by risk management concerns regarding worker entry buffer zones based upon the screening level dispersion models. Several model refinements were presented by developers representing industry groups. These platforms included, the Probabilistic Exposure and Risk Model for Fumigants (PERFUM), Fumigant Exposure Modeling System (FEMS), and the Soil Fumigant Exposure Assessment Model (SOFEA). Each of these models is based on the ISCST3 dispersion model algorithm. However, each model processes ISCST3 output differently. For previous assessments, HED and EFED scientists have chosen to use PERFUM, considering factors such as the applications that the model platform offers and relative ease of use.

There are several refinements which PERFUM handles which the above screening models do not. First, a time series of hourly volatility flux values, which can be measured during the field volatility studies, can be considered coincident with hourly meteorological conditions. This modeling scheme is most representative to meteorological conditions that would exist throughout different times of the day when off-gassing events occur in the field. PERFUM uses the flux time series which is repeated over five years of hourly meteorological conditions. Meteorological data used in the modeling come from such sources as the National Weather Service observation sites or state observation sites such as CIMIS (California Irrigation Management Information System). Processed meteorological data files have been developed for areas where the use of soil and structural fumigants are most prevalent. Sites where processed meteorological data are available include Bakersfield (CA), Ventura (CA), Yakima (WA), Flint (MI), Tallahassee (FL), Bradenton (FL), and Philadelphia (PA). The second refinement includes the consideration of averaging periods for EECs besides a peak exposure duration.

Since site-specific rather than generic downwind meteorology is used in PERFUM, the model predicts concentrations at a grouping of receptors within multiple radii from the edge of a treated field. **Figure M-4** illustrates the source and receptor configuration that is built-in to PERFUM (right) as well as the frequency distribution of temporally varying wind speeds and direction that is considered in the model as depicted by the wind rose (left). Factors such as Pasquill-Gifford turbulent stability classes are also considered in PERFUM and are calculated hourly from the raw hourly meteorological observations in the processed meteorological files. The PERFUM model is publically available on the web at <http://www.exponent.com/ProjectDetail.aspx?project=450> (Accessed 8/17/2011) (Reiss, 2006).

Figure M-4. Illustration of the spatial and temporal aspects of the source to receptor configuration in PERFUM. The wind rose (left) illustrates the frequency distribution of variations in wind speed and wind direction that PERFUM accounts for in the transport of the vapor plume from the treated source to receptors (right).



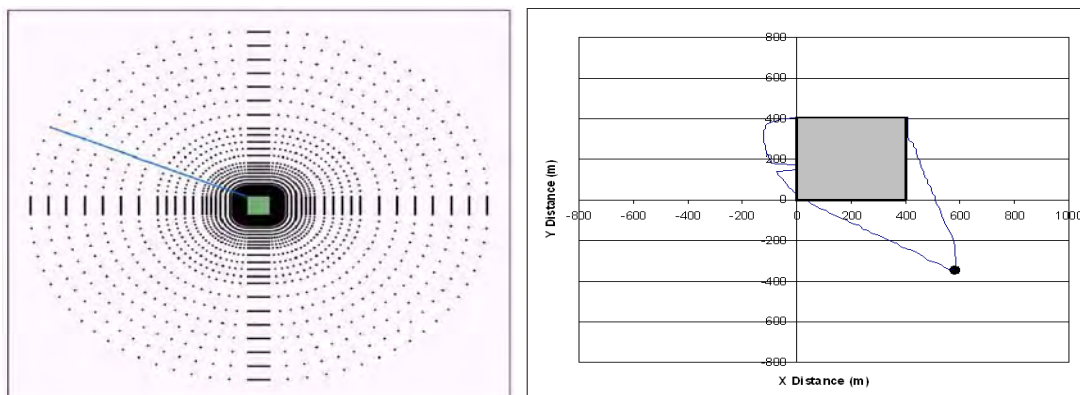
The PERFUM model processes the ISCST3 predicted concentrations into ranked percentile distributions by the averaging period and receptor ring distance from the edge of the field. Essentially, flux rates based on all available and acceptable field volatility studies can be input into separate PERFUM files and run with all of the available meteorological data regions and field. The user should note that flux rates should be scaled to the application rate for the risk assessment. In addition, since the highest EECs will result from the largest source size, an 80-acre field is often used as the basis for the air exposure risk quotients like in the tier 1 modeling. Furthermore, the receptor ring distances from the edge of the field and the receptor height are fixed in the model.

For the acute risk quotient, EFED selects the highest 90th percentile EEC predicted by the model accounting for both the time of day (averaging period) and the distance from the edge of the field. In most cases, the controlling concentration results from the inner-most receptor ring. Since ISCST3 (and hence, the PERFUM model's) area source algorithm is based on a numerical integration of point sources over the treated field, it follows that the maximum concentration would occur in the vicinity of the edge of the field given that plume elements from the field would accumulate as the wind travels over the area source (USEPA, 1995). This phenomenon is best illustrated in Figure 5-3.

The 90th percentile PERFUM predicted buffer zone can be used to estimate the distance from the edge of the field given that the appropriate LOC which is entered, if there is a risk of concern determined for terrestrial organisms. **Figure M-5** shows schematics illustrating the difference in the development of the PERFUM buffer zone distribution at one time step for the whole field versus the maximum concentration distributions. The maximum concentration percentile distribution conveys the probability that there will be an exceedance over time only, and the whole field percentile distribution conveys the probability that there will be an

exceedance over time and space. The whole field and maximum concentration distributions are developed by PERFUM considering each averaging period interval throughout the five-year meteorological period. In this risk assessment, the 90th percentile concentration and subsequent downwind distance to reach the LOC is identified from the averaging period interval possessing the highest whole field concentration distribution 90th percentile concentration. The user should note that PERFUM does not calculate a matrix of distances from the edge of the field to the LOC for each wind direction or class of wind directions. Rather, the buffer zone distributions in PERFUM are developed based on the maximum distance to the LOC which would occur along the prevailing wind direction axis.

Figure M-5. PERFUM whole field (left) versus maximum concentration (right) distributions at one time step.



Attachment M-2 shows a sample excerpt from a PERFUM output file. The excerpt shows the particular concentration array binned by percentile and downwind distance at a specific time of day where and when the maximum 90th percentile concentration was identified for the various uses at 400 lbs.a.i./A including the Forestry Nursery, Nursery and Ornamentals, Sweet Potatoes, Athletic Fields, and Golf Courses uses. The PERFUM model was run referenced by application rate since flux rates are directly related to the application rate. Therefore, the file shown in Attachment M-2 represents all of the uses at 400 lbs. a.i./A. Two-day hourly profiles of flux rates in the file shown were run concurrently with 5-years of Ventura, CA meteorological data, repeated over other meteorological day.

ATMOSPHERIC DISPERSION MODEL APPLICATION FOR STRUCTURAL FUMIGANTS

The screening approach and refined modeling approach using PERFUM is discussed in detail in Section 3.1 of the risk assessment. Section 3.1 describes the source parameters such as release direction, stack diameter, stack gas temperature, gas stream flow velocity, stack height, and emission or flux rates and related scenarios used to determine the various parameterizations into PERFUM. However, besides this discussion, the information conveyed in Figures M-4 and M-5 still apply as these describe how PERFUM treats gas plume behavior in the atmosphere.

Attachment M-3 shows a sample excerpt from a PERFUM output file. This excerpt shows the same type of array as shown in Attachment M-2. Since there are exceedances with the LOC in the various scenarios modeled, the 90th percentile concentration spatial profile, referenced to a

ring number corresponding to a certain downwind distance, is used to identify the downwind distance where air concentrations are predicted to be below the LOC. The file selected in Attachment M-2 is consistent with the highest calculated RQs which resulted from the horizontal release scenario from a 250,000 ft.³ building, 6-hour release scenario. One-day hourly profiles of emission rates in the file shown were run concurrently with 5-years of Bakersfield, CA meteorological data, repeated over each meteorological day.

Attachment M-1. SCREEN3 sample output file for methyl bromide soil fumigant uses.*

*Note – modeling input file is reflective of normalized flux to $1 \mu\text{g}/\text{m}^2\text{s}$ from a 100-acre field.

17:13:27

*** SCREEN3 MODEL RUN ***

*** VERSION DATED 96043 ***

Methyl Bromide Soil Fumigant Unit Modeling

SIMPLE TERRAIN INPUTS:

SOURCE TYPE = AREA
EMISSION RATE ($\text{G}/(\text{S}-\text{M}^{**2})$) = .100000E-05
SOURCE HEIGHT (M) = .0000
LENGTH OF LARGER SIDE (M) = 636.1000
LENGTH OF SMALLER SIDE (M) = 636.1000
RECEPTOR HEIGHT (M) = .0000
URBAN/RURAL OPTION = RURAL

THE REGULATORY (DEFAULT) MIXING HEIGHT OPTION WAS SELECTED.

THE REGULATORY (DEFAULT) ANEMOMETER HEIGHT OF 10.0 METERS WAS ENTERED.

MODEL ESTIMATES DIRECTION TO MAX CONCENTRATION

BUOY. FLUX = .000 $\text{M}^{**4}/\text{S}^{**3}$; MOM. FLUX = .000 $\text{M}^{**4}/\text{S}^{**2}$.

*** FULL METEOROLOGY ***

*** SCREEN AUTOMATED DISTANCES ***

*** TERRAIN HEIGHT OF 0. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES ***

DIST (M)	CONC (UG/M^{**3})	STAB	U10M (M/S)	USTK (M/S)	MIX HT (M)	PLUME HT (M)	MAX DIR (DEG)
-----	-----	----	-----	-----	-----	-----	-----
1	165.3	6	1	1	10000	0	45
100	174.9	6	1	1	10000	0	45
200	183.4	6	1	1	10000	0	45
300	191.1	6	1	1	10000	0	45
400	196.8	6	1	1	10000	0	45
500	117.5	6	1	1	10000	0	45

600	86.36	6	1	1	10000	0	45
700	71.78	6	1	1	10000	0	45
800	62.51	6	1	1	10000	0	45
900	55.92	6	1	1	10000	0	45
1000	50.95	6	1	1	10000	0	45

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND 1. M:

450. 200.0 6 1.0 1.0 10000.0 .00 45.

*** SUMMARY OF SCREEN MODEL RESULTS ***

CALCULATION	MAX CONC	DIST TO	TERRAIN
PROCEDURE	(UG/M**3)	MAX (M)	HT (M)

SIMPLE TERRAIN	200.0	450.	0.
----------------	-------	------	----

** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

Attachment M-2. PERFUM sample output file for methyl bromide soil fumigant uses.

**** PERFUM Output File**

Version 2.5.1 - compiled on 7/2/2008

Run finished on: 12/04/2011 at 19:05

**** Basic information about the model run**

Scenario Type: SF

Source of flux data: CDPR Commodity Permit Conditions

Source of meteorological data: Ventura, CA

ISCST3 meterological file: ..\PERFUM2\MET\vt.MET

Field size (acres): 9.999

Length in x-direction (m): 201.20

Length in y-direction (m): 201.20

Grid density: FINE

**** Toxicity Inputs**

Human Equivalent Conc (ug/m3) : 38830.0

Uncertainty factor: 1.0

Threshold (ug/m3): 38830.0

** Exposure Assumptions

Exposure averaging period (hours): 1
Distribution averaging time (hours): 1

** Time Assumptions

Starting year: 1995
Ending year: 1999
Application Start Hour: 15

** Fumigant Flux Profiles

Flux rates for day number: 1

Hour	Flux Rate
	283.480
1	224.580
2	177.770
3	140.710
4	111.460
5	88.390
6	70.200
7	55.860
8	

9	44.540
10	0.140
11	27.210
12	236.570
13	653.960
14	1063.660
15	1310.930
16	1377.870
17	1313.540
18	1176.150
19	1010.310
20	843.830
21	691.390
22	559.110
23	448.130
24	357.080

Flux rates for day number: 2

HOURLY	Flux Rate
	1.640
1	1.360
2	1.130
3	0.940
4	0.790
5	0.660
6	0.550
7	0.460
8	0.390
9	35.590
10	28.510
11	22.890
12	

13	18.420
	14.860
14	12.020
15	9.740
16	7.920
17	6.450
18	5.270
19	4.310
20	3.540
21	2.910
22	2.400
23	1.980
24	

** All flux rates in micrograms per meter squared per second

----- Number of Periods with Buffer Length Estimates -----

Period	Valid Periods	Calm Periods
--------	---------------	--------------

	1772	22
1	1771	23
2	1754	40
3	1700	94
4	1544	250
5	1312	482
6	1036	758
7	909	885
8	897	897
9	956	838
10	1016	778
11	1070	724
12		

13	1110	684
	1153	641
14	1179	615
15	1237	557
16	1354	440
17	1496	298
18	1647	147
19	1722	72
20	1730	64
21	1746	48
22	1764	30
23	1768	26
24		

----- Definition of Flux Averaging Periods -----

Period 1: Hours 15 to 15
Period 2: Hours 16 to 16
Period 3: Hours 17 to 17
Period 4: Hours 18 to 18
Period 5: Hours 19 to 19
Period 6: Hours 20 to 20
Period 7: Hours 21 to 21
Period 8: Hours 22 to 22
Period 9: Hours 23 to 23
Period 10: Hours 24 to 24
Period 11: Hours 1 to 1
Period 12: Hours 2 to 2
Period 13: Hours 3 to 3
Period 14: Hours 4 to 4
Period 15: Hours 5 to 5
Period 16: Hours 6 to 6
Period 17: Hours 7 to 7
Period 18: Hours 8 to 8

Period 19: Hours 9 to 9
Period 20 : Hours 10 to 10
Period 21 : Hours 11 to 11
Period 22 : Hours 12 to 12
Period 23 : Hours 13 to 13
Period 24 : Hours 14 to 14

----- PERFUM Model Results -----

Concentration distribution results for rings the field

Ring No. Distance (meters)

1	5.
2	7.
3	10.
4	15.
5	20.
6	30.
7	50.
8	70.
9	80.
10	90.
11	100.
12	120.
13	150.
14	180.
15	210.
16	240.
17	270.
18	300.

19	360.
20	420.
21	480.
22	540.
23	600.
24	720.
25	840.
26	960.
27	1080.
28	1200.
29	1320.
30	1440.

Concentration distribution for an application rate of 400.0 for Flux Profile Day No. 1 for Averaging Period 6

The maximum reported concentration is 10 times the rounded threshold concentration, which is 388500.0. Concentrations reported at this level should be interpreted as greater than or equal to it.

[illegible]

60	389	389	389	0	0	0	0	0	0	0	0	0	0	0	0
65	1943	1943	1166	389	389	389	0	0	0	0	0	0	0	0	0
70	5828	5051	5051	4274	2720	1166	389	389	389	389	0	0	0	0	0
75	8159	7382	7382	6605	5828	4274	1943	389	389	389	389	389	0	0	0
80	10490	9713	9713	8936	8159	6605	4274	2720	1943	1166	389	389	389	389	389
85	12821	12821	12044	11267	10490	8936	6605	4274	3497	3497	2720	1943	389	389	389
90	16706	16706	15929	15152	14375	12044	9713	7382	6605	5828	5051	4274	2720	1943	1166
95	22145	22145	21368	20591	19814	18260	15152	12821	12044	10490	9713	8936	6605	5828	4274
97	25253	25253	24476	24476	23699	22145	19037	16706	15152	14375	13598	12044	9713	8936	7382
99	29138	29138	29138	29138	29138	28361	26030	23699	22145	21368	20591	18260	15929	14375	12821
99.9	33023	33023	33023	33023	33023	33023	30692	28361	26807	26030	25253	22922	20591	19037	17483

Attachment M-3. PERFUM sample output file for methyl bromide structural fumigant uses.

**** PERFUM Output File**

Version 2.5.1 - compiled on 7/2/2008

Run finished on: 10/14/2011 at 17:14

**** Basic information about the model run**

Scenario Type: GRN

Source of flux data: Application Rate

Source of meteorological data: Bakersfield, CA

ISCST3 meterological file: ..\PERFUM2\MET\baka.MET

Field size (acres): 0.077

Length in x-direction (m): 17.60

Length in y-direction (m): 17.60

Grid density: FINE

**** Toxicity Inputs**

Human Equivalent Conc (ug/m3) : 155319.0

Uncertainty factor: 1.0

Threshold (ug/m3): *****

** Exposure Assumptions

Exposure averaging period (hours): 1
Distribution averaging time (hours): 1

** Time Assumptions

Starting year: 1999
Ending year: 2003
Application Start Hour: 1

** Additional assumptions for greenhouse scenario

Greenhouse source type: Area
Height of greenhouse + stack (m): 0.0
Greenhouse height (m): 22.9
Adjusted greenhouse height (m): 11.4
Source of flux data: Manually entered by user

** Fumigant Flux Profiles

Flux rates for day number: 1

HOUR	Flux Rate
	9679.629
1	8758.491
2	7925.010
3	7170.846
4	6488.449
5	5870.992
6	9679.629
7	8758.491
8	7925.010
9	7170.846
10	6488.449
11	5870.992
12	9679.629
13	8758.491
14	7925.010
15	7170.846
16	6488.449
17	5870.992
18	9679.629
19	8758.491
20	7925.010
21	7170.846
22	6488.449
23	5870.992
24	

----- Definition of Flux Averaging Periods -----

Period 1: Hours 1 to 1
Period 2: Hours 2 to 2
Period 3: Hours 3 to 3
Period 4: Hours 4 to 4
Period 5: Hours 5 to 5

Period 6: Hours 6 to 6
Period 7: Hours 7 to 7
Period 8: Hours 8 to 8
Period 9: Hours 9 to 9
Period 10 : Hours 10 to 10
Period 11 : Hours 11 to 11
Period 12 : Hours 12 to 12
Period 13 : Hours 13 to 13
Period 14 : Hours 14 to 14
Period 15 : Hours 15 to 15
Period 16 : Hours 16 to 16
Period 17 : Hours 17 to 17
Period 18 : Hours 18 to 18
Period 19 : Hours 19 to 19
Period 20 : Hours 20 to 20
Period 21 : Hours 21 to 21
Period 22 : Hours 22 to 22
Period 23 : Hours 23 to 23
Period 24 : Hours 24 to 24

----- PERFUM Model Results -----

Concentration distribution results for rings the field

Ring No. Distance (meters)

1	5.
2	7.
3	10.
4	15.
5	20.

6	30.
7	50.
8	70.
9	80.
10	90.
11	100.
12	120.
13	150.
14	180.
15	210.
16	240.
17	270.
18	300.
19	360.
20	420.
21	480.
22	540.
23	600.
24	720.
25	840.
26	960.
27	1080.
28	1200.
29	1320.
30	1440.

Concentration distribution for an application rate of ***** for Flux Profile Day No. 1 for Averaging Period 14

The maximum reported concentration is 10 times the rounded threshold concentration, which is *****.
Concentrations reported at this level should be interpreted as greater than or equal to it.

[illegible]

20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
80	1554	1554	1554	0	0	0	0	0	0	0	0	0	0	0	0
85	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554
90	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554
95	4661	4661	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554
97	10875	7768	4661	4661	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554	1554
99	17089	13982	10875	7768	4661	4661	4661	1554	1554	1554	1554	1554	1554	1554	1554
99.9	41945	35731	29517	20196	13982	10875	10875	7768	4661	4661	1554	1554	1554	1554	1554