Appendix A
Detailed Description of the PERFUM Modeling System

A.1 Features of the PERFUM Modeling System

The PERFUM modeling system was developed to assist risk assessors and risk managers in understanding the potential for bystander exposures and risk following fumigant applications. The system includes two programs: (1) the main modeling program PERFUM, and (2) the risk management tool PERFUM_MOE. The EPA regulatory dispersion model ISCST3 can be programmed to output all of the necessary of information to estimate buffer zones; however, the estimate would require significant post-processing, and the generation of very large ISCST3 output files. Instead, PERFUM integrates the ISCST3 computer code, with minor modifications as described below, to perform the buffer zone calculations efficiently and accurately.

The PERFUM system includes the following features:

- Algorithms to estimate the probability of being exposed to a given concentration of interest if one is at the perimeter of a buffer zone specified by the user. The model also outputs the probability of being exposed to a given concentration if it is assumed that a person is at the location with the maximum downwind exposure. The latter probabilities are analogous to the methodology used by CDPR to estimate buffer zones for methyl bromide.

- For a given buffer zone estimate, the PERFUM_MOE program can be used to generate a probability distribution of margins of exposure for a person at a random location along the perimeter of the buffer zone. This calculation will allow risk managers to gauge the potential for exposures above a given concentration threshold, and the margin by which any exposures exceed these thresholds. The PERFUM_MOE program also calculates the margins of exposure for the distribution of maximum concentrations around the field (i.e., not including other areas around the field that have concentrations below the maximum).

- PERFUM performs all of the buffer zone calculations on a monthly basis also, outputting the buffer zone distributions for each month. This is useful for looking at buffer zones for fumigants that are used in well-defined use seasons.

- PERFUM performs all of the buffer zone calculations for up to 10 user-supplied application rates. Buffer zone requirements for methyl bromide in California are a function of the application rate. Therefore, this feature allows quick calculations of buffer zones for multiple potential application rates.

- PERFUM includes an option to treat the flux rates of the fumigants in a probabilistic manner that incorporates the measurement uncertainty in the flux study.

- The report shows that the starting time of the application and the diurnal profile of the flux rates can have a large impact on the potential buffer zones. PERFUM allows for an explicit treatment of the application start time and the subsequent diurnal profile of the flux rates.

- PERFUM is relatively easy to use for any user familiar with ISCST3. It only requires a minimum of input information. For a 1 acre field, the model runtime is on the order of several minutes with a modern desktop computer. For a 40 acre field (the largest so far tested), the runtime is about 15-20 minutes.

- The PERFUM and PERFUM_MOE programs contain about 60 error messages to assist users in identifying run problems. Most of the error messages between PERFUM and PERFUM_MOE are identical. A description of the error messages and potential solutions are listed later in the appendix.

- The program creates a file to store warning messages that identify potential run problems, but for which execution is not stopped (like the error messages). A description of the warning messages and potential solutions are listed later in the appendix.

The next subsection provides a detailed description of the program structure and algorithms.

A.2 Structure of the PERFUM Code

PERFUM was developed in FORTRAN 95 using the Lahey 95 compiler. The FORTRAN code includes extensive commenting to assist interested users in following the structure of the code and calculations. The FORTRAN code has been printed out and provided as an attachment to the report. It is also available electronically on the CD-ROM. For the ISCST3 portion of the code, only the portions that were changed for PERFUM are provided. The PERFUM code includes a main program (PERFUM), six subroutines, and two modules.

- *PERFUM_INI*: Used to initialize variables used in the run.
- *ISCST3*: EPA's ISCST3 model, but changed from a main program to a subroutine called by PERFUM.
- *HRBUFFER*: Called from ISCST3 to sum the hourly concentrations for a period and match the receptor point in ISCST3 to the receptor point in PERFUM.
- *DAYCALC*: Called from ISCST3 after the completion of dispersion calculations for each 24-hour period to calculate the 24-hour averages for each receptor point, and estimate the buffer distance for each spoke. In PERFUM_MOE, this subroutine is used to estimate the concentration at the user-supplied buffer distance for each spoke.
- *SPLINT*: For each spoke, SPLINE calculates an array of second derivatives of the concentration with respect to distance for input into SPLINT. In PERFUM_MOE, this subroutine calculates an array of second derivatives of the distance from the field with respect to concentration.
- *SPLINE*: For each spoke, calculates the distance from the field to the threshold concentration from a cubic spline interpolation. In PERFUM_MOE, the subroutine calculates the concentration at the user-supplied buffer zone for each spoke.
- *BUFFER1*: FORTRAN module for PERFUM that declares variables available in the main program and all of the subroutines (including the ISCST3 subroutine).
- *MAIN1*: FORTRAN module for the ISCST3 program. This module was not modified from the EPA code, but was made available in the PERFUM main program and subroutines so that ISCST3 variables could be used.

Main Program

The main program performs several purposes. The first part of the code opens the main input file (the CONTROL.TXT file), which includes the names of all of the other input files, output file names, and other important information needed for the run. The detailed format of the CONTROL.TXT file is discussed below. Briefly, the input files needed by PERFUM include the ISCST3 input file, a coordinate file that lists the receptor points (supplied with the modeling software for different field sizes and density), and the t-distribution file (supplied with the modeling software). The control file also names the ISCST3 output file and the PERFUM output file (usually labeled PERFUM.OUT). The other information that is needed include the starting and ending years of the model run, the starting hour of the application, the toxicity threshold concentration, the coefficients of variation for the measurement uncertainty of different flux rates, and the application rates for which to conduct the modeling run. This part of the program contains extensive error checking to assure the consistency of the input information.

The main program opens two TEST files (TESTFILE1 and TESTFILE2), which output the ISCST3 results for a single period (TESTFILE1) and the buffer length estimates for each spoke for that period (TESTFILE2). This allows any interested user the ability to check the calculations for a single period.

The main program opens a file of t-values from a t-distribution, which are used in the probabilistic simulation of the flux rates. The file is called TDIST11.CSV and is supplied with the PERFUM software, although the user could construct an alternative file if desired. The t-values were constructed with the TINV function in Microsoft Excel® assuming 11 degrees of freedom. Most of the flux studies contain 12 data points, and the regressions to estimate the period flux rates have 11 degrees of freedom. The structure of the TDIST file is simply 2000 random t-values on separate rows. The file was examined to assure that the t-values at the upper and lower percentiles closely approximated a t-distribution with 11 degrees of freedom. Alternative t-distribution files have been developed to test the representativeness of the t-value file program with the program. The buffer zone estimates with the alternative files were always virtually identical at the 95th percentile.

An alternative to this approach would be the use of a random number generator built into the program. However, the advantage of using a pre-defined file of random

numbers is that the results are repeatable for multiple runs. Also, when the PERFUM_MOE program is run with a buffer zone estimate from PERFUM, each flux period on each day of the simulation will be assigned the same uncertainty as in the PERFUM run. Therefore, there would be no bias between the PERFUM_MOE and PERFUM runs for the same scenario. Additionally, it is desirable from a regulatory perspective for users to get the same results for a given model scenario, whereas there could be small differences between users if a random number generator were used.

The main program also opens and reads the coordinate file, which contains the receptor coordinates for the modeling run. These coordinates refer to the coordinate system used in ISCST3. The coordinate file expects a header line, followed by sequential lines with four comma-delimited columns containing the x-coordinate, y-coordinate, distance from the field (ring distance), and spoke number. The PERFUM software supplies 10 different coordinate files for use. There are coordinate files for both a fine and a coarse grid system. The coarse grid system runs faster (about 4 times faster), but may underestimate the buffer zones at the highest percentiles (>99th percentile). The fine grid system runs slower, but more accurately estimates buffer zones at the highest percentiles**.** The coordinates in the coordinate file must match the receptor coordinates in the ISCST3 input file. If not, an error message will be given when the first ISCST3 calculations are made. The program also checks that the coordinate file is balanced, meaning that it has the same number of spokes in each ring.

The main program establishes 24-hour periods for the concentrations to be estimated with the application starting time as the first hour followed by the next 23 hours. With the FLUX_PERIOD variable, each hour of the model run period is assigned a period value starting with one, and numbered sequentially. For the hours on the first day before the application start time and the hours on the last day after the application start time, a value of -9 is given for the FLUX_PERIOD variable and calculations are not performed for these hours.

The main program calls ISCST3 as a subroutine, where the vast majority of the runtime processing occurs. After returning from the ISCST3 subroutine, the main program writes the final output file, which includes a repeat of the key input information and all of the calculated distributions. All of the buffer zone estimates are in meters. The user should verify that the emission rates and coefficients of variance all match the intended inputs.

Finally, the main program outputs a few final warning messages, if necessary. These include:

- If there were any errors in the interpolation algorithm in the DAYCALC subroutine, the number of errors is outputted.
- If there were any buffer zone estimates that were larger than the maximum receptor distance in the coordinate file (and thus unknown), the number of these is outputted. This tends to occur a few times per run in the 40 acre fields, but it is not a significant problem, so long if there were fewer of these spokes compared to the total number of spokes estimated. For example, if there were buffer lengths for 100,000 spokes estimated in a model run, and 1000 had estimates that were greater than the maximum distance, the percentile estimates would only be inaccurate at the above the (1 – 1000/100000) 99^{th} percentile. The program prints out the upper percentile that the estimated are reliable, when large buffers are reported.
- The number of spokes with non-monotonic concentration arrays (described later).

Subroutine PERFUM_INI

The PERFUM_INI subroutine simply initializes many of the variables used in the model to zero.

Subroutine ISCST3

The ISCST3 subroutine is simply the EPA ISCST3 model reconfigured as a subroutine. The computer code for the model was downloaded from the EPA website and recompiled. The EPA developers used the Lahey95 FORTRAN compiler, which is the same compiler used to develop PERFUM, so there was no difficulties in recompiling the ISCST3 model.

To integrate the ISCST3 model into PERFUM, a few minor changes were made to the ISCST3 code. All changes in the ISCST3 program are documented with comment statements in the code with "CRR" in the first columns of the line to denote a comment by the PERFUM model developer. The changes to the main ISCST3 program include:

- The GETCOM subroutine in ISCST3 was removed. This subroutine was used to accept the user input of the input and output file names from the command line (or DOS prompt). Since ISCST3 is not loaded from the command line in PERFUM, the input and output file names for ISCST3 are instead loaded into the PERFUM CONTROL.TXT input file.

- The main ISCST3 program (now a subroutine) has a STOP statement at the end of the program, which was removed to allow execution back into PERFUM after the ISCST3 calculations are made.

- The update to the screen that was written after each day of execution was removed, and instead a similar statement was added to the DAYCALC subroutine.

Most of the substantive changes were made in the ACALC subroutine, which is where ISCST3 calculates the receptor concentrations for area sources. The following changes were made in this subroutine:

- A USE statement was added to allow the use of the variables in the PERFUM module BUFFER1.

- Several CYCLE statements were removed, which had the purpose of advancing the program when the concentration was zero to the next receptor in the loop that goes through all of the input receptors. Instead, GOTO statements were added to allow each and every receptor to pass through the portion of the code which called the PERFUM subroutines. This change was necessary to assure that the PERFUM DAYCALC subroutine would be called whenever ISCST3 advanced into a new 24-hour period as defined in PERFUM.

- For each receptor point and hour, the flux period is defined with the FLUX_PERIOD variable using the date variables in ISCST3.

- For each receptor and hour, the HRBUFFER subroutine is called in PERFUM to add the concentrations for the period.

- When a period is finished and the first receptor for the next period is detected, the DAYCALC subroutine in PERFUM is called to calculate the period

concentrations and perform the buffer distance estimates for the previous period.

Subroutine HRBUFFER

This subroutine receives concentration estimates from ISCST3 for each receptor for each non-calm hour. The program matches the receptor coordinates in ISCST3 with the coordinate in PERFUM so that the program knows the ring and spoke for each coordinate. After the match is made, the subroutine adds the hourly concentration at the receptor to an array that is summing the hourly concentrations, so that the period average can be calculated later.

This subroutine also performs the probabilistic treatment of the flux rate, which is done in a special manner to accurately simulate the measurement uncertainty in the flux studies. The measurement uncertainties in the flux studies are input into the model as coefficients of variance (CVs) for each measurement period (from 2 to 12 hours in duration). However, ISCST3 is an hourly model and thus generates a concentration estimate for each hour. To correctly simulate the measurement uncertainty in the flux studies, the same deviation from the mean must be used to perturb fluxes (or concentrations) in a given period, across the hours corresponding to that period. Therefore, when the HRBUFFER routine encounters the first concentration estimate for a new period, the model calculates deviations for each of the flux periods for the 24-hours. The deviation is defined as follows:

$$Deviation(period) = \left(\frac{CV(\%)}{100}\right) * t - value \qquad \text{(A-1)}$$

with a random *t-value* drawn for each of the sub-24-hour measurement periods. For each hourly concentration that passes through the array, the flux measurement period corresponding to that hour is determined and the deviation applied to the concentration estimate, as follows:

$$Conc = Conc + Conc * Deviation(period) \qquad \text{(A-2)}$$

This calculation is mathematically equivalent to applying the deviation to the flux period average, as desired, since the flux and concentration are directly proportional

in the model[1]. If, instead, random deviations were applied to each hour within a flux measurement period, the overall uncertainty would be underestimated.

DAYCALC Subroutine

The DAYCALC subroutine performs several functions. First, the subroutine calculates the period average concentrations. The HRBUFFER subroutine provides a summation of the concentration over the period for each receptor. The DAYCALC routine divides this summed concentration by the maximum of the number of non-calm hours (i.e., the number of hours that ISCST3 was run for the period) and 75% of 24 (or 18). The latter rule is an implementation of EPA's calms processing and duplicates the calculation results in ISCST3.

The DAYCALC subroutine also estimates the buffer distances for each spoke for each period. There are three options for estimating the buffer distance for a spoke depending on the concentrations:

- If the concentration at the second ring is greater than the threshold concentration (true for most significant buffer distances), a cubic spline interpolation is conducted. The cubic spline interpolation is accomplished by calls to the SPLINT and SPLINE subroutines, which are canned routines from the commonly used Numerical Recipes FORTRAN library. The program performs a check of the interpolation estimate to assure that it falls between the rings that bound the threshold concentration. If so, a linear interpolation is conducted. This reality check assures that there are no gross errors in the interpolated concentrations.

- If the concentration at the second ring is less than or equal to the threshold, there are not enough points to do a cubic spline interpolation. If the concentration at the first ring is greater than the threshold, a linear interpolation is conducted between the first and second rings. If the concentration at the first ring is below the threshold, the buffer distance is assigned the distance from the field for the first ring if the concentration at the first ring is half or more than the threshold, and assigned a zero buffer distance otherwise. If the concentration at the first ring is zero, the buffer distance is assigned as zero. It is acknowledged that the buffer estimates

[1] Press et al. (1992) "Numerical recipes in FORTRAN 77: the art of scientific computing.

below the second ring (usually 30 meters) are not as accurate as the estimates beyond the second ring, but these estimates have no impact on the upper percentile estimates, which are typically well beyond 30 meters.

- If the concentration estimate at the last ring is above the threshold, then receptor coordinates were insufficiently far from the field to estimate the buffer zone. In this case, the model assigns the largest ring distance as the buffer zone and prints a warning to the warning output file.

The subroutine produces estimates of buffer distance for each spoke within a period and the maximum buffer distance for the period. These buffer distances are converted to the nearest integer, and an array which stores the frequency of each buffer distance occurring is updated. This results in an efficient storage of the results. After the frequency arrays are updated for a period, all of the concentration estimates can be flushed from memory, which results in an efficient memory management and smooth execution.

A.3 Running the PERFUM Model

PERFUM Input and Output Files

To run the PERFUM program, go to the command prompt in the directory for which the program is stored and type PERFUM. Users can also run the program by double-clicking on the PERFUM executable. However, it is recommended that the program be run from the command prompt because, on some systems, error messages are not visible when run from Windows. If the directory with the PERFUM executable is added to the file directory path, the program can be run from any directory.

The input and output files for PERFUM are listed in **Table A.1**. The principal input file for PERFUM is the CONTROL.TXT file, which contains the names of all of the other input and output files, and the values of the key variables. Instructions for completing the CONTROL.TXT file are provided below. The user must also prepare an ISCST3 input file, just as they would if they were running ISCST3 alone. The ISCST3 input file must contain the identical receptor coordinates as the PERFUM coordinate file, and the program checks to assure this. Example ISCST3 input files are provided for each of the 10 field scenarios provided with PERFUM, which include five different field sizes (1, 5, 10, 20, and 40 acres) with both a coarse and a fine grid option.

The program requires two other input files. First, the random t-distribution file is required and a useable file is provided with the PERFUM software. The user may substitute an alternative file if desired. A receptor coordinate file is also required, specifying the locations of each receptor that ISCST3 will estimate the concentration. The PERFUM program provides 10 receptor files for five different field sizes and both a coarse and a fine grid. The coarse grid runs more quickly and provides estimates that are accurate for most purposes, while the fine grid runs slower but provides more accurate estimates for the upper percentiles.

The PERFUM program has several output files. The main output file, PERFUM.OUT, contains all of the calculated percentiles, including using the buffer distance probabilities using the PERFUM approach and the maximum concentration approach. The file also contains the buffer distance probabilities on a monthly basis. At the beginning of the output file, the most important input information is repeated so that the user can assure that the model correctly read the input data.

PERFUM also outputs the normal ISCST3 output file, which contains a summary of the run and results, and lists any errors that occurred in the run. The user should check this file to determine if there were any errors in the ISCST3 portion of the model run. For the PERFUM part of the run, any run warnings (listed below) are printed in the WARNINGS.OUT file. All error messages are printed to the screen and execution is halted. Finally, for users who wish to check the calculations in

Table A.1. Summary of Input and Output Files in PERFUM

Name of File	Type of File	Description
CONTROL.TXT	Input file	Identifies the names of all of the other input and output files, and the values of key variables.
[ISCST3].INP	Input file	Input file for ISCST3 which identifies hourly emission rates, field coordinates, receptor coordinates and the meteorological file. Can be given any 8-character prefix name. Example files provided with program for each field size, and for coarse and fine grids.
TDIST11.CSV	Input file	Contains 2000 random t-values. File supplied with program, but alternative files of the same format can be substituted.
COORD*.CSV	Input file	Specifies the coordinates of the receptors relative to the field, and the ring and spoke of each receptor. Program supplies 10 coordinate files, for 5 field sizes and for coarse and fine grids.
PERFUM.OUT (or PERFUM_MOE.OUT)	Output file	PERFUM or PERFUM_MOE output file. Contains percentiles of buffer lengths or margins of exposure.
[ISCST3].OUT	Output file	ISCST3 output file. Contains summary of input data, some of the concentration estimates, and a list of errors or warnings.
WARNINGS.OUT	Output file	List of warnings for PERFUM model runs.
TEST1.OUT	Output file	For interested users, contains the buffer length estimates for one test day for checking.
TEST2.OUT	Output file	For interested users, contains the period average concentrations for each receptor for the test day.

PERFUM, a single day can be selected for a PERFUM run (labeled the TEST day), and the program will output the buffer length estimates for each spoke (TEST1.OUT) and the concentration predictions at every receptor (TEST2.OUT).

Setting up the Input Files

Table A.2 lists the required structure of the CONTROL.TXT file. The CONTROL.TXT file is the main input file for both PERFUM and PERFUM_MOE. Because of the similarity in the information required by the programs, identical CONTROL.TXT files are used for a given scenario, with a few lines in the file not read by each of the programs, as appropriate. The format requires that each piece of information be provided on certain line numbers, and in most cases, that the information be entered in a particular format. For example, all numbers are specified as real numbers or integers, which is a requirement in FORTRAN programming. Error messages may be generated if numbers are input in the wrong format. For real numbers, the number of decimal places is also specified. The file is structured so that PERFUM only begins reading the input starting on column 31 of all lines. Columns 1-30 are reserved for descriptions of the required inputs. When entering data into any line, do not use tabs but rather advance the cursor with the space bar. While not visible, the FORTRAN compiler may recognize the tabs and misread the information.

Table A.2 is relatively self-explanatory, but a few items bear more detailed explanations:

- The user is allowed 50 characters to identify any file name. If the input file is in the same directory as PERFUM, there is no need to identify a directory path. However, the user may also have input files in other directories and identify them with the full DOS path name (e.g., c:\buffer\coord1fine.csv).

- The application start hour defines the 24-hour period that calculations are estimated. For example, if the start hour is 8am, the period estimates are made for 8am-8pm. Users should apply the ISC convention for defining hours. ISC numbers each hour from 1-24. For example, hour 1 refers to midnight to 1am, and hour 9 refers to 8am-9am. Therefore, for an application starting at 8am, the start hour should be 9.

- Lines 23-46 are used to delineate the measurement periods of the flux estimates from the flux field study. These periods are used in the model to assign the correct coefficient of variation corresponding to the measurement

error for each period. For example, if there are five measurement periods, the users should assign each hour either 1, 2, 3, 4, or 5. In the examples provided with the program, the first flux period (i.e., when the application started) is defined as 1, and the periods that follow are numbered sequentially. However, the model does not require that the first period be defined as 1, but simply that all hours are defined. The user is free to assign all 24 hours with a different period, and assign CVs to each period.

- Line 50+NF specifies the number of application rates that the user wants to model. The limit is 10, and at least one rate must be specified. The application rates are specified on the lines that follow. The first application rate specified must be the largest rate, and must correspond to the flux rates specified in the ISCST3 input file.

Table A.2. Format of the CONTROL.TXT File

Line Number	Information	Description	Format (all input starts on column 30)
1	Header line	Description of model run. Not read by program	50 CHARACTER String
2	Header line	Delineates portion of CONTROL file to read in ISCST3 input and output file names	Not read by program
3	ISCST3 input file	Names the ISCST3 input file	50 CHARACTER String
4	ISCST3 output file	Names the ISCST3 output file	50 CHARACTER String
5	Header line	Delineates portion of the CONTROL file for PERFUM input information.	50 CHARACTER String
6	Flux data source	Text string to enter source of flux data. Repeated in output file, but has no effect on calculations.	50 CHARACTER String
7	Meteorological data source	Text string to enter source of meteorological data in ISCST3 run. Repeated in output file, but has no effect on calculations.	50 CHARACTER String

Line Number	Information	Description	Format (all input starts on column 30)
8	Field size	Text string to enter the field size. Repeated in output file, but has no effect on calculations.	50 CHARACTER String
9	Begin year	Beginning year of PERFUM run (use 4 digit years, i.e., 1999)	4-DIGIT INTEGER
10	End year	Ending year of PERFUM run (can be the same as the begin year, if running 1 year of data) (use 4 digit years, i.e., 1999)	4-DIGIT INTEGER
11	Application start hour	Starting hour of the application using ISCST3 hour convention.	2-DIGIT INTEGER
12	Coordinate file	Names the receptor coordinate input file (example provided with software)	50 CHARACTER String
13	Warning file	Names a file to store any PERFUM run warnings	50 CHARACTER String
14	Output file	PERFUM output file (usually PERFUM.OUT). Not read in PERFUM_MOE program.	50 CHARACTER String
15	Margin of exposure file	PERFUM_MOE output file (usually MOE.OUT). Not read in PERFUM program.	50 CHARACTER String

Line Number	Information	Description	Format (all input starts on column 30)
16	Threshold	Toxicity threshold in $\mu g/m^3$.	REAL number with one decimal point (e.g., 150.0)
17	t-distribution file	List of 2000 t-values. Provided with model software.	50 CHARACTER String
18	Buffer length	Buffer zone estimate in meters. Only read by PERFUM_MOE	REAL number with one decimal point (e.g., 100.0)
19	Test file 1	Names test file 1	50 CHARACTER String
20	Test file 2	Names test file 2	50 CHARACTER String
21	Test day	Specifies test day in year, month, day, in the following format (99 01 01). Use two-digit year and skip space between year and month and month and day.	50 CHARACTER String
22	Header line	Delineates the definition of the hourly flux periods	Not read by program
23-46	Hour flux period for hours 1-24	Specifies a user-defined integer period for each flux measurement.	2-DIGIT INTEGER
47	Header line	Delineates the definition of the coefficients of variance	Not read by program
48	Number of flux periods, NF	Specifies the number of flux measurement periods	2-DIGIT INTEGER

Line Number	Information	Description	Format (all input starts on column 30)
49 to 48+NF	Coefficient of variance by flux period	Specifies the coefficient of variance (as a percent) for each flux period specified above (lines 23-46).	REAL number with one decimal point (e.g., 25.3)
49+NF	Header line	Delineates the definition of the number of application rates	Not read by program
50+NF	Number of application rates, NA	Specifies the number of application rates to model	2-DIGIT INTEGER
51+NF to 50+NF+NA	Application rates	Application rate. The largest application rate, and the one corresponding to the flux rates specified in the ISCST3 file, must be the first application specified. The program returns an error if the first application rate is not the largest.	REAL number with one decimal point (e.g., 175.0)

The following key information must be provided in the ISCST3 input file:

- It must include an hourly emissions profile, using the HROFDY card to specify flux rates for each hour of the day. It is important to note that the emission rates specified in the HROFDY card must correspond to the maximum application rate specified in the control file. There is no way for the program to check that these inputs are consistent.
- It must include the specification of the field area coordinates with the LOCATION card, and the field size with the SRCPARAM card. For the 10 field scenarios available with PERFUM, the example ISCST3 input files have the correct specifications.
- In the runs used in this report, the file specifies the FLAGPOLE card at 1.5 to set the receptor height at 1.5 meters, a typically breathing height. The user is free to change this value.
- The name of the meteorological data file must be specified.
- The user is free to specify any type of output files available in ISCST3, including plot and post files.

An alternative formulation to PERFUM would be to have the user enter the emission rates into the PERFUM input file and choose which receptor coordinate scenario to run, and then have PERFUM create an ISCST3 input file. This approach would have the advantage of reducing the potential for discrepancies between the two input files, but would lessen the flexibility of the ISCST3 portion of the program.

Coordinate Files

The user needs to specify a coordinate file specific to the field size of the run. The PERFUM software includes 10 coordinate files listed in **Table A.3**. The fine grid files will produce more accurate results at the upper percentiles (>99th), but the coarse grid files will run faster. If the user is only interested in the 95th percentile or below, the coarse grid files should be sufficient.

The user must be sure that the coordinates in the coordinate file match those in the ISCST3 input file, or the program will give an error and halt execution.

Table A-3. Receptor Points for Various Field Sizes for the Fine Grid

Grid Type	Field Size (acres)	Number of Spokes	Number of Distances	Number of Receptors (Spokes*Distances)
Fine	1	96	28	2,688
	5	132	28	3,696
	10	152	28	4,256
	20	188	28	5,264
	40	232	28	6,496
Coarse	1	24	28	672
	5	33	28	924
	10	38	28	1,064
	20	47	28	1,316
	40	58	28	1,624

Running PERFUM and PERFUM_MOE in Batch Mode

The PERFUM software includes two simple DOS batch files that can be used to run PERFUM or PERFUM_MOE in batch mode (i.e., run multiple scenarios consecutively without interfacing with the computer between runs). The files are named RUNEM.BAT and RUNFUM.BAT. The purpose of the RUNEM.BAT file is

to call the RUNFUM.BAT file and give it an 8-digit extension that identifies the run. For example, MN01BKAS could be used to identify the Manteca flux data (MN) for a 1 acre field (01) and Bakersfield-ASOS meteorological data (BKAS). For each run that the user wishes to conduct, the RUNEM.BAT file needs the following statement (the 8-digit identifier above is used as an example):

CALL RUNFUM MN01BKAS

The user should prepare CONTROL.TXT files with the 8-digit identifier added to the filename, (e.g., CONTROL.MN01BKAS.TXT).

The purpose of the RUNFUM.BAT file is to first change the name of the user-supplied CONTROL file to CONTROL.TXT so that the program recognizes it as a PERFUM input file. Following the run, the RUNFUM.BAT file changes the output files (including the PERFUM output file and warning file) to include the 8-digit identifier. Therefore, when the next PERFUM run is made, these files will not be overwritten. Alternatively, the user could also have different output file names specified in each CONTROL.TXT file. Also, the RUNFUM.BAT file changes the CONTROL.TXT file back to its original name (including the 8-digit identifier) so that, for the next run, the CONTROL file can be changed to CONTROL.TXT. The RUNFUM.BAT file for PERFUM is as follows:

RUNFUM.BAT

```
REN CONTROL.%1.TXT CONTROL.TXT
PERFUM (runs the PERFUM model)
REN PERFUM.OUT PERFUM.%1.OUT
REN WARNINGS.OUT WARNINGS.%1.OUT
REN CONTROL.TXT CONTROL.%1.TXT
```

The REN command changes name of the files, and the *%1* identifies the 8-digit identifier from the RUNEM.BAT file. There are analogous files for PERFUM_MOE. The RUNFUM.BAT is name RUNMOE.BAT for PERFUM_MOE.

The user can simply type RUNEM.BAT at the command prompt or double-click on it from Windows. The user must be sure that there are no files named CONTROL.TXT, WARNINGS.OUT, or PERFUM.OUT in the directory prior to starting the batch run, or the REN command will fail.

A.4 Error and Warning Messages in the PERFUM Model

PERFUM and PERFUM_MOE contain over 60 error messages to ensure that all input information is entered properly and all calculations are done accurately. The error messages are largely the same between the PERFUM and PERFUM_MOE programs. **Table A.4** lists all of the error messages in PERFUM and PERFUM_MOE, and suggests possible solutions to these errors.

There are also a few warning messages in PERFUM that are printed to the WARNINGS.OUT file. The difference between a warning and error message is that the program halts execution if an error message is given. The warning messages include:

- A warning is given if the concentration at the last ring (1440 meters in the coordinate files supplied with the program) is greater than the threshold concentration. If this occurs, an accurate estimate of the buffer distance for that spoke cannot be calculated. However, if it only occurs a few times, the estimate of the buffer zone percentile is only biased at the very highest percentiles. If any of these warnings are detected, the PERFUM program outputs a message at the end of execution, which indicates the number of these warnings and the upper percentile that the buffer zone estimates are valid. It should be noted that a buffer zone of 1440 meters is well beyond the distance that would be considered viable in the marketplace; therefore, there is little interest in accurately calculating buffer zones beyond this distance.

- The program performs a cubic spline interpolation to calculate the buffer distance for each spoke. After the interpolation, the program performs a reality check by testing that the concentrations at the rings nearest the interpolated estimate bound the threshold concentration. If this occurs, the program instead performs a linear interpolation between the two adjacent points to more accurately estimate the buffer distance. Nonetheless, the program prints a warning message to the WARNINGS.OUT file to alert the user that this occurred. A few of these warnings in a given run is no cause for concern, but if this warning occurs for a significant number of buffer distances

(>1%), the user may want to remove several of the inner buffer distances and re-run.

- Due to crosswinds, occasionally the concentration at the second ring can be greater than the first ring. If this occurs, the program, removes the concentration at the first ring to achieve a better interpolation. If, for some reason this fails, the program prints a warning message that a non-monotonic concentration distribution occurred.

Table A.4. List of Error Messages in PERFUM and PERFUM_MOE

Error Number	Description of the Error	Possible Solutions
901	CONTROL.TXT file not found	Check that CONTROL.TXT file is the same directory as the PERFUM executable.
902	WARNINGS.TXT file not found	Check that the CONTROL.TXT file is properly formatted, and that the WARNINGS.OUT file is specified on line 13. Check that the name of the file does not exceed 50 characters.
903	TESTFILE 1 not found	Check that the CONTROL.TXT file is properly formatted, and that the TESTFILE1 is specified on line 19. Check that the name of the file does not exceed 50 characters.
904	TESTFILE 2 not found	Check that the CONTROL.TXT file is properly formatted, and that the TESTFILE2 is specified on line 20. Check that the name of the file does not exceed 50 characters.
905	t-Distribution file not found	Check that the CONTROL.TXT file is properly formatted, and that the t-distribution file is specified on line 17.

Error Number	Description of the Error	Possible Solutions
		Check that the name of the file does not exceed 50 characters. Check that the file is in the specified directory, or in the PERFUM model directory if no directory is specified.
906	Receptor coordinate file not found	Check that the CONTROL.TXT file is properly formatted, and that the coordinate file is specified on line 12. Check that the name of the file does not exceed 50 characters. Check that the file is in the specified directory, or in the PERFUM model directory if no directory is specified.
907	Output file not found	Check that the CONTROL.TXT file is properly formatted, and that the output file name is specified on line 14. Check that the name of the file does not exceed 50 characters.
910	Error reading ISCST3 input file name	Check that the CONTROL.TXT file is properly formatted, and that the ISCST3 input file name is specified on line 3.
911	Error reading ISCST3 output file name	Check that the CONTROL.TXT file is properly formatted, and that the ISCST3 output file name is specified on line 4.
912	Error reading header string for flux data	Check that the CONTROL.TXT file is

Error Number	Description of the Error	Possible Solutions
		properly formatted, and that the flux data description is specified on line 6.
913	Error reading header string for meteorological data	Check that the CONTROL.TXT file is properly formatted, and that the meteorological data description is specified on line 7.
914	Error reading header string for field size	Check that the CONTROL.TXT file is properly formatted, and that the field size description is specified on line 8.
915	Error reading the START YEAR of the run	Check that the CONTROL.TXT file is properly formatted, and that the START YEAR is specified on line 9. Enter START YEAR as a 4-digit integer.
916	Error reading the END YEAR of the run	Check that the CONTROL.TXT file is properly formatted, and that the END YEAR is specified on line 10. Enter START YEAR as a 4-digit integer.
917	Error reading application start hour	Check that the CONTROL.TXT file is properly formatted, and that the application star hour is specified on line 11. Enter application start hour as a 1 or 2-digit integer.
918	Error reading receptor coordinate file name	Check that the CONTROL.TXT file is properly formatted, and that the coordinate

Error Number	Description of the Error	Possible Solutions
		file is specified on line 12. Check that the coordinate file name is 50 characters or less.
919	Error reading warning file name	Check that the CONTROL.TXT file is properly formatted, and that the warning file is specified on line 13. Check that the warning file name is 50 characters or less.
920	Error reading PERFUM or PERFUM_MOE output file name	Check that the CONTROL.TXT file is properly formatted, and that the output file is specified on line 14. Check that the file name is 50 characters or less.
921	Error reading threshold value	Check that the CONTROL.TXT file is properly formatted, and that the threshold is specified on line 16. Check that value is a real number with one digit after the decimal place.
923	Error reading *t*-distribution file name	Check that the CONTROL.TXT file is properly formatted, and that the t-distribution file name is specified on line 17. Check that the file name is 50 characters or less.
924	Error reading TESTFILE 1 name	Check that the CONTROL.TXT file is properly formatted, and that the TESTFILE1 name is specified on line 19.

Error Number	Description of the Error	Possible Solutions
		Check that the file name is 50 characters or less.
925	Error reading TESTFILE 2 name	Check that the CONTROL.TXT file is properly formatted, and that the TESTFILE 2 name is specified on line 20. Check that the file name is 50 characters or less.
926	Error reading test file date	Check that the CONTROL.TXT file is properly formatted, and that the test file data name is specified on line 20. Check that a year, month, and day are specified, with two integers each and a space between year and month, and month and day.
927	Error reading flux rate periods	Check that the CONTROL.TXT file is properly formatted, and that the flux rate periods are specified on lines 23-46. Check that each period is a 1 or 2-digit integer.
928	Error reading CVs for flux rates	Check that the CONTROL.TXT file is properly formatted, and that the CVs are specified on lines 49 to 48+NF. Check that each CV is real number with 1 digit after the decimal place.

Error Number	Description of the Error	Possible Solutions
929	Error reading application rates	Check that the CONTROL.TXT file is properly formatted, and that the application rates are specified on lines 51+NF to 50+NF+NA Check that each application rate is real number with 1 digit after the decimal place.
930	START YEAR is out of bounds	START_YEAR must be between 1975 and 2010
931	END YEAR is out of bounds	END_YEAR must be between 1975 and 2010
932	START YEAR can not greater than END YEAR	END YEAR must be equal to or greater than the START YEAR
933	Application start hour out of bounds	Application start hour must be between 1 and 24
934	Threshold concentration out of bounds	Threshold concentrations must be greater than zero
935	Flux period out of bounds	Each hour must have a flux period between 1 and 24
936	Number of flux periods out of bounds	The number of flux periods must be between 1 and 24
937	Mismatch between the number of flux periods specified and actually assigned.	The number of separate flux periods specified on lines 23-46 must equal the number of flux period specified on line 48.
938	Number of application rates out of bounds	The number of application rates must be

Error Number	Description of the Error	Possible Solutions
		between 1 and 10.
939	Application rate error	All application rates must be positive.
940	Application rate error	The first application rate specified must be the largest.
941	Flux rate read error – reached end of file before reading all flux rates	The CONTROL.TXT file may not be properly formatted.
942	CV read error – reached end of file before reading all CVs	The CONTROL.TXT file may not be properly formatted. Check that the number of flux periods specified on line 48, equals the number separate CVs that are specified.
950	t-value read error – reached end of file before reading all 2000 t-values	Check that the t-value file has 2000 t-values.
951	Coordinate file formatting error	The distances from the field (i.e., rings) must proceed from lowest to highest
952	Number of rings out of bounds	The number of rings in the coordinate file cannot exceed 50.
953	Coordinate file formatting error	The spokes identification numbers in the coordinates must proceed from lowest to highest.
954	Number of spokes out of bounds	The number of spokes in the coordinate file cannot exceed 232.
955	Unbalanced coordinate file	The coordinate file must have the same number of spokes for each ring

Error Number	Description of the Error	Possible Solutions
956	Too many years	The number of years of data cannot exceed five.
957	Error in the number of periods estimated by PERFUM – too few periods for number of years specified	Possible coding problem that should be brought the attention of the model developers.
958	Error in the number of periods estimated by PERFUM – too many periods for number of years specified	Possible coding problem that should be brought the attention of the model developers.
959	A flux period not assigned for a given hour. Detected in MAIN program.	Possible coding problem that should be brought the attention of the model developers.
960	Coordinate mismatch between PERFUM and ISCST3	Check that ISCST3 has the identical coordinates as specified in PERFUM
961	A flux period not assigned for a given hour. Detected in HRBUFFER subroutine.	Possible coding problem that should be brought the attention of the model developers.
970	A full day of calm hours in meteorological file	Remove this day from the meteorological file and rerun.
972	Error in interpolation of concentrations across a spoke	May be a coding problem. However, if there are only a few of these errors, the estimates are not likely to be significantly affected.
973	Incorrect number of concentrations processed through the DAYCALC	Possible coding problem that should be brought the attention of the model

Error Number	Description of the Error	Possible Solutions
	subroutine.	developers.
980	Interpolation error in SPLINE subroutine.	Possible coding problem that should be brought the attention of the model developers.
981	Mismatch in years between PERFUM and ISCST3	Check that the years specified for the PERFUM run match the years in ISCST3 meteorological file
982	Valid period not obtained in ISCST3 subroutine	Possible coding problem that should be brought the attention of the model developers.