Exponent®

User's Guide for the Probabilistic Exposure and Risk model for FUMigants

PERFUM

Version 3.0

Prepared by

Exponent
1800 Diagonal Road, Suite 500
Alexandria, VA 22314

Sponsored by

U.S. Environmental Protection Agency
Office of Pesticide Programs
Health Effects Division

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1.0 INTRODUCTION

The Probabilistic Exposure and Risk model for FUMigants (PERFUM) was developed to address the issue of bystander exposures to fumigants following applications. Following application of fumigants, some of the applied material may volatilize from the field and be carried downwind, causing potential exposure to persons in the vicinity of the application. The highest exposures will be closest to the field, with the atmosphere dispersing the fumigant gas to lower concentrations as the plume moves downwind. Both the U.S. Environmental Protection Agency (EPA) and the California Department of Pesticide Regulation (CDPR) have used PERFUM for regulatory decisions. Other international agencies have also used PERFUM.

The model has evolved to include other capabilities including the modeling of fumigant emissions from applications in enclosures and modeling of semi-volatile pesticides that are not necessarily fumigants.

One function of PERFUM is to establish potential buffer zones. The purpose of a buffer zone is to establish a distance from the edge of the field where the concentration of the fumigant is at or below a level assumed to be safe. The major factors that influence the required buffer distance are the flux rate of the fumigant, the meteorological conditions that influence gas dispersion, the size of the field and the toxicity of the compound. These factors represent the major inputs to PERFUM.

PERFUM can be used to establish a probability that a given buffer zone will not result in an exceedance of a user-specified concentration. The probability is largely a factor of the variability in potential meteorological conditions following an application. The model can also be used to model the effect of the flux rate on the buffer zone size.

The first version of PERFUM was submitted to the U.S. EPA in the summer of 2004. EPA convened a FIFRA Scientific Advisory Panel (SAP) meeting to review the model in August of 2004. The SAP meeting was held on August 24-25, 2004, and the review can be found on the EPA website along with a detailed report on the model by Reiss and Griffin (2004). The EPA was satisfied with the SAP review and decided that the model could be used for regulatory purposes. EPA first used PERFUM in its preliminary fumigant risk assessments which were publicly released in July 2005. Version 2 was released in 2006 and included expanded capabilities to model emissions from enclosures where fumigants were applied.

This user's manual describes the revised version of PERFUM called PERFUM3. PERFUM3 includes several additional capabilities from the first version. The most significant changes include:

- The model now includes three separate dispersion models. In addition to ISCST3, the user can now also use AERMOD or CALPUFF to estimate the underlying air concentrations.

- A Graphical User Interface (GUI) has been built.

- The user can change the receptor grid distances and select longer distances than previously allowed.

- The distributions are now calculated using the P^2 algorithm (Jian and Chlamtac, 1985). Previously, a binning method was used where the number of buffer zones in certain specified ranges was counted. This method was necessary because it was not possible to store all of the values in memory so the counting method was used. The P2 algorithm allows a distribution to be constantly updated based on new values, though removing the need to store them in memory. The P^2 algorithm allows for a more accurate and precise estimate of distribution percentiles.

- An improved algorithm for estimating emissions from enclosures.

- The user can specify specific dates within a year to run the model.

2.0 CONCEPTS

The topics in this section provide a general description of the PERFUM approach to estimating probability of exposure at the perimeter of the buffer zone.

2.1 Dispersion Modeling

The core of PERFUM3 is the ISCST3, AERMOD, and CALPUFF dispersion models, which have been used for regulatory risk assessment for stationary sources for many years. PERFUM originally only included ISCST3. EPA eventually replaced ISCST3 with AERMOD, so AERMOD is now included. ISCST3 remains a part of the model given its historical use in fumigant risk assessment, and because in some cases, fluxes have been estimated using ISCST3 with a back-calculation technique. CALPUFF is an alternative dispersion model with some advanced capabilities.

The purpose of an air dispersion model is to estimate the concentration of an airborne compound at any receptor point downwind given the emission rate (or flux rate) of the compound and a characterization of the meteorology in the atmosphere. For a fumigant application, dispersion models require the following input information:

- The emission rate of the compound from the field for every time period of interest. For an area source, we typically call the emission rate a flux rate. The flux rate is defined as the amount of mass volatilized per unit area per unit time. Typical units of the flux rate are $\mu g/m^2/sec$ or lbs/acre/day. For enclosures, the emission rate could be from an area, volume, or point source. For enclosures the units are either grams/second (point sources) or $\mu g/m^2/sec$ (area or volume sources).

- The dimensions of the field or enclosure, and the coordinates of receptor points relative to the field dimensions where the concentrations are to be estimated. The development of the receptor grids is discussed later in this section.

- The averaging period for risk assessment needs to be specified. This averaging period should match the averaging period recommended for the toxicity level of the fumigant. For fumigants, the averaging period for acute risk assessment could range from 1 to 24 hours.

- A characterization of the meteorological conditions affecting dispersion in the atmosphere. These parameters include the wind speed, wind direction, and the atmospheric stability. The needed data vary according to the dispersion model.

For regulatory modeling applications for EPA's air program, dispersion models are typically run with five years of historical meteorology data to characterize the potential meteorological variability in a given source area (EPA, 2005).

A few notes are necessary regarding how CALPUFF is used within PERFUM. When performing CALPUFF runs, there are several dozen parameters which can be set depending on the modeling scenario. The user can define the type of the sources modeled, whether chemical

reactions or deposition are modeled or not, the algorithm used for dispersion coefficient calculations, the coordinate system, and other more advanced options.

In PERFUM runs, many of these parameters are either set to their default values (for example, terrain adjustment parameters) or not utilized (for example, parameters related to chemical transformation). The parameters with their default values or those that are not utilized in the PERFUM applications are not explicitly written out in the CALPUFF input file. Only those parameters that are using non-default values are required to be written to the input file.

In fumigation modeling, the crucial impacts are found very close to the fumigated field or enclosure (the receptors in the modeling domain are placed within three kilometers from the source). Meteorological data from a single meteorological station will be sufficient to represent the meteorological conditions within such a small area. Therefore, CALPUFF uses meteorological data prepared by AERMET, as opposed to the more advanced 3-dimensional wind field simulations. Thus, CALPUFF uses the same meteorological data that are used in AERMOD runs. Note that in CALPUFF, valid meteorological data should be available for all modeled hours, or in other words, no missing data are allowed for the CALPUFF runs. In cases where there are gaps in the AERMET surface and profile data files, missing hours should either be interpolated or substituted from data at a nearby station.

The dispersion coefficient in CALPUFF can be computed using five different methods (selected using parameter MDISP). Current EPA regulatory requirements allow for the choice between two methods, either internally calculated dispersion factors or using PG dispersion factors (MDISP = 2 or 3). For PERFUM applications the MDISP parameter is set to 2. This will use the micrometeorological variables provided in the AERMET surface data file (u*, w*, L, etc.) as input to internally calculating sigma v, sigma w and deriving the dispersion coefficients. This calculation is consistent with the data available in the AERMET files.

For area sources (e.g., polygon, circular and area enclosure) a non-circular puff (a “slug”) is used by setting the parameter MSLUG=1. A slug is an elongated puff in the direction of the wind during release. During the initial time-step the new end of the slug will be “attached” at the source. This results in a more accurate representation of near-field concentrations. Puffs are used for point and volume enclosures by specifying the parameter MSLUG=0.

AERMOD and ISCST3 are run in the regulatory default modes.

PERFUM includes the beta LOWWIND options in AERMOD. Please consult the AERMOD user guide for more details.

2.2 Modeling Framework

It is possible to use a dispersion model to estimate downwind concentrations for a given set of flux data and meteorological assumptions. However, the major drawback of this approach is its deterministic nature. It only provides a single estimate of the buffer zone for a given meteorological situation. Furthermore, as it has been applied prior to PERFUM, it does not account for the diurnal variability in flux rates, which is a potentially critical factor in estimating the buffer zones. The most important aspect of a next generation model is the capability to use actual meteorological data. By using the historical data files of measured meteorological

conditions, the model can assemble a distribution of potential exposures that could occur following application. Therefore, risk managers will be able to better assess the probabilities of exposures of concern occurring.

The purpose of the PERFUM approach is to get closer to an estimate of the probability of exposure for someone at the perimeter of the buffer zone. Therefore, risk managers could know that for a given buffer zone, a person at the perimeter of the buffer zone would be exposed to a concentration less than the concentration of concern for a certain percentage of the time. The phrase "closer to an estimate of the probability of exposure" is important to bear in mind. For several reasons that are discussed in the report, the concentration estimates at the buffer perimeter are upper-bound, conservative estimates of exposure, and thus it is not a true probability of exposure.

One approach is to focus on the maximally exposed location for each set of meteorological conditions. In other words, for a given set of 24-hour meteorological conditions, this approach considers only the location at the farthest distance from the field that is equal to the threshold concentration. The approach that is developed in this report builds upon this later approach to consider all of the locations around the field, instead of only the maximally exposed location. Therefore, in addition to the distribution of concentrations at the maximum exposed location, a distribution is established that considers all of the locations around the field, and calculates the upper percentile of this larger distribution, which could be used to establish a buffer zone. This approach more closely approximates a probability of exposure for someone at the perimeter of the buffer zone; or, alternatively, a population distribution for people near the field (although we are speaking about locations, where there may not be a person). CDPR used the maximally exposed location and the approach considering all of the locations around the field to estimate the percentile level of methyl bromide buffer zones derived using the CDPR standard meteorological conditions (Johnson, 2001).

> **Note:** It is important to think of "locations" instead of "exposures," because, for a given field, it is unknown whether an individual will actually be at the location around the buffer zone that has the highest concentrations.

The two distributions that are output by PERFUM are illustrated in Figure 1, which is a simplified schematic of the output of the model for a single day. The schematic assumes a fumigant where the target MOE is 100 (it could be different for other fumigants) and assumes that the buffer zone is set based on the 95th percentile (the exact percentile to use is the choice of the regulators).

The first approach, **the whole field approach**, is represented by the inner ring. With the whole field approach, the buffer zone is selected such that a large portion (in this case, 95%) of the buffer zone perimeter has an MOE greater than or equal to the target. A small sliver of the buffer zone perimeter (5% as shown in the figure) may have an MOE less than 100. The MOE scenario in PERFUM can be used to examine the actual range of MOEs below the target that could potentially exist within the buffer zone. The whole field approach makes the assumption of equal probability that a person could be at any location around the field. This will likely not be true for individual fields, but should be true, on average, across the many fields where applications will occur.

The other approach, **the maximum concentration approach**, is represented by the outer ring. In this approach, the buffer zone is defined such that there is no location with an MOE below the target for a specified percentage of applications (e.g., 95%). This approach is analogous to the maximally exposed individual (MEI) approach and the probabilities around it represent the probability that the MEI will have a given exposure based on historical variability in meteorology.

It is important to remember that the concentration and buffer zone estimates from PERFUM represent an upper-bound for exposure for several reasons:

- There is not necessarily someone at the location of the maximum concentration.
- A person may not spend a total of 24-hours at the perimeter of the buffer, and thus would have a lower 24-hour average exposure than is estimated by this approach.
- A person may be indoors and the indoor concentrations may be lower than the outdoor concentrations, which is not accounted for with this approach.

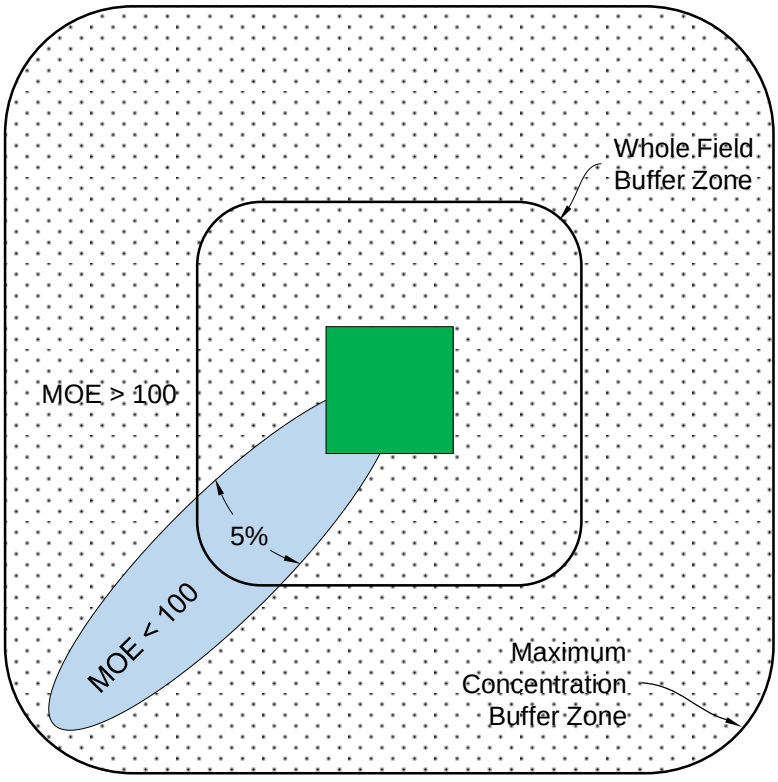


Figure 1. Whole field vs. maximum concentration approach

3.0 MODELING APPROACH

3.1 Basics of the PERFUM Approach

Although the dispersion models are run as a subroutine in PERFUM, it still runs in basically the same manner and the user has much of the flexibility inherent in the underlying dispersion models. The model is typically run for 5 years of meteorological data, but for a different reason than that of the EPA Office of Air & Radiation which typically runs the model for 5 years of data for permitting applications. In most air office applications, the source is continuously emitting and the model is run to generate a 5-year time-series of concentration estimates. However, fumigants are generally applied about once per year. In this application, the model is essentially run in a probabilistic mode to generate a distribution of daily average concentrations over a 5-year period that represents the possible range of downwind concentrations depending on when the fumigant is actually applied. If one assumes that there is an equal probability of a fumigant application occurring for any day of the year (a simplification, which is not necessarily true), the daily average concentration distribution generated from a 5-year run could be used to develop a probability of exposure. One model run is required for each combination of the flux rate profile, meteorological station, and field size.

Another important aspect of the PERFUM approach is the use of the actual hourly flux profile from the flux studies. Specifically, the dispersion models allows the flux rate to vary by hour-of-day. Therefore, the flux estimates from each period of the studies (periods typically range from 2 to 12 hours) are input into the model for the particular hour-of- day that the period measurement occurred. This allows the model to account for the day-night variability in flux rate, and account for the higher fluxes during the day than typically occur for morning applications, which are the norm. The conditions for dispersion are most conducive during the daytime, and the flux rates are highest during the daytime, particularly for a morning application. Therefore, the use of diurnal flux rates represents an important refinement that will increase the accuracy of the downwind concentration estimates. Additionally, PERFUM allows the user to specify the starting hour of the application, and estimates the average concentrations from this hour forward. This is not possible in most dispersion models. For example, all 24-hour average concentrations output by ISCST3 and AERMOD are based on a midnight to midnight average. PERFUM calculates a 24-hour average starting with the application starting hour and continuing through to the next day.

The ISCST3 subroutine is run assuming rural, flat terrain, consistent with most agricultural applications. The model is run in regulatory mode, which includes the use of the calms processing routine.

3.2 Development of the Receptor Grid

To estimate buffer zones, we need to estimate concentrations with the dispersion model at various distances from the field to accurately determine the distances in each direction before the concentration is below the reference concentration. Dispersion models allows the user to establish a receptor grid of data points around a source in which the concentration is estimated. In the original version of PERFUM, the receptors grids were constructed with a GIS program for different field sizes and included as inputs within PERFUM. However, this limited the

number of field sizes and shapes that the user could apply (at least without creating their own receptor grids).

PERFUM2 included algorithms to automatically establish the receptor grid. Whereas in the original version of PERFUM, the ISCST3 input files were pre-built and supplied with the program, PERFUM2 automatically created the ISCST3 input files, including all of the receptor coordinates. The user only needs to specify the length (x-direction) and width (y-direction) of the field. The total area of the field is any area between 0.001 and 160 acres. This increased flexibility allows the user to model any field size between 0.001 and 160 acres. The user can also model any square or rectangular shape, provided that the aspect ratio is not greater than 10. The aspect ratio is defined as the ratio of the largest side divided by the smaller side, and if the aspect ratio is greater than 10, ISCST3 gives a warning indicating potential inaccuracies in the concentration estimates. Therefore, PERFUM does not allow fields with an aspect ratio greater than 10.

The receptor grid established in PERFUM is built with rings and spokes. A ring is a set of coordinates surrounding the field at a specified distance from the field. A spoke represents a straight line from the edge of the field with receptors on each ring. The rings and spokes are shown in Figure 2, which is an example coordinate system for a 5 acre field. The rings around the field are clearly shown, and the blue line represents an example of a spoke.

In PERFUM3, the user can now specify the ring distances in a file called RINGS.TXT that it stored in the model directory. Normally, the user should utilize the default RINGS.TXT file, which includes 16 ring distances at 1, 5, 10, 15, 25, 50, 100, 150, 200, 300, 400, 500, 750, 1000, 1500, and 2500 meters. The nested spacing is necessary for accurate estimates of the buffer zone near the field where the concentration may change most rapidly. Farther from the field, less receptors are needed to estimate the buffer zone. If the user desires to change the ring distances, the format of the file is simply the number of rings on the first line and the rings on each successive line in increasing order. The first and second ring distance must always be 1 and 5 meters. The longest ring distance allowed is 10,000 meters.

The model software includes both a coarse and fine grid option. With the coarse grid, the model runs much faster (by about a factor or four), but the estimates at the upper percentiles are slightly less accurate. For most applications, the coarse grid system is adequate, but the fine grid can be used if the user desires more accurate estimates in the range of the 99th percentile. For the coarse grid, spokes are established approximately every 35 meters off each side, while for the fine grid; spokes are established approximately every 9 meters. At the corners, spokes are established every 18 degrees for the coarse grid, and every 5 degrees for the fine grid.

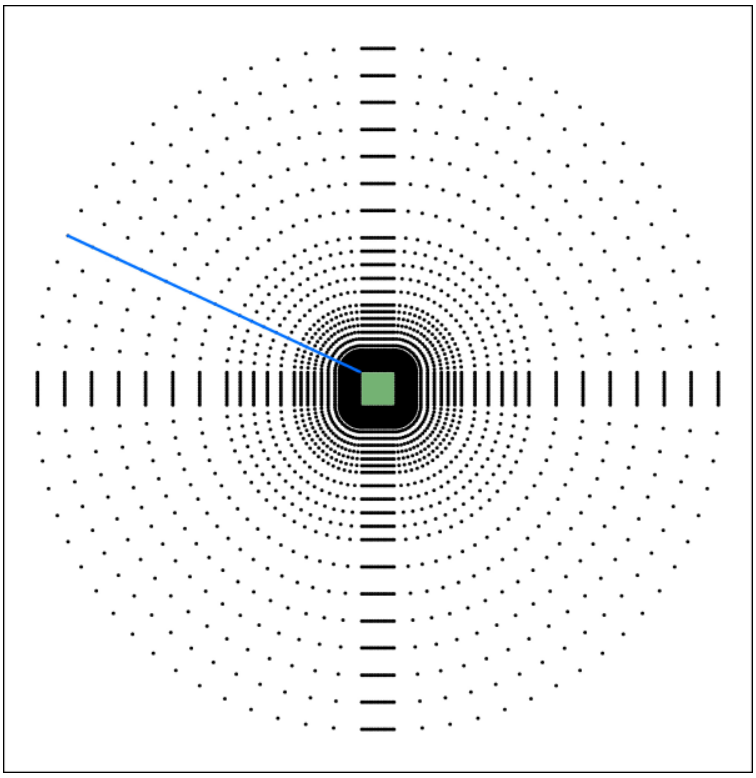


Figure 2. Receptor grid for a 5 acre field

3.3 Meteorological Data

The dispersion models use different file formats for meteorological data. ISCST3 requires a single file with hourly data and includes both the surface data and mixing height data. AERMOD and CALPUFF use the same file format and have separate files for surface and upper-air data. CALPUFF can actually accept other file formats, but in PERFUM, CALPUFF is set to use only AERMOD-formatted files. PERFUM can accommodate any ISCST3- or AERMOD-formatted file.

Several ISCST3-formatted files are provided with the program and have been selected based on their potential to represent fumigant growing regions. Each file includes five years of historical data. The use of a 5-year dataset is recommended for PERFUM3 and is the standard for regulatory dispersion modeling (EPA, 2005).

3.4 PERFUM Output

PERFUM outputs the following information:

- The percentile distribution of the buffer lengths using a) the whole field approach including all of the distances around the field, and b) the maximum concentration approach including only including the maximum daily concentration. Percentiles are included from the 1st to the 99th percentile, in increments of one percentile. The model

includes both a raw output file (*.OUT extension) and a plot file (*.PLT extension). The raw output file contains a detailed summary of the input assumptions and presents an overview of the output. The plot file contains only the output data, but in more detail that the OUT file, and is in a comma-delimited format that can easily be read into a spreadsheet to allow the user to create tables and plots more readily.

- The percentile distribution can be output for up to 10 user-specified application rates. This is a useful tool for establishing buffer zone tables. Both the raw output file and the plot file contain the results for each application rate.

- The program outputs the buffer lengths on a monthly basis to assist in seasonal analysis. This could be helpful in locations where the seasonal pattern of application is well understood. The raw output file contains these results, but the plot file does not.

- The contour file (*.CTR extension) outputs the coordinates around the field corresponding to the whole field buffer zone for a user-specified percentile. The contours represent the buffer distances separately calculated for all of the different spokes at the specified percentile. This file is useful for developing graphical displays of the buffer zones. It shows the actual directions from the field where concentrations above the threshold level could occur.

- The BUFFMAX.OUT file contains maximum concentration distribution buffer zones for each day of the simulation.

4.0 SCENARIO TYPES

4.1 Polygon

The POLY scenario is used to model the typical agricultural pesticide application where pesticide volatilizes from a field following an application. The user needs to enter the field size lengths. The field size can be any area from 0.001 to 160 acres and an aspect ratio (length of largest side to length of smallest side) of less than 10.

Fluxes must be entered as $g/m^2/sec$. Up to 5 days of fluxes following application area allowed and the flux can start at any hour of the day.

4.2 Circular

The CIR scenario is used to model a circular field application. This may occur for chemigation applications. The inputs for the CIR scenario are the same as for the POLY scenario, except that a radius is entered instead of field lengths. The maximum entered radius is 500 meters.

4.3 Margin of Exposure

The MOE scenario estimates the distribution of the margins of exposure at the perimeter of the buffer (assuming someone is at the perimeter and outdoors for the entire averaging period). For the purposes of this report, the margin of exposure (MOE) is defined as follows:

$$\text{MOE} = \frac{\text{HEC or NOEL}}{\text{Exposure}}$$

where the HEC is the Human Equivalent Concentration, the concentration assumed to have no effect in an animal and converted to a human equivalent value. The No Observed Effect Level (NOEL) would be used with human study data. The MOEs can be compared to the required uncertainty factor for risk assessment. The MOE scenario model uses the buffer length estimate from a PERFUM scenario, or any other buffer length that the user is interested. The buffer length needs to be entered by the user. As with the buffer lengths, percentiles are included from the 1st to the 99th percentile, in increments of one percentile. The MOE essentially provides an estimate of the number of fold that the HEC or NOEL is above the exposure estimate. If one only wants the buffer zone estimate, this scenario does not need to be run. The purpose of this program is to provide additional information for risk management. The MOE scenario is currently not designed to be run for the ENCL scenario.

4.4 Enclosure

Applications are also made in greenhouses and other structures, which represents a completely different type of exposure scenario as the application occurs indoors and instead of escaping from the soil the fumigant must first escape the enclosure before causing ambient exposures. These are modeled with the ENCL scenario.

Emissions from enclosures can be modeled as either an area source, volume, or point source. A point source corresponds to a facility with a stack or vent to the outside, which represents the

primary release point for the applied fumigant. An area source represents a facility without a stack or vent where the fumigant primarily escapes through natural ventilation. The user can also specify a release height (in meters) that is sometimes put as half of the building height to represent emissions occurring at a range of distances from ground-level. For volume sources, the emissions are modeled as coming from the building sides and tops. For point sources, the stack or vent is assumed to be located in the center of the facility.

The user has the option of manually entering flux emissions (presumably from flux study data) or using the flux model provided in PERFUM. Entered fluxes are in $\mu g/m^2/sec$ for area and volume sources. The user needs to account for the different assumed release areas for an area (only top of building) or volume (top of building, plus sides) source. Point source emissions are in g/sec.

The flux model in PERFUM is based on a mass-balance of the applied fumigant within the facility using a simple one-compartment box model as follows (Godfrey, 1983) (Equation 1):

$$V\frac{dC}{dt} = -QC$$

where *V* is the volume of the facility, *C* is the air concentration of the fumigant, and *t* is the time since application. Equation 1 can be separated to give the following integral (Equation 2):

$$\frac{-1}{R}\int_0^C \frac{dC}{-C} = \int_0^t dt$$

where *R* is the air exchange rate of the facility defined as *Q/V*. The solution to this integral is as follows (Equation 3):

$$C(t) = C_o \exp(-Rt)$$

where C_o is the initial concentration in the building. C_o is estimated by calculating the mass of chemical in the building at time zero using the building application rate (entered as $lbs/1000\ ft^3$ of building volume) and the building volume. The air exchange rate (*R*) determines the release rate of the chemical in the building. For each hour of the simulation, the loss rate of chemical is calculated by difference in building concentration over the hour using equation 3.

The typical process for a building fumigation includes a treatment period (i.e., the period while the fumigant is working), and an aeration period where the fumigant is vented or removed from the building. PERFUM3 models these periods separately. During treatment, some amount of the application will be lost. Therefore, a retention rate variable has been added to the model. Typically, the retention rate should be 100% during treatment because all of the application mass is in the building at time=0. For aeration, the retention rate should be set to the percentage of the original application mass left in the building at the start of aeration. Thus, if 10% of the mass was lost during treatment, the retention rate should be set to 90% for aeration.

The user is able to specify an air exchange rate for the treatment and aeration periods. For example, during the treatment period, sometimes windows and door cracks are sealed to

minimize product loss, resulting in a low air exchange. During the aeration period, window and doors are opened (passive aeration) or air is forced out by ventilation (forced aeration), resulting in a generally higher air exchange rate during aeration.

The user has the following options in developing an enclosure scenario:

- The source can be modeled as a point source (stack or vent), or area source or volume source (natural ventilation from a building). For point sources, the stack is assumed to be in the center of the building.

- The enclosure dimensions need to be specified, including the length, width, and height of the building.

- Whether the flux rates (or emission rates for a point source) are calculated with the theoretical model (C) or entered manually from study data (E).

- The application rate in lbs per 1000 ft^3 of enclosure space.

- The air exchange rate in turnovers per hour needs be specified for the treatment and aeration periods when using the calculation method.

- For point sources, the stack height (above the top of the building), stack diameter, stack temperature, and stack exit velocity.

If a point source is specified, PERFUM will call the Building Profile Input Program (BPIP) to calculate downwash parameters, if necessary (EPA, 1993). This capability in PERFUM was accomplished by compiling the BPIP source code provided by U.S. EPA on its website, and calling it as a subroutine. Edits were made to allow the variables in PERFUM to be used in BPIP, but no changes to the actual computation algorithms were made. The user can review the normal output of the BPIP program in the BPIP subdirectory.

5.0 INPUT FILE FORMAT

The GUI will automatically create the PERFUM3 input file. But the user can also run the model without the GUI by typing PERFUM3 at the command prompt in a directory with the model executable and input file.

Table 1. Input file format

Line Number(s)	Description (including units, if applicable)	Type of Field
1	Header information describing the scenario types	n/a
2	Scenario type (POLY, MOE, CIR, ENCL)	3-4 character string
3	Dispersion model (ISCST, AERMOD, CALPUFF)	5-7 character string
4	Output type (CONC only, later versions will include DDEP and WDEP for wet and dry deposition)	4-character string
5	Header for ISCST portion of file	n/a
6	Surface meteorological station ID	5-digit integer
7	Upper-air meteorological station ID	5-digit integer
8	Meteorological data file (full directory name)	200-character string
9	Header for AERMOD/CALPUF portion of file	n/a
10	Surface meteorological station ID	5-digit integer
11	Upper-air meteorological station ID	5-digit integer
12	Surface data file (full directory name)	200-character string
13	Upper air data file (full directory name)	200-character string
14	Anemometer height (meters)	Real number
15	Header for AERMOD LOWWIND beta option	
16	AERMOD LOWWIND beta option (0: default, 1, 2, or 3)	Integer
17	Header for dimensions and receptor information	n/a
18	Field length in x-direction (meters)	Real number
19	Field length in y-direction (meters)	Real number
20	Receptor height (meters)	Real number
21	Grid density (C-coarse/F-fine)	1-character string
22	Question on performing monthly calculations (Y/N)	1-character string
23	Header line to separate inputs for ENCL scenario	n/a
24	Flux estimation (C=calculated, E=entered)	1-character string
25	Source type for ENCL (P=point/A=area)	1-character string

Line Number(s)	Description (including units, if applicable)	Type of Field
26	Building height (meters)	Real number
27	Adjusted building height (meters)	Real number
28	Stack height (above the building height) (meters)	Real number
29	Stack diameter (meters)	Real number
30	Stack exit velocity (m/sec)	Real number
31	Stack gas exit temperature (Kelvin) (user 0 to release at ambient temperature)	Real number
32	Application rate (lbs/1000 ft3)	Real number
33	Air exchange rate (per hour)	Real number
34	Retention rate (fraction)	Real number
35	Additional information for circular source	N/A
36	Radius of circle (meters)	Real number
37-42	Reserved for deposition calculations	
43	Header line to separate general inputs	
44	Flux data source description	60-character string
45	Number of simulation days (days)	Integer
46	Averaging period (hours)	Integer
47	Distribution averaging period (hours)	Integer
48	Beginning year of simulation	4-digit integer
49	Ending year of simulation	4-digit integer
50	Date range 1	Date range
51	Date range 2	Date range
52	Staring hour of simulation	Integer
53	File name for PERFUM output file	12-character string
54	File name for PERFUM plot file	12-character string
55	File name for PERFUM contour file	12-character string
56	Contour percentile	Real number
57	HEC or NOEL (µg/m3)	Real number
58	Uncertainty factor	Real number
59	Buffer length for MOE scenario	Real number
60	Header line to separate application rate part of file	n/a
61	Number of application rates	Integer

Line Number(s)	Description (including units, if applicable)	Type of Field
62-71	Application rates (lbs/acre)	Real
72	Header line to separate flux rate data part of file for main source	n/a
73-96	Hourly flux rates for main source (μg/m^2/sec) for area sources and grams/second for point sources)	Real or scientific notation

6.0 USING PERFUM

The graphical user interface (PERFUM-GUI) is the recommended system for configuring and running PERFUM3 scenarios. The following sections cover the GUI and its features.

6.1 PERFUM-GUI Overview

The PERFUM-GUI is designed to manage multiple scenarios in a single integrated environment, and introduces the Perfum project file type which can store settings for many scenarios in a single file. The main window is shown in Figure 3.

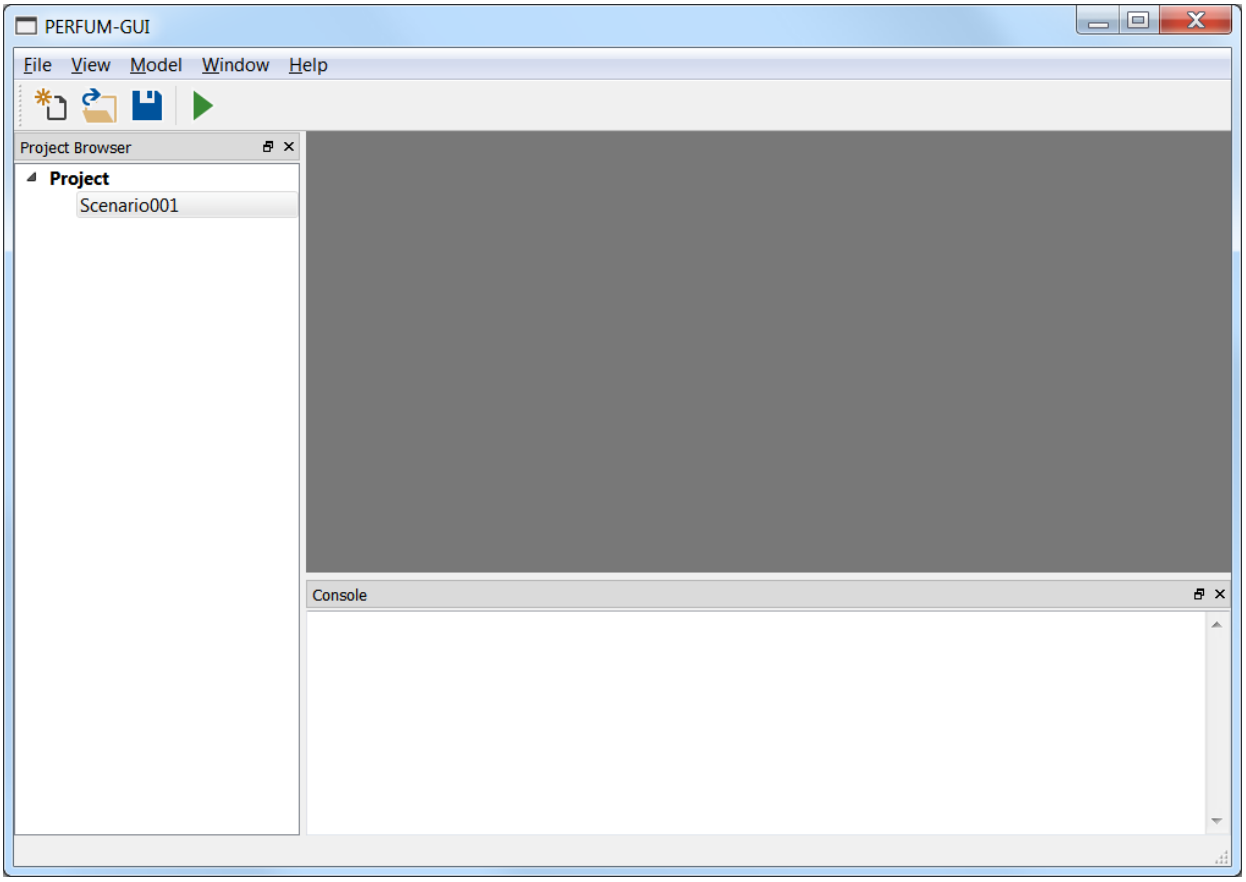


Figure 3. PERFUM-GUI main window

The main window is divided into the Project Browser, Console and Workspace:

- **Project Browser:** manages all of the scenarios in a project. Most options are accessed via the context menu displayed when right clicking a scenario.

- **Console:** captures informational messages and errors from PERFUM and dispersion models while running.

- **Workspace:** the central area which contains all windows related to a specific scenario, such as Properties, Input File Viewer and Plots. Multiple windows can be open for one or more scenarios.

The main project controls are available in the menus and toolbar:

New Scenario: creates a new scenario with default settings.
Open File or Project: opens an existing input file (.inp) or project (.perfum).
Save Project: saves all loaded data to the project file.
Run Model: opens the run dialog to start or monitor progress of runs.

The **Scenario Context Menu**, shown in Figure 4, is the central point for managing all actions related to a specific scenario. This menu is accessed by right clicking a scenario in the Project Browser.

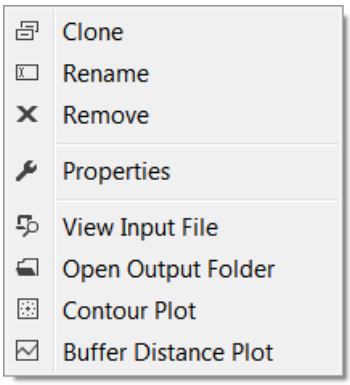


Figure 4. Scenario context menu

Clone: copies all data from one scenario to a new scenario.
Rename: changes the name of the scenario.
Remove: removes the scenario from the project; original files are not deleted.
Properties: opens the main settings dialog.
View Input File: shows a preview of the generated INP file.
Open Output Folder: opens the output folder in Windows Explorer.
Contour Plot: plots the user-specified contour and receptor grid.
Buffer Distance Plot: plots buffer distance by percentile.

> **Warning:** Cloning a scenario copies all information, including name and output folder. To prevent overwriting output from other runs, make sure to change the output folder, or set output folder to automatic and rename before starting a run.

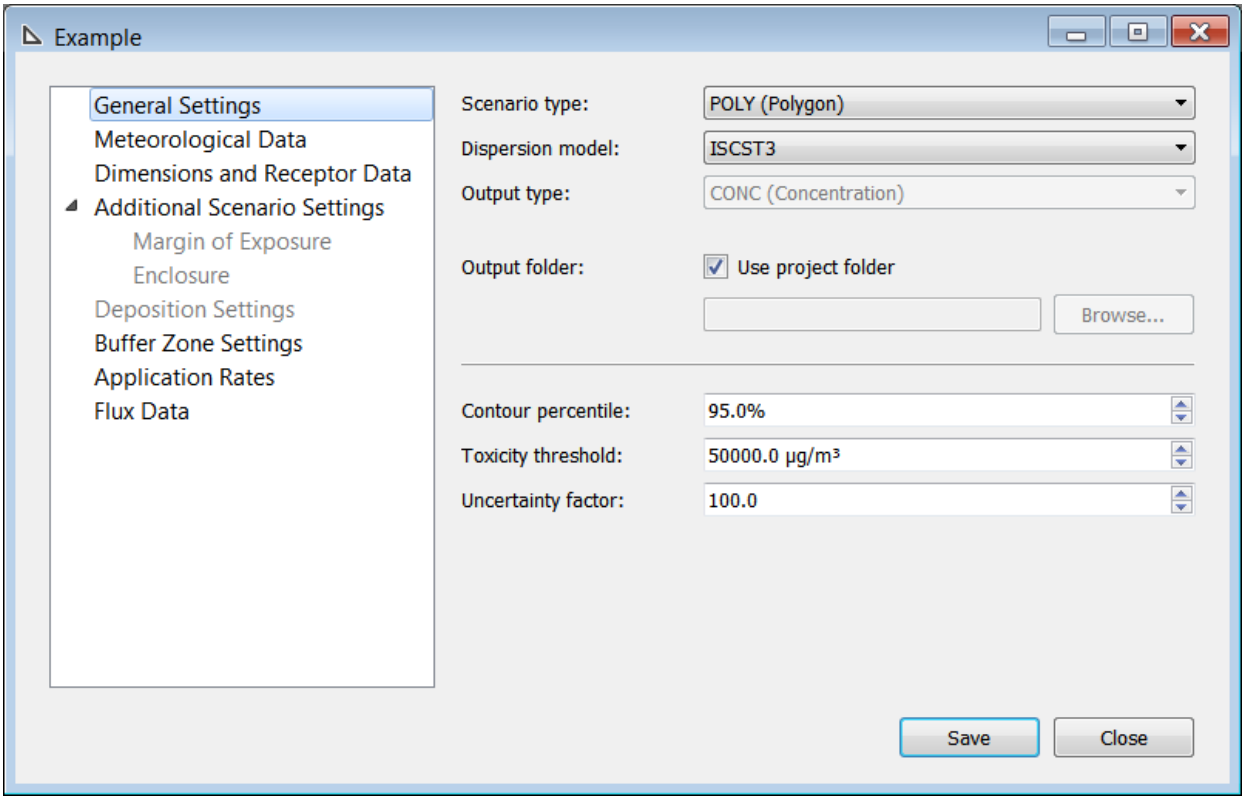
These options are detailed in the following sections.

6.2 Scenario Properties

The Scenario Properties window is divided into a number of functionally-related pages (pathways) for configuring the model. Only the required information for a particular scenario type or dispersion model is shown.

The options available on each page are detailed in the following sections.

6.2.1 General Settings



The General Settings page includes options applicable to all models, as follows:

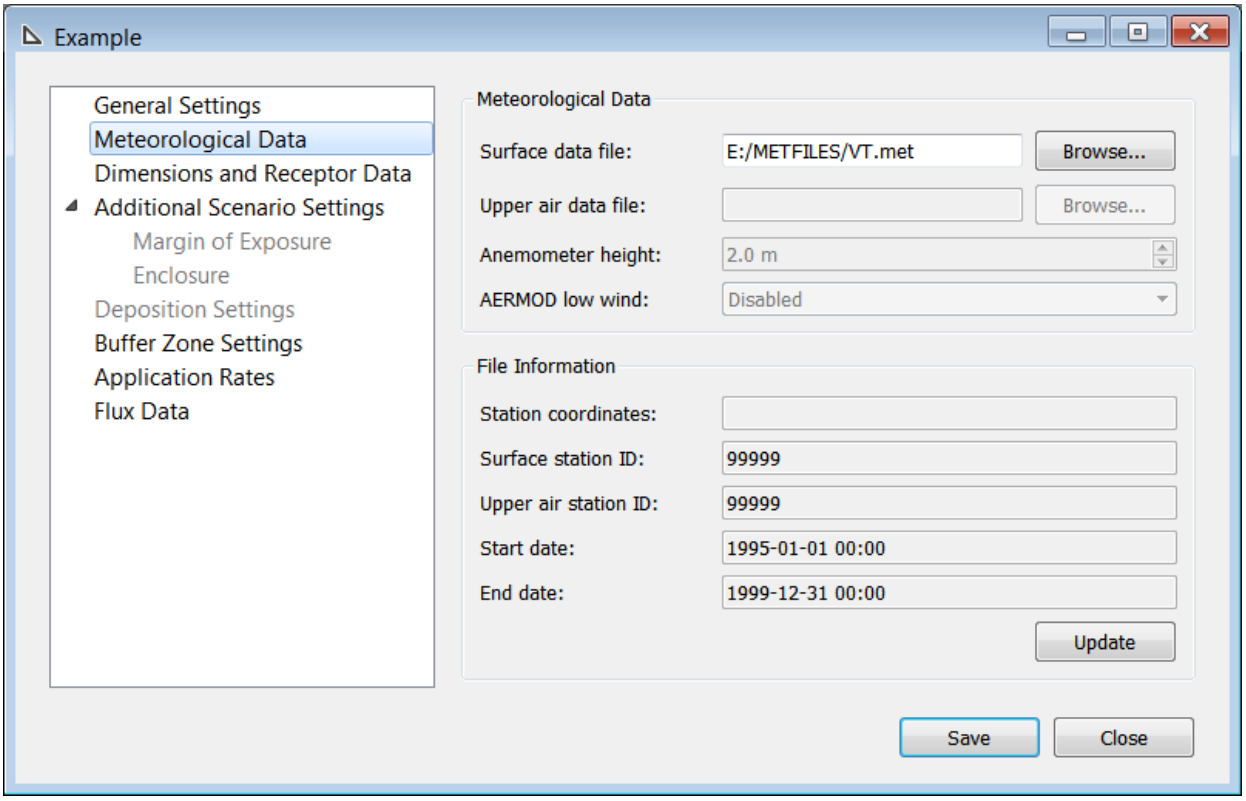
- **Scenario type**: POLY, CIR, MOE or ENCL
- **Dispersion model**: ISCST3, AERMOD or CALPUFF
- **Output type**: only CONC available; DDEP and WDEP options (dry and wet deposition) are in development and currently disabled.
- **Output folder:** allows the user to specify either a custom folder to store all model inputs and outputs, or by using the project folder option, PERFUM-GUI will automatically create subdirectory with the same name as the scenario in the .perfum project folder. The project folder option is recommended for easy file management.

- **Contour percentile:** used to generate the PERFUM.CTR file containing the coordinates around the field corresponding to the whole-field buffer zone at this percentile.

- **Toxicity threshold:** corresponds to the NOEL (for a human study) or the HEC (for an animal study).

- **Uncertainty factor:** the uncertainty factor is a factor that accounts for uncertainty in the NOEL or HEC. The NOEL or HEC is divided by the uncertainty factor to determine the toxicity level of concern.

6.2.2 Meteorological Data



The Meteorological Data page provides options to read ISCST3-formatted data files (*.MET) and AERMOD files (*.SFC, *.PFL). Available options depend on the selected dispersion model.

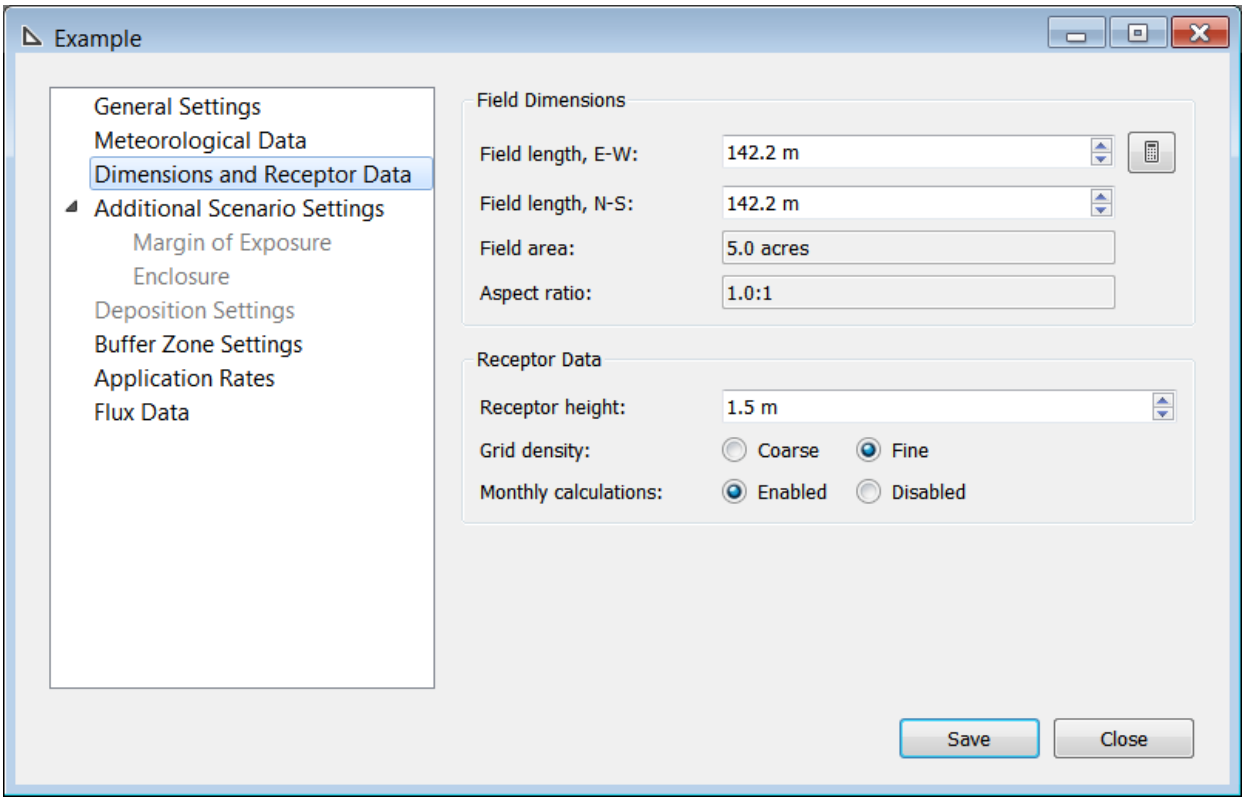
> **Note:** A short path with no spaces is recommended for the surface and upper air data files.

Anemometer height is required for AERMOD files.

AERMOD low wind enables the beta LOWWIND options, which are intended to address concerns regarding model performance under low wind conditions. Refer to the AERMOD user's guide and Model Change Bulletin #8 (December 10, 2012) for details.

Station identification information, start date and end date are automatically read from the surface data file when saved. To manually refresh, click **Update**.

6.2.3 Dimensions and Receptor Data



Field dimensions for a rectangular field can be specified directly as East-West and North-South length in meters, or calculated from field area in acres and X:Y aspect ratio by clicking the calculator button ( ). The maximum field area is 160 acres and maximum aspect ratio is 10:1; if the field lengths result in a number outside of the valid range, the field area and/or aspect ratio fields will turn red and PERFUM will report an error when run.

For a circular field, field dimensions are entered using radius.

Receptor options are as follows:

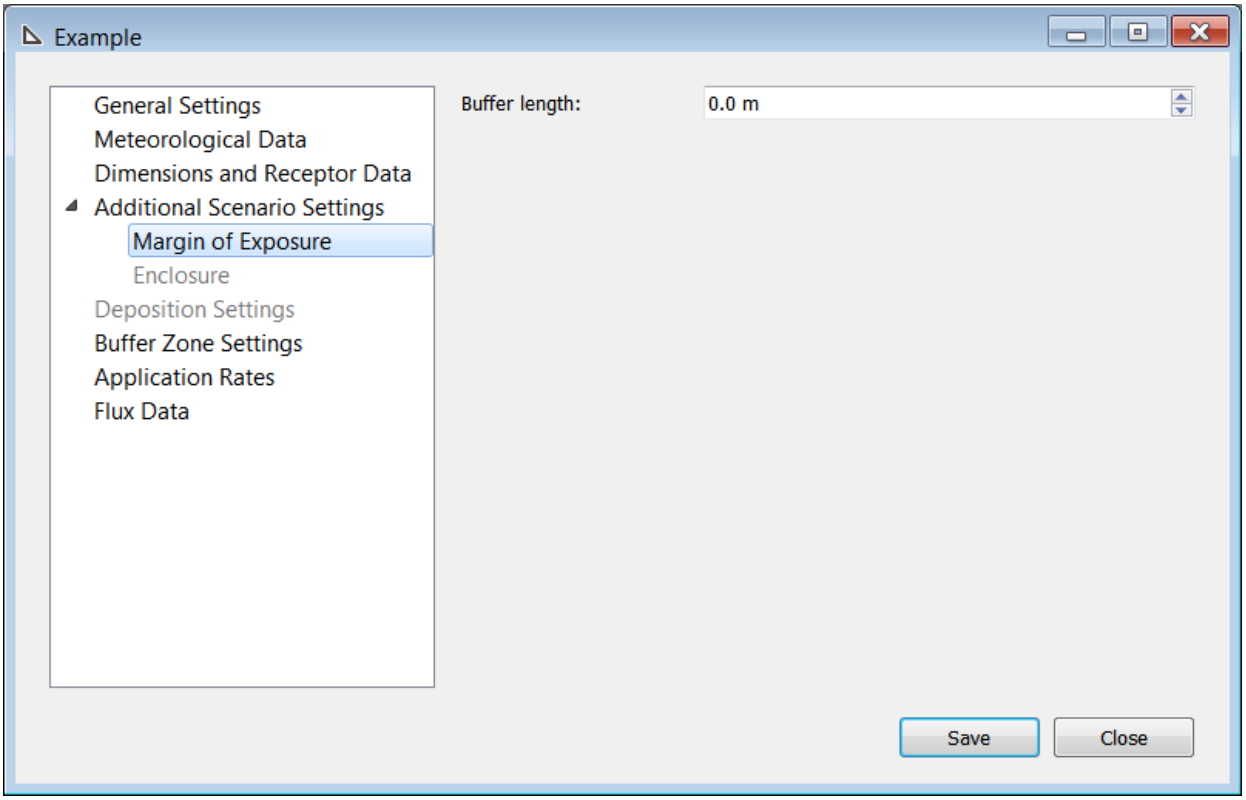
- **Receptor height** is 1.5 meters by default, which represents a typical breathing height for a person.

- **Grid density** allows a coarse or fine receptor grid. For the coarse grid, spokes are established approximately every 35 meters off each side, while for the fine grid; spokes are established approximately every 9 meters. At the corners, spokes are established every 18 degrees for the coarse grid, and every 5 degrees for the fine grid.

Runs using the coarse grid will complete about 4 times faster, at the cost of possibly decreased contour resolution and reduced accuracy of estimates at upper percentiles (typically, above the 99th percentile).

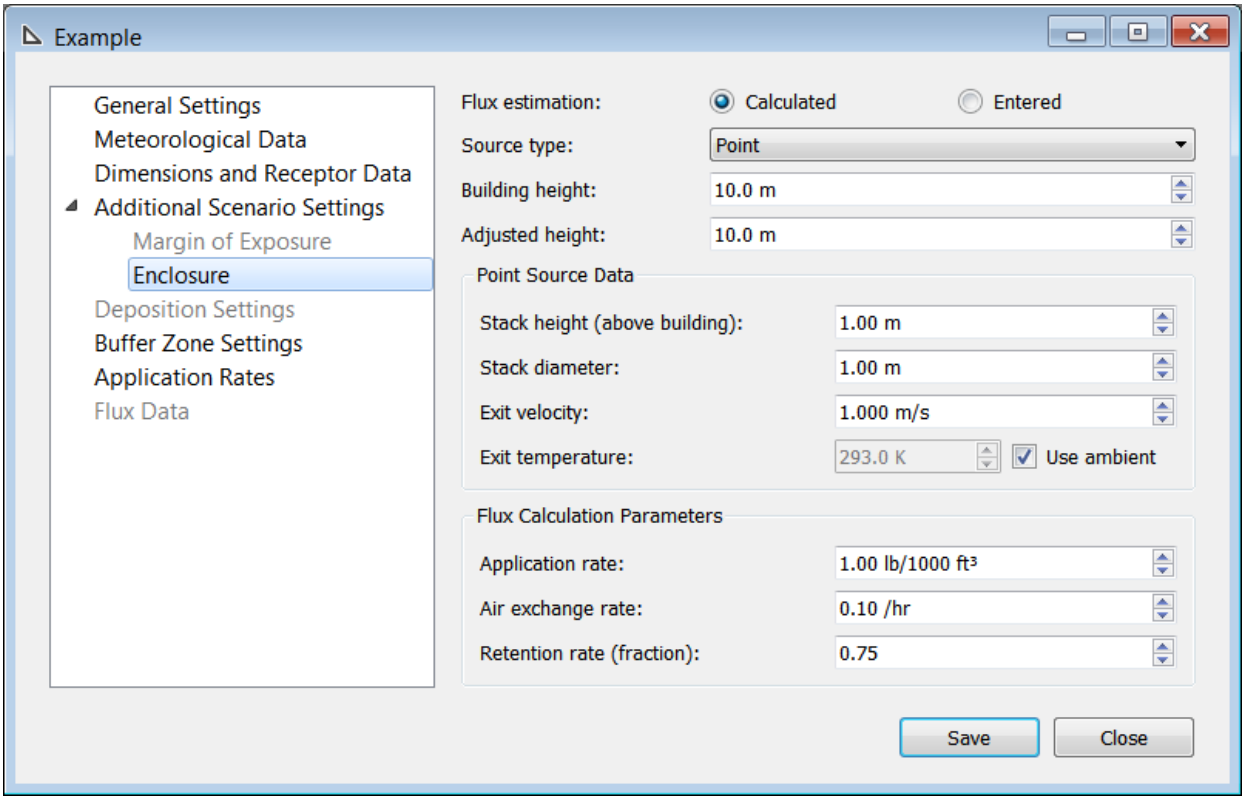
- **Monthly calculations** outputs the buffer lengths on a monthly basis to assist in seasonal analysis. This could be helpful in locations where the seasonal pattern of application is well understood.

6.2.4 Additional Settings: Margin of Exposure

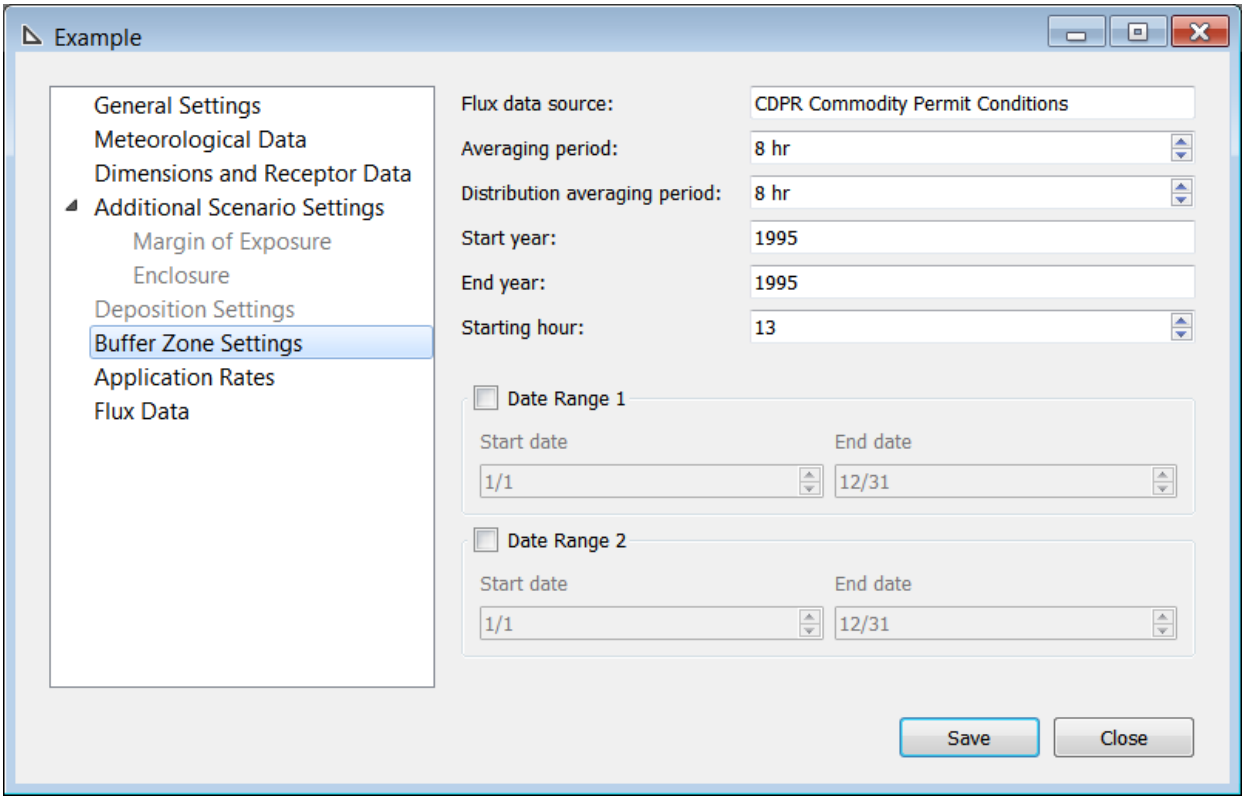


The MOE scenario buffer length is entered on this page. This can be a buffer length from a previous PERFUM run, or any other buffer length of interest.

6.2.5 Additional Settings: Enclosure



6.2.6 Buffer Zone Settings



- **Flux data source:** an optional description which may be entered for reference purposes.

- **Averaging period:** the averaging period corresponds to relevant averaging period for the toxicity data. It should be selected in conjunction with toxicologists and corresponds with the NOEL or HEC. In order to order to create a 5-year repeating sequence of periods, the averaging period is constrained to factors of 24 (1, 2, 3, 4, 6, 8, 12, 24).

- **Distribution averaging period:** This option allows the user to select a larger time period (larger than the averaging period) to consolidate the distribution output in PERFUM. For example, if the user selects a distribution averaging period of 8 and an averaging period of 1, PERFUM will calculate 1-hour average concentrations and buffer distances based on these concentrations, but when outputting the final distributions, the program will consolidate the buffer distances into three 8-hour blocks. This option allows the user to reduce the large amount of information that could potentially be output by PERFUM when a small averaging period is selected.

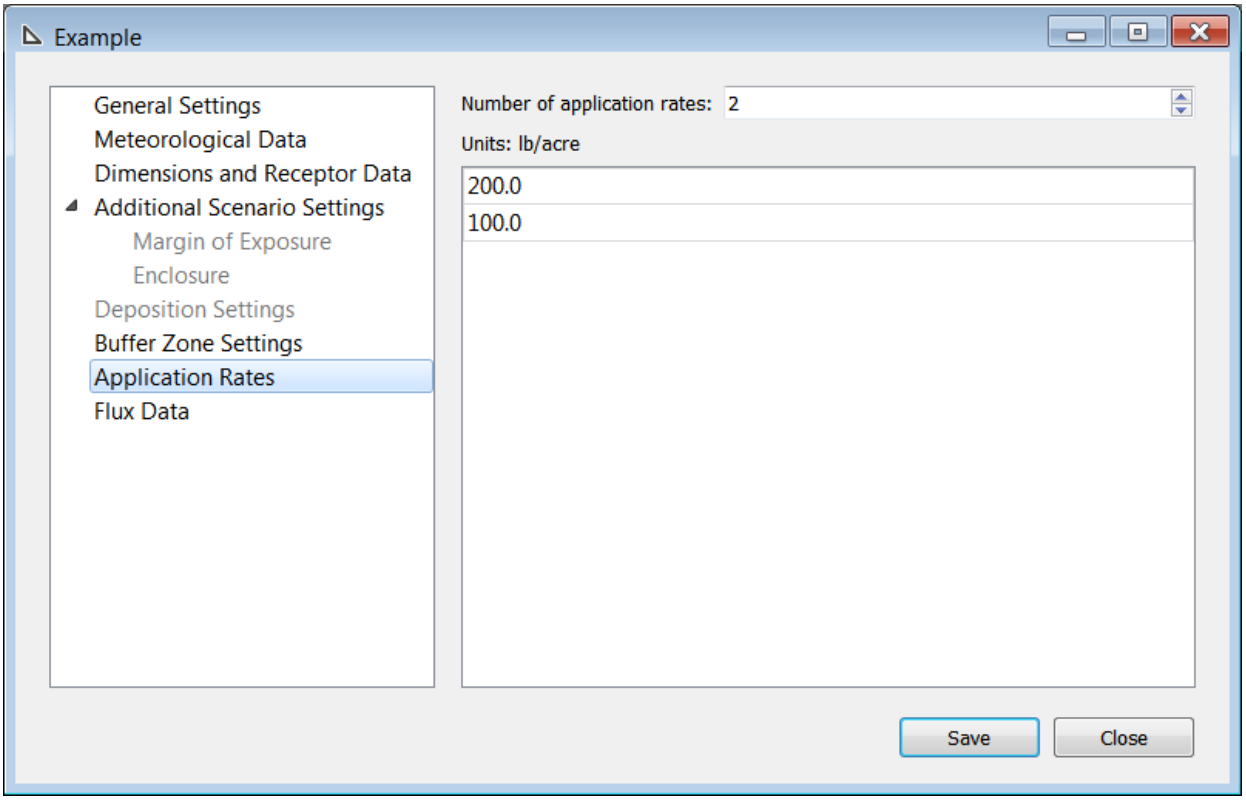
  If the averaging period and the distribution averaging period are the same, there will be no consolidation of the distributions.

- **Start year** and **End year**: automatically constrained to the year range in the surface data file. Changing these fields allows a subset of years to be processed.

- **Starting hour:** corresponds to the start of the application. PERFUM will estimate concentrations from this hour forward and into the next day, spanning 24 hours.

- **Date range:** allows the model to run for only part of a year for up to two contiguous date ranges. This option is useful for modeling particular application seasons. Currently only supported by the AERMOD and ISCST3 models.

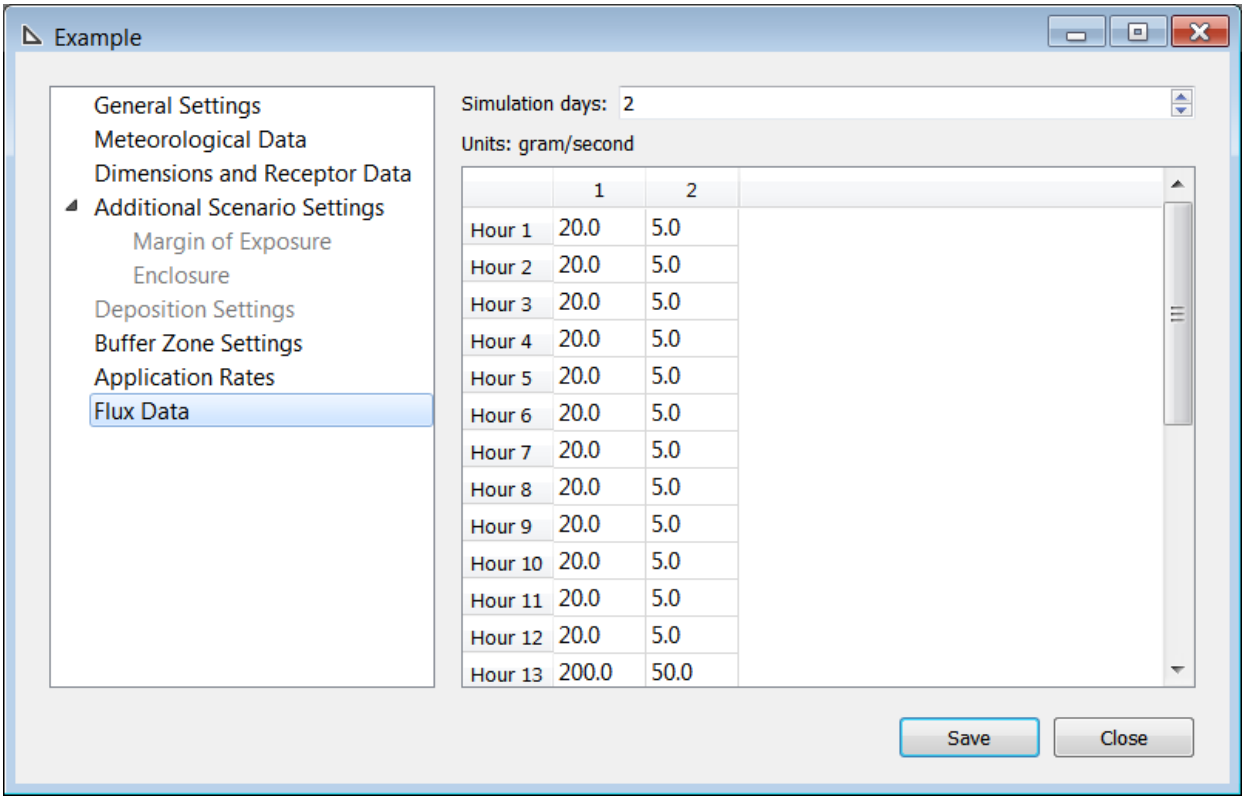
6.2.7 Application Rates



Up to 10 application rates can be specified for a single scenario, but the first rate must be the largest and must correspond to the hourly flux data. The application rate units are lb/acre for all scenarios except ENCL, where units are lbs/1000 ft^3.

Application rates should be entered as lbs/acre, not lbs/treated acre, for the mass balance checking algorithms in PERFUM to work properly

6.2.8 Flux Data



Hourly flux rates, or specifically emission rates for an ENCL scenario, are specified for up to 5 simulation days.

The hourly flux rates are entered in a specific manner. The flux rates should be entered corresponding to the hour of day in the flux study. The hours are numbered 1-24, and correspond to 1-hour blocks starting with hour 1 as midnight-1am. Therefore, if the study started at 9am the first flux rate should be listed on hour 10 (9am-10am is the tenth hour of the day). The flux rates are specified through hour 24, and then from hour 1 to hour 9, all in the first column. If there is a second simulation day, the first hours of the second day (still 9am in this example) is entered for hour 10 in the second column of values and the process is completed.

By selecting multiple cells and using the **Ctrl-C** and **Ctrl-V** keyboard shortcuts, flux data can be copied and pasted to and from Microsoft Excel for ease of editing.

This page is used for all scenario types except ENCL with the flux option ‘C’ (calculated).

6.3 Input File Viewer

The input file viewer, shown in Figure 5, shows the generated INP file based on the properties entered in the GUI. Only the necessary fields for a specific scenario type or dispersion model are populated, and as a result the generated INP file may not match an imported INP file.

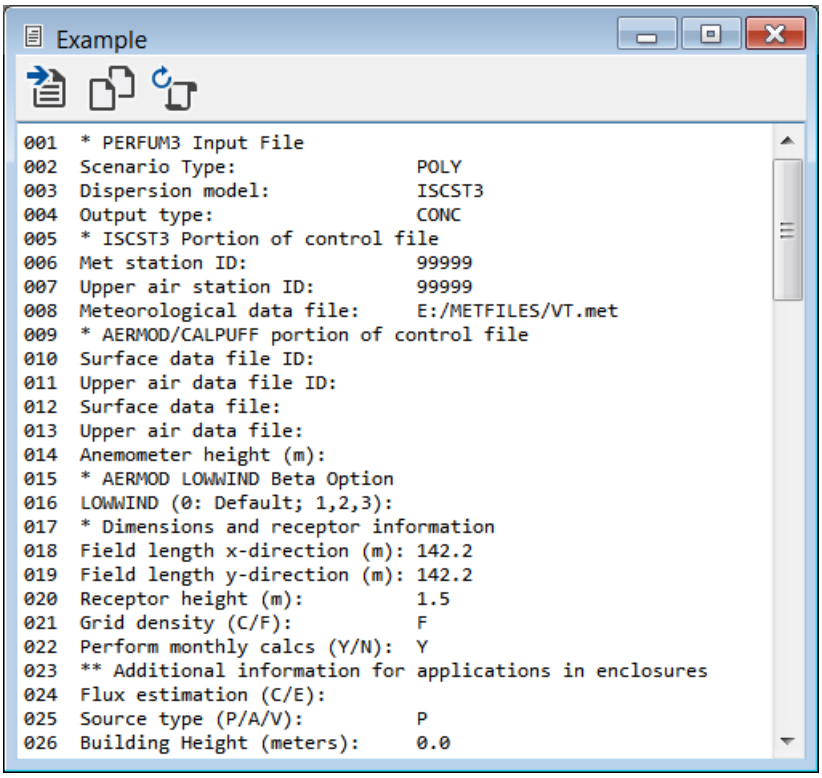


Figure 5. Input file viewer

The generated input file is copied to PERFUM.INP and used by the PERFUM3 command line executables. The viewer can be open at the same time as properties, and the preview will automatically refresh when properties are saved.

Toolbar actions are as follows:

Export File: exports to a new .INP file
Copy to Clipboard: copies the input file text to the clipboard.
Refresh: forces a refresh of the displayed input file; normally not used.

6.4 Run Model Window

The Run Model window summarizes all currently loaded scenarios, controls one or more runs, and displays progress and process status information. Messages from PERFUM and the dispersion model subroutines are printed to the Console.

6.5 Plotting

The PERFUM GUI includes an interactive plotting system based on gnuplot. Two plot types are currently available, and are accessed from the scenario context menu:

- **Contour Plot:** plots the receptor grid (grid.dat file) and the contour for the whole-field buffer percentile specified under General Settings (95.0% by default).

- **Buffer Distance Plot:** plots the whole-field and maximum concentration buffer distances for the first 24 hours after the application.

Sample plots are shown in Figure 6 and Figure 7.

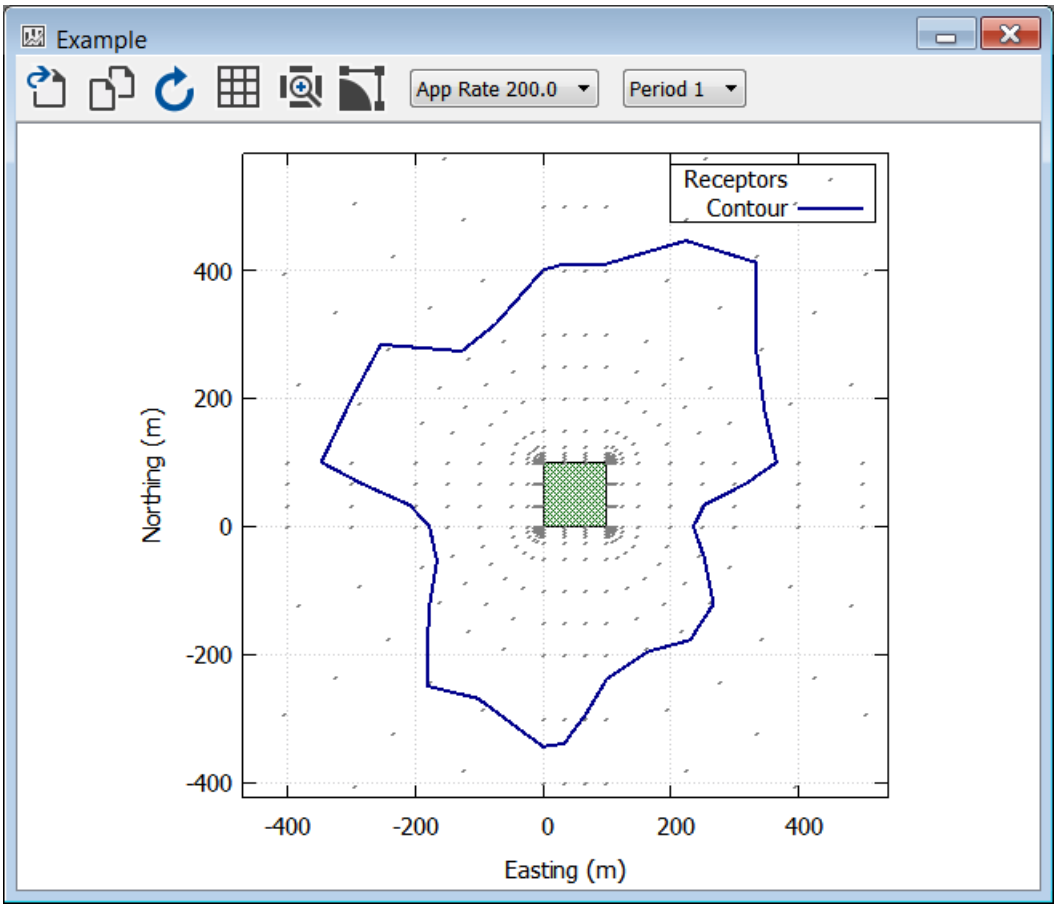


Figure 6. Contour plot window

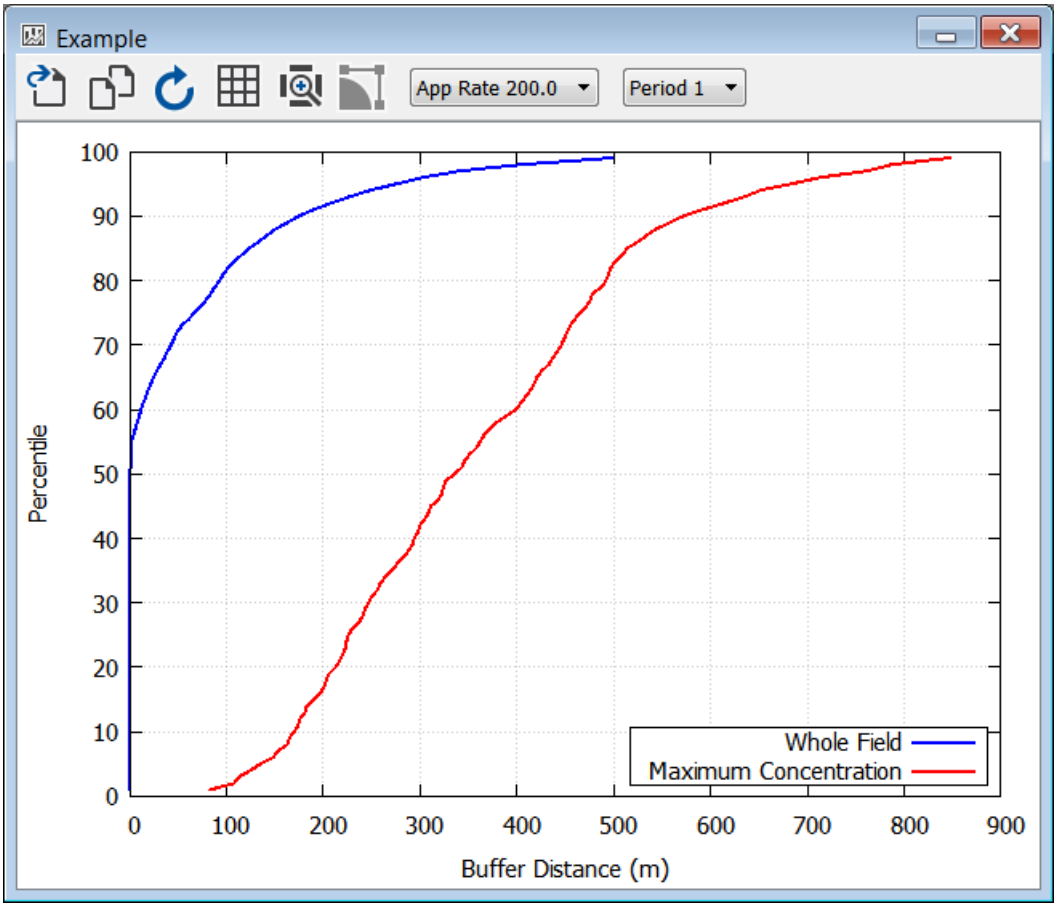


Figure 7. Buffer distance plot window

Options for graphics export, plot appearance and data selection are provided on the toolbar:

Export Plot: exports the current view to a PDF, PNG or SVG file.
Copy to Clipboard: copies an image of the current view to the clipboard.
Refresh: force replot; normally unused.
Toggle Grid: turns the background grid on and off.
Zoom to Fit: zooms to the extent of the loaded data.
Toggle Smoothing Spline: contour only; fits a smooth curve to the points.

The **App Rate** and **Period** drop down lists select subsets of the data for plotting.

In addition, several keyboard and mouse shortcuts are available to control the plot appearance:

- To change the size of the plot, resize the window.
- To zoom in on a specific area, right click at the first corner of the area, then right click again at the opposite corner.
- Click an item in the legend to turn it on or off.

- To pan up/down, move the mouse wheel.
- To pan left/right, hold Shift and move the mouse wheel.
- To zoom in/out, hold Ctrl and move the mouse wheel.

7.0 MODEL APPLICATION EXAMPLES

This section contains example scenarios for each of the scenario types in PERFUM:

- Polygon
- Circular
- Margin of Exposure
- Enclosure

To demonstrate the use of PERFUM, an example dataset has been developed. The model will be run with this dataset for the POLY, MOE, and CIR scenarios, though the field dimensions will be defined differently for the CIR scenario. Additional assumptions will be made for the ENCL scenario. For the field applications, we have assumed two days of flux data. The assumed flux values are listed in Table 2. Additional assumptions are listed in Table 3. All of the scenarios are included in a PERFUM project file called UsersGuide which is included in the Examples directory.

Table 2. Flux rates for hypothetical field application

	Flux Rates (µg/m2/sec)	
Hour	**Day 1**	**Day 2**
13	200	50
14	200	50
15	200	50
16	200	50
17	200	50
18	200	50
19	100	25
20	100	25
21	100	25
22	100	25
23	100	25
24	100	25
1	20	5
2	20	5
3	20	5
4	20	5
5	20	5
6	20	5
7	20	5
8	20	5
9	20	5
10	20	5
11	20	5
12	20	5

Table 3. Additional assumptions for hypothetical field scenario

Parameter	Assumed Value
Grid Density	Coarse
Number of Simulation Days	2
Averaging Period	8 hours
Distribution Averaging Period	8 hours
Meteorological Data Station	Raleigh, North Carolina
Contour Percentile	95
HEC	50,000 $\mu g/m^3$
UF	100
Field Size	5 acres

For the purposes of these simulations, a meteorological data file from Raleigh, North Carolina for 1990 was used. Both ISCST3- and AERMOD-formatted files were produced and are included in the **EXAMPLES** directory.

7.1 POLY Scenario

The single field scenario was run with the assumptions listed in Tables 3 and 4.

Figure 8 shows a plot of the whole field buffer distances for first period after the application, including results for each dispersion model. Figure 9 shows the same plot for the maximum concentration distribution. The 95th whole field percentile values are higher using ISCST3 (95 meters) compared to AERMOD (63 meters) and CALPUFF (51 meters). For the maximum concentration distribution, the 95th percentile buffer zones were highest using AERMOD (259 meters), followed by ISCST3 (193 meters), and then CALPUFF (100 meters).

Different models use different algorithms for calculation of dispersion parameters which can yield different concentration impacts. One difference between AERMOD and CALPUFF is the treatment of calms. AERMOD skips the hours with calms (no wind), while CALPUFF switches to calm wind mode calculation and produces results even for the calm hours. In AERMOD when modeling light winds at night, a meander algorithm is used which spreads concentrations in all directions including up wind (this option is implemented differently depending on the value of LOWWIND parameter). The meandering algorithm is not used in CALPUFF.

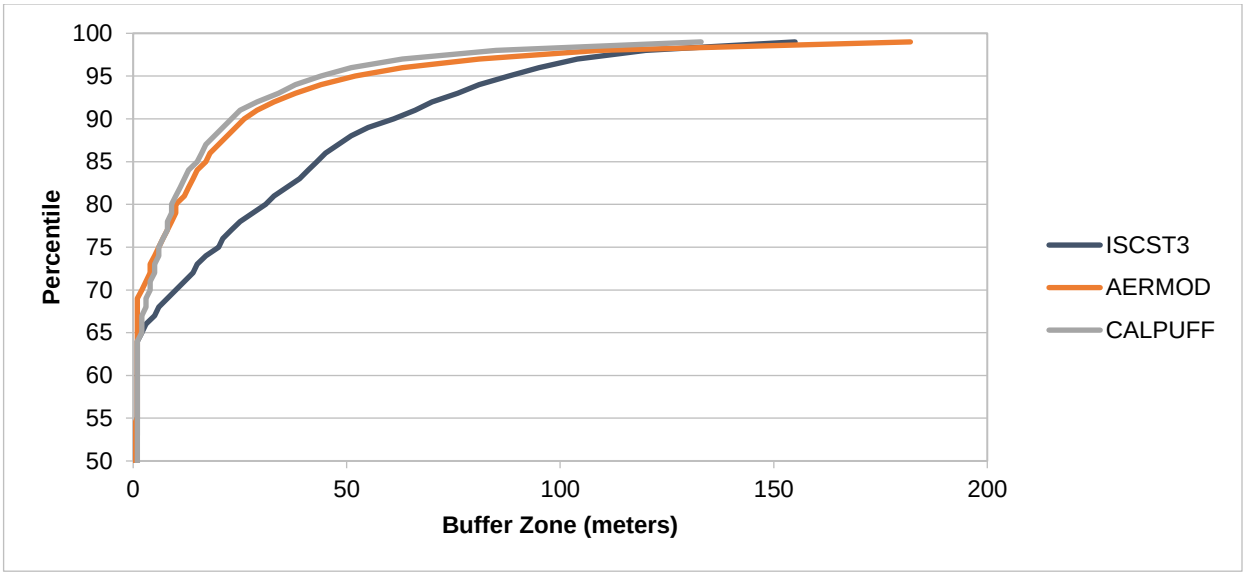


Figure 8. Whole field buffer zone distribution for first period after the application for example scenario

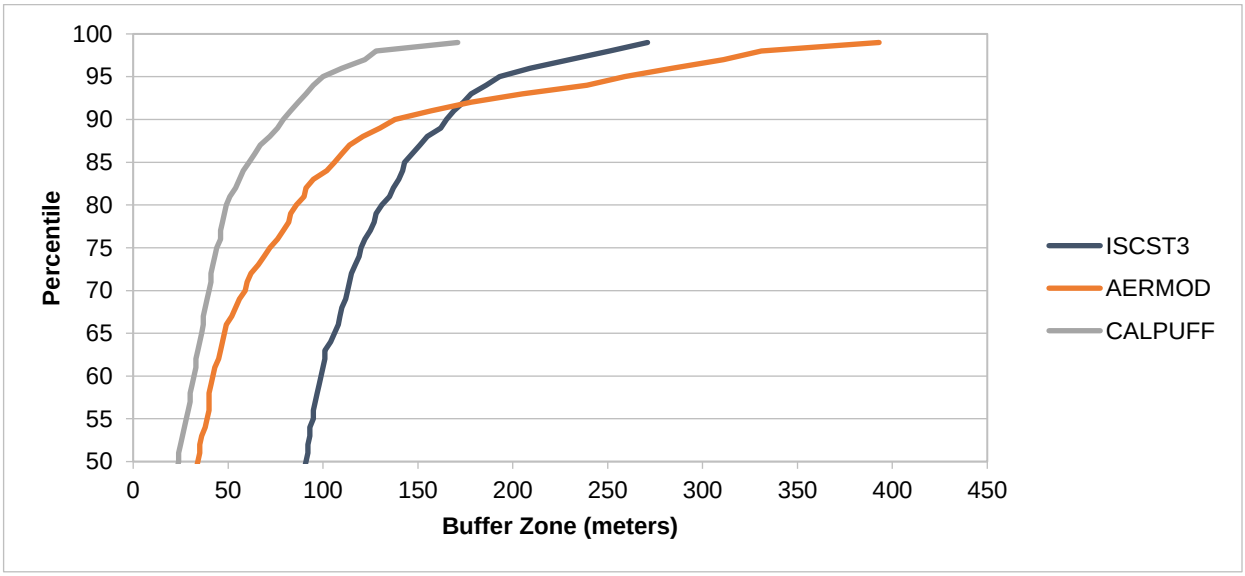


Figure 9. Maximum concentration buffer zone distribution for first period after the application for example scenario

The results for the second period after the application are shown in Figure 10 (whole field) and Figure 11 (maximum concentration). Using CALPUFF yielded significantly lower buffer zones (23 and 74 meters for 95th percentile for whole field and maximum concentration, respectively) than ISCST3 (64 meters for 95th percentile whole field and 212 meters for 95th percentile maximum concentration) and AERMOD (52 meters for 95th percentile whole field and 284 meters for 95th percentile maximum concentration).

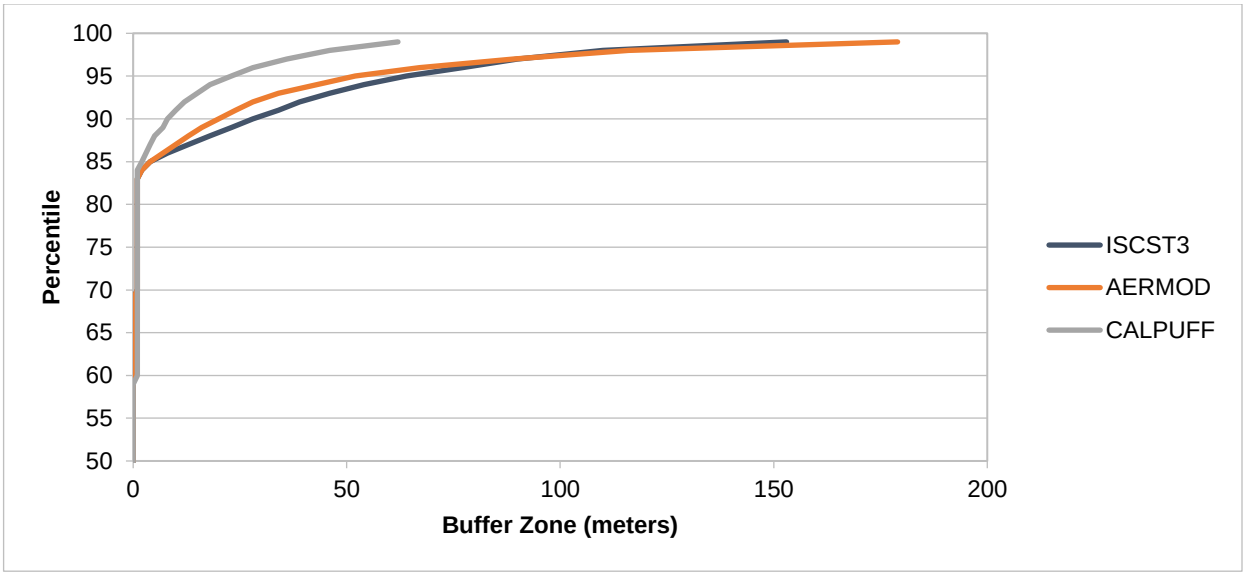


Figure 10. Whole field buffer zone distribution for second period after the application for example scenario

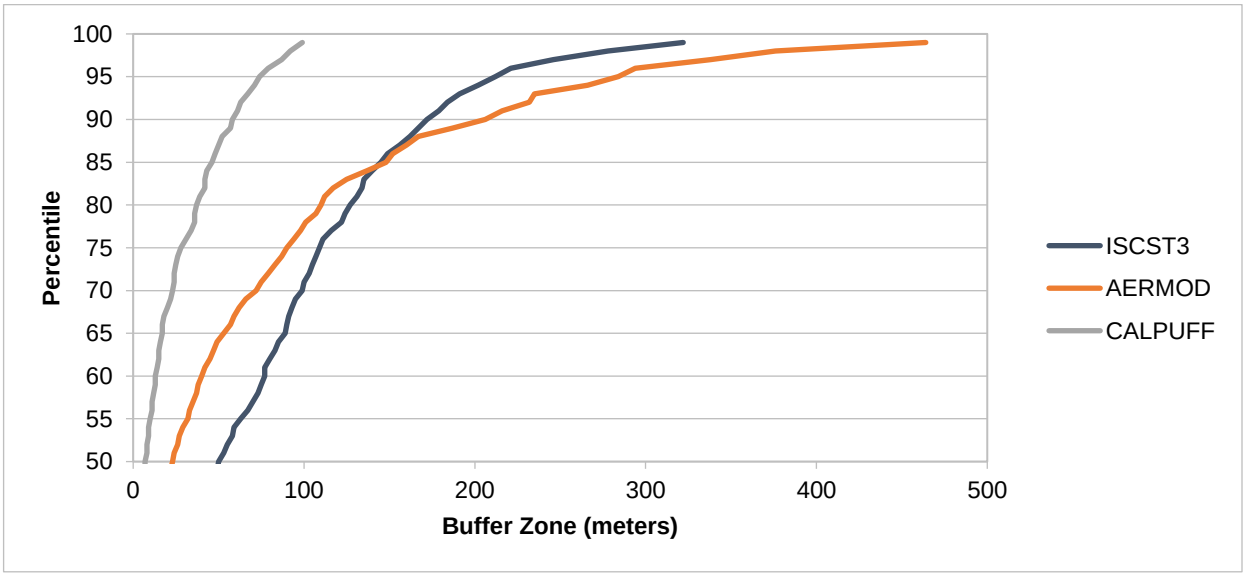


Figure 11. Maximum concentration buffer zone distribution for second period after the application for example scenario

Figure 12 shows a plot of the monthly buffer zones for period 1 using AERMOD. The buffer zones during the Spring and Summer months are often less than half of the buffer zones during the winter months. The reason is that wind speeds are generally greater during the summertime and the longer days result in fewer hours with low turbulence.

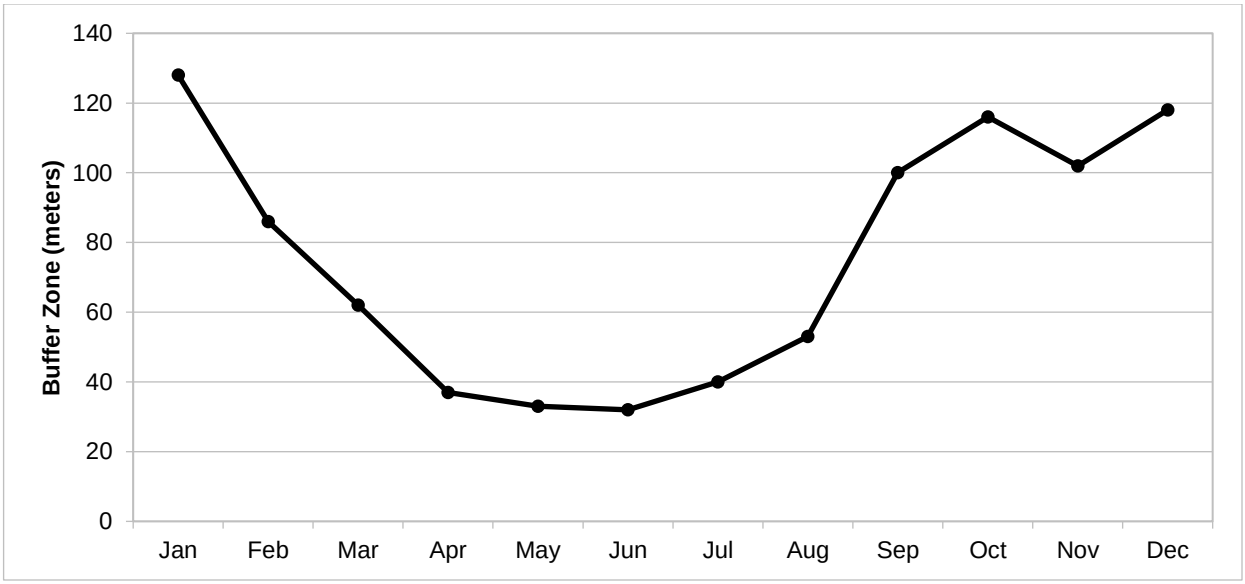


Figure 12. Monthly buffer zones for period 1 after the application using AERMOD

Finally, Figure 13 shows a plot of the contour file for the first period after the application using AERMOD. The file shows the 95th percentile buffer distance calculated separately for each spoke to show the directional range of the buffer distances. The plot shows that the buffer distances are highest in the northwest quadrants from the field edge. PERFUM predicts that buffer zones are smallest to the east.

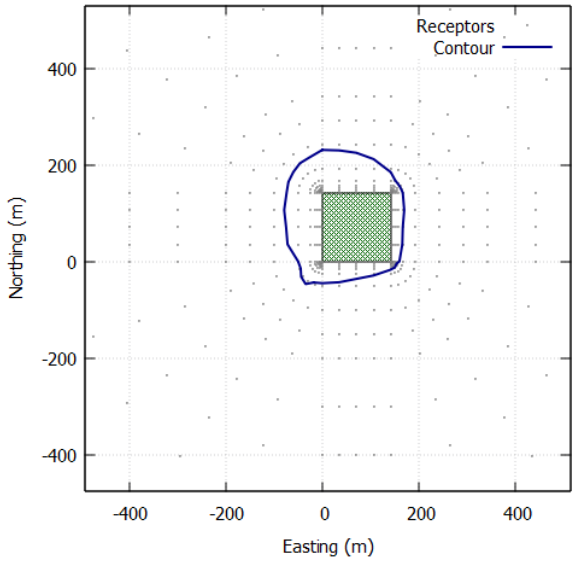


Figure 13. 95th percentile buffer distance for period 1 after the application using AERMOD

7.2 MOE Scenario

To demonstrate the margin of exposure scenario, a buffer length of 260 meters was entered, which corresponds to the 95th percentile of the maximum concentration distribution for the first period after the application using AERMOD.

Figure 14 shows the whole field MOEs for the first period after the application. As expected, the MOE is 100 (or very close to it) at the 95th percentile, as the buffer zone entered into the MOE scenario was defined to be 100 at the 95th percentile. These plots are useful for examining the MOEs at the upper-end of the risk distribution.

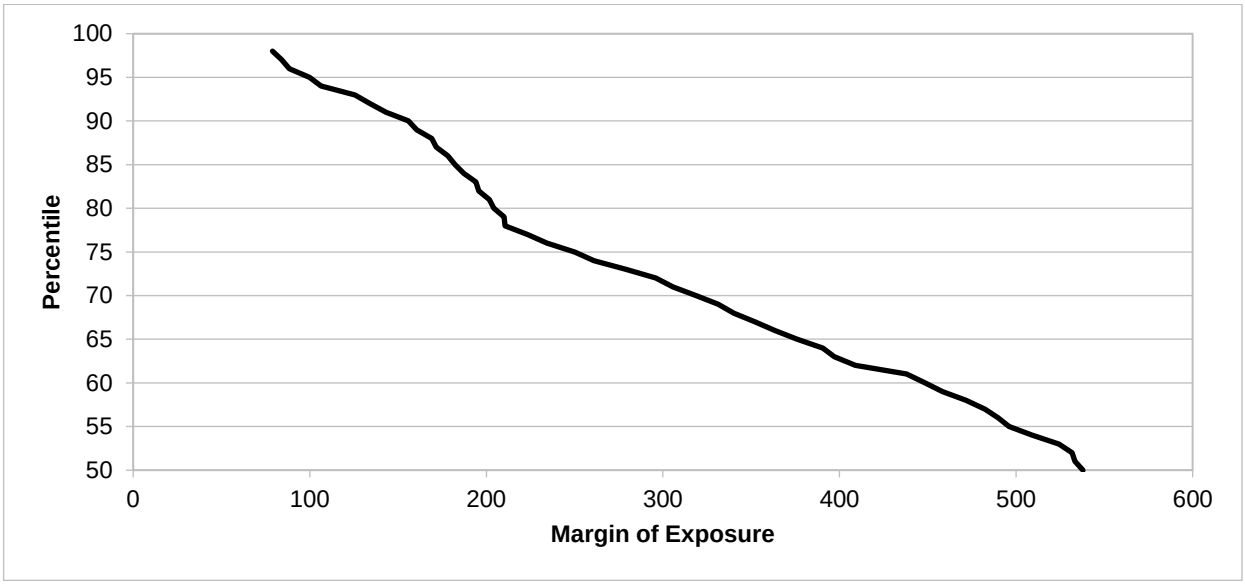


Figure 14. Whole-field MOEs for the first period after the application

7.3 CIR Scenario

A circular source was run with a radius of 80.2 meters, which yields a 5 acre field as with the POLY scenarios. AERMOD was used as the dispersion model. Otherwise, all of the same assumptions for the POLY scenario were used. The 95th percentile whole field buffer zones were 57 and 63 meters for periods 1 and 2, respectively. The 95th percentile maximum concentration buffer zones were 253 and 257 meters for periods 1 and 2, respectively. These values are very similar to the AERMOD POLY scenario with a square field.

7.4 ENCL Scenario

To demonstrate the enclosure scenario, a 10 meter by 10 meter enclosure was assumed, with a building height of 10 meters (total volume = 1,000 m^3). The fine grid was used because the point source algorithms run very fast and the area of the building is small relative to agricultural fields. The theoretical method was chosen to estimate the flux rates. The application rate was 1.0 lbs/1,000 ft^3. An aeration rate was assumed with an air exchange rate of 3.0 per hour with a retention rate of 75%. Point, area and volume sources were modeled. The stack height (above the building) was 1 meter with a stack diameter of 1 meter. The stack exit velocity was

calculated to be 1.06 m/sec for the point source simulation and was calculated from the building volume, air exchange rate, and stack area. Finally, a toxicity level of 5,000 μg/m^3 with a 100-fold uncertainty factor was assumed. Simulations were performed using AERMOD. Table 3 summarizes the enclosure scenario assumptions.

Table 4. Assumptions for the enclosure scenario

Parameter	Assumed Value
Grid Density	Fine
Number of Simulation Days	1
Averaging Period	24 hours
Distribution Averaging Period	24 hours
Meteorological Data Station	Raleigh, North Carolina
Contour Percentile	95
HEC	5,000 μg/m^3
UF	100
Enclosure dimensions	10 x 10 x 10 meters
Flux rates	Calculated
Application rate	1 lb/1000 ft^3
Aeration rate	3 per hour
Retention rate	75%
Stack height above building (point only)	1 meter
Stack diameter (point only)	1 meter
Exit velocity (point only)	1.06 m/sec
Dispersion model	AERMOD

Figure 15 shows the maximum concentration distribution for each of the source types. The lowest buffer zones are for the point source example where the buffer zones were zero below the 98th percentile. The point source scenario has lower buffer zones because the source is elevated above the building and there is momentum for the release through the stack that elevates the plume further above the building. The 95th percentile buffer zones were 72 and 81 meters for the area and volume source scenario, respectively. The area source has zero buffer zones below the 80th percentile, whereas the volume source has non-zero buffer zones for all scenarios. This makes sense since the area source emits all of the mass at the top of the building whereas the volume source emits a lot of the mass through the sides where it will reach the ground quicker.

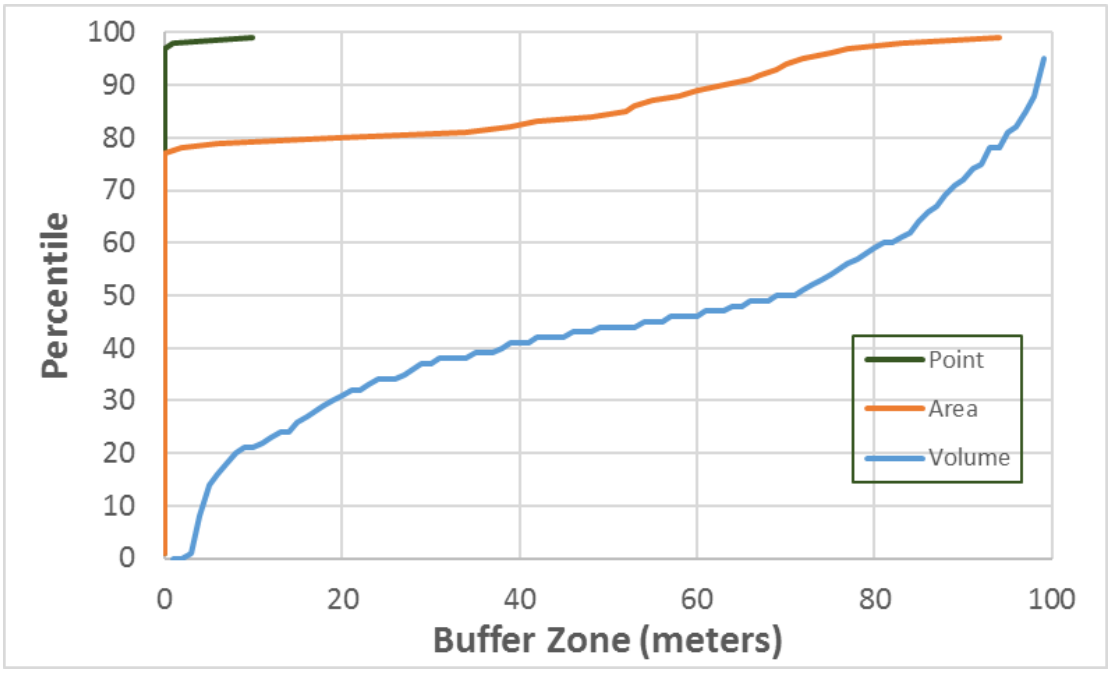


Figure 15. Maximum concentration distribution for the enclosure scenario example using three source types and AERMOD

ERROR CODES

Error Number	Description
901	PERFUM.INP file not found
902	Unknown scenario type: Must be POLY, ENCL, MOE, or CIR (USE ALL CAPS).
903	Error reading met station ID
904	Error reading upper-air station ID
905	Error reading source x-dimension
906	Error reading source y-dimension
907	Field size must be > 0.001 acres and <= 160 acres
908	Invalid grid density choice. Must be C or F
909	Error reading enclosure app rate
910	Enclosure application rate must be between 0.01 and 30 lb/1000 ft3
911	Invalid flux choice. Must be C (calculated) or E (entered)
912	Error reading air exchange rate
913	Air exchange rate must be between 0.001 and 100 per hour
914	Error reading retention rate
915	Error reading scenario type
916	Error reading source type for enclosure scenario
917	Enclosure source type must be P, V or A
918	Error reading enclosure source height
919	Invalid enclosure height - must be > 0 and < 50 meters
920	Exceeded receptor limit. Reduce number of receptors
921	Retention rate must be between 0.001 and 1.0
922	Error reading dispersion model selection
923	Error reading enclosure air exchange rate
924	Receptor height must be between 0 and 5 meters
926	Error reading enclosure stack diameter
927	Error reading receptor height
928	Error reading aeration AER
929	Error reading header string for flux data
930	Error reading monthly identifier
931	Error reading header string for field size

Error Number	Description
932	Error reading the number of simulation days
933	Number of simulation days between 1 and 5
934	Error reading the averaging time
935	Averaging time must be between 1 and 24.
936	Averaging time must be a factor of 24
937	Error reading the distribution averaging time
938	Distribution averaging time is less than the averaging time
939	Distribution averaging time must be an even multiple of the averaging time
940	Distribution averaging time must be less than or equal to 24
941	Distribution averaging time must be a factor or 24
942	Error reading START YEAR of model run
943	START YEAR is must be between 1975 and 2030
944	END YEAR must be between 1975 and 2030
945	Error reading END YEAR of model run
946	START YEAR cannot be greater than the END YEAR
947	Error reading application start hour
948	Application starting hour must be between 1 and 24
949	Error reading meteorological file name
950	Error reading PERFUM output file name
951	Error reading plot file name
952	Error reading contour file name
953	Error reading contour percentile
954	Contour percentile must be between 1 and 99.9
955	Error reading POD
956	Error reading uncertainty factor
957	Uncertainty factor must be > 1
958	Monthly identifier must be Y or N.
959	Error reading buffer length
960	Buffer length must be >0 and <1440 meters
961	Error reading the number of application rates
962	The number of application rates must be between 1 and 10
963	Error reading application rates

Error Number	Description
964	Active application rates must be greater than zero
965	Inconsistent application rates for enclosure scenario
966	Error reading ISCST3 input file name
967	Error reading ISCST3 output file name
968	The first specified application rate must be the largest
969	Error reading flux rates
970	Less than 24 hours of flux data input
971	All fluxes must be entered as real numbers and there must be the same number of flux rates as simulation days
972	Unknown dispersion model entered. Must be ISCST3, AERMOD, or CALPUFF (USE ALL CAPS).
973	UNUSED
974	Aspect ratio of source must be <10
975	Error reading output type
976	FORMAT(' INPUT ERROR : Error reading enclosure stack height
977	Unknown output type entered. Output type can be CONC or DDEP (USE ALL CAPS).
978	Error reading AERMOD/CALPUFF surface file
979	Error reading AERMOD/CALPUFF upper air file
980	Error reading crop circle radius
981	Crop circle radius must be greater than 0 and less than 500 meters.
982	Error reading adjusted building height
983	Adjusted building height must be less than or equal to actual height.
984	Error entering exit velocity
985	Error entering release temperature
988	Error reading RINGS.TXT file
9881	Error reading RINGS.TXT file. Number of rings should not exceed 30. Check value of the first line in RINGS.TXT.
9882	Error reading RINGS.TXT file. Number of rings indicated in the first line of RINGS.TXT is larger than the number of ring sizes provided in the file.
989	First ring in rings.txt must be 1 meter
990	Second ring in rings.txt must be 5 meters
991	Ring distances must be monotonic
992	Error reading first dayrange

Error Number	Description
993	Error reading second dayrange
994	Error reading anemometer height
995	Anemometer height must be between 2 and 15 meters
996	Error reading low wind speed option for AERMOD
997	Invalid LOWWIND identifier. Value must be 0, 1, 2 or 3
701	Error entering Air Diffusion
702	Error entering Water Diffusion
703	Error entering Cuticular Resistance
704	Error entering Henrys law
705	Error entering Atmospheric half-life
709	Deposition run available with AERMOD only. Choose concentration run (CONC) instead.
710	Warning: Enclosure stack height. Should be greater than 0 and less than 50 meters
711	Warning: Enclosure stack diameter. Should be greater than 0.0001 m and less than 20 m
712	Warning: Enclosure exit velocity. Should be greater than 0 and less than 20 m/s
713	Warning: Enclosure exit temperature. Should be either between 283-313K, or 0K in which case, ambient temperature is modeled
714	Warning: Air diffusion. Should be between 0.01 and 0.2 cm2/s
715	Warning; Water diffusion. Should be between 0.1e-5 and 2.e-5 cm2/s

VERSION HISTORY

The topics in this section describe significant changes made to PERFUM over the life of the model since 2004.

Version 2.0.0

Version 2.0.0 (PERFUM2) was released on June 6, 2008.

Changes were made to expand the capabilities of the model to be able to accommodate a wider range of scenarios, including any field size less than 160 acres, irregular field shapes, the effect of multiple fields, and greenhouse applications. It was not necessary to make any significant corrections to the program, and PERFUM2 gave very similar results as the original version of PERFUM (very small differences are possible as explained below).

The major changes in PERFUM2 included:

- The incorporation of two multiple field scenarios (since removed in PERFUM3) and a greenhouse scenario into the model.

- The consolidation of the prior program PERFUM_MOE into PERFUM2 so that the MOE algorithm can be run as a scenario within PERFUM2 without the need for an additional program.

- The development of algorithms to construct the receptor grid within PERFUM2 instead of using a pre-built receptor grid as in the original version. The use of the pre-built receptor grids in the original version limited the number of field sizes and field shapes that the user could apply without developing their own receptor grids. PERFUM2 allowed the user to specify the length and width of the field and then constructs an appropriate receptor grid. Because the placement of the receptors were not completely identical in PERFUM2 for a field size and shape included in the original version of PERFUM, there was a possibility that the results between PERFUM and PERFUM2 could differ by small amounts (~5 meters for buffer zones). This is well within the assumed error range for the model. The user still has the option of using a fine or coarse grid.

- The propagation of the uncertainty of the flux rates was removed. This feature in the original version of PERFUM allowed the user to enter an uncertainty for each flux rate, which allowed the flux rates to be included as a probabilistic variable in the model. There were several reasons for this decision: (a) the use of this method does not separate variability (caused by meteorology) and uncertainty (as modeled for the flux rates) as is desirable in probabilistic modeling, which was pointed out by the SAP, and which is discussed in the literature (e.g., Cullen and Frey, 1999), (b) EPA did not make use of this feature in its preliminary risk assessments for fumigants other than iodomethane, (c) there is more variability in the measurements among different flux studies than uncertainty within a single flux study, thus looking at the results across different flux studies is the most useful way to understand the potential variability in buffer zones

across different applications, and (d) the application of this feature required a significant effort to develop the required inputs.

- The inclusion of algorithms to estimate the concentration distribution at different distances from the field.

- The inclusion of algorithms to estimate the concentration distribution within the near-field activity zone (since removed).

Other minor changes in PERFUM2 included:

- The input file name has been changed from CONTROL.TXT to PERFUM.INP.

- The prior version of PERFUM had "test files" that outputted detailed results for a single day specified by the user. The purpose of the test files was to allow a thorough checking of results for a subset of the simulation. This was no longer considered necessary given the wider usage of PERFUM since its development. Therefore, this feature was removed.

- There was a warning file in the original version which included messages of potential problems in a PERFUM run. This file has been removed, and all error and warning messages print to the screen and execution is halted.

Version 1.0.0

Version 1.0.0 was released on July 28, 2004. Initial release.

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