WORKBOOK FOR GAUSSIAN MODELING ANALYSIS OF AIR CONCENTRATION MEASUREMENTS

Bruce Johnson, Terrell Barry, and Pamela Wofford

September 1999
Revised May 2010

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First things first, but not necessarily in that order.

Doctor Who

Preface to 2010 Revision

Over the intervening years since the first Workbook, we have gained more experience with these techniques. This revised version reflects our experience. We have tightened some of the statistical procedures. We eliminated the major axis regression approach (Johnson 1999) . The only known major axis algorithm was implemented in FORTRAN but failed under certain conditions. The simple regression method presented here is easy to understand and conduct with any conventional regression package. The WEATH5 (Johnson 1999) program has been updated and recompiled in Fortran 95. It is now WEATH6A. Separate documentation is available for WEATH6A (Johnson 2010) . For determining hourly sun altitude, we have dropped the SUNFIX (Johnson 1999) program in favor of the US Navy Astronomical Applications Department Data Services web site. In April 2010 we taught a 1-day course in using ISCST3. The course materials are all contained in a Tutorial appended to this report. Examples and problems in that tutorial are referenced in the Workbook text. A new section, "Topics Since 1999", provides an introduction to some of the concepts and procedures which have arisen since the first version.

Gaussian modeling and related procedures have been used to interpret and analyze air monitoring studies for various fumigants including methyl bromide, chloropicrin, MITC and 1,3-dichloropropene. The methyl bromide permitting program classifies methyl bromide application types using back-calculation estimates of volatilization. For fumigant data analysis, the Department of Pesticide Regulation (DPR) uses the U.S. Environmental Protection Agency (U.S. EPA) Gaussian model, Industrial Source Complex Short Term Version 3 (ISCST3) (U.S. EPA, 1995). The U.S. EPA Office of Air and Radiation and Office of Air Quality Planning and Standards administers the program which reviews and accepts candidate models and "preferred." "alternative," or "screening," and maintains air dispersion model codes. This process insures uniformity in the models and modeling procedures among users. The "preferred" model status is required for State Implementation Plan (SIP) revisions for existing sources and for New Source Review and Prevention of Significant Deterioration (PSD) programs (40 CFR 51, Federal Register, 2005). The "preferred" models related to DPR applications are the AMS/EPA

Regulatory Model (AERMOD) (Cimorellli et al. 2004) and CALPUFF (Scire et al., 2000). The 'alternative' model status allows for reviewed models to be used in regulatory applications with case-by-case justification (Section 3.2, Appendix W, 40 CFR 51, Federal Register 2005). The reviewing authority in this case is DPR and the 'alternative" model related to DPR applications is ISCST3. Since the 1990's, DPR has used ISCST3 extensively to estimate off-site fumigant air concentrations. The ISCST3 model was a "preferred" model prior to the promulgation of AERMOD in December, 2006. Improvements gained by use of AERMOD were not implemented in the area source portion of that model. The back-calculation procedure presented in this document uses area sources exclusively. Thus, a shift from ISCST3 to AERMOD is neither required, nor presents any advantage. The use of CALPUFF has been considered. However, CALPUFF is a complex model that requires extensive meteorological inputs that are not generally available. While it is likely CALPUFF will be integrated into the DPR modeling program eventually, at this time it is not in use.

Historically the ISCST3 model was developed within the context of simulation of industrial smoke-stack discharges which in the ISCST3 vernacular are called point sources. The wide emphasis of ISCST3 use has been for point sources. At DPR an important use of ISCST3 has been to simulate area sources. This document has been created to explain how we have used the ISCST3 for area sources and to provide a resource for our colleagues who may have to use this model for their own area source calculations.

INTRODUCTION.

1.1. **Purpose of this document**
    1.1.1. **Scope**. This document presents procedures used to model field applications, distinct from applications associated with commodities (space fumigations) or homes (structural fumigations)..
    1.1.2. **Record.** Environmental Monitoring (EM) has analyzed many studies. This document provides a summary of our current procedures.
    1.1.3. **Consistency.** This document establishes modeling analysis guidelines.
1.2. **Knowledge and skill requirements**. The optimum combination is knowledge and skill in both quantitative and computer methods. Below is a list of the most important knowledge and skills required to perform these modeling analyses.
    1.2.1. **Concepts**
        1.2.1.1.**Mathematical and statistical** concepts can be found in introductory textbooks.

$$\tan(\theta) = \frac{\sin(\theta)}{\cos(\theta)}$$

$$57.3^o = 1.0 \; radian$$

$$360^o = 2\pi \; radian$$

            1.2.1.1.1. regression
            1.2.1.1.2. confidence intervals
            1.2.1.1.3. trigonometry and geometry
                1.2.1.1.3.1.sin, cosine, tangent, arctangent
                1.2.1.1.3.2.angles-degrees versus radians
        1.2.1.2.**Computer.** Ability to understand and use both DOS and Windows. Knowledge of path, subdirectory tree structures and ascii files, regardless of how files are deleted, renamed or copied.
            1.2.1.2.1. DOS commands- copy, delete, rename, dos file names
            1.2.1.2.2. ascii files
            1.2.1.2.3. subdirectory tree structures
            1.2.1.2.4. comma delimited data

An ascii file generally contains only printable characters such as numbers and letters.

        1.2.1.3.**Physical science** - Primarily meteorology, though other physical sciences may aid in discovering why a particular analysis is not successful. Some of the following references can help understand these concepts including Beychok (1994), Stull (1988), Turner (1994), Wark and Warner (1981) and Zannetti

(1990).

     1.2.1.3.1.   boundary layer stability
         1.2.1.3.1.1.inversion height
         1.2.1.3.1.2.mixing height
         1.2.1.3.1.3.temperature profiles
         1.2.1.3.1.4.convective mixing
         1.2.1.3.1.5.nighttime stable boundary layer
         1.2.1.3.1.6.neutral stability
     1.2.1.3.2.   Gaussian equation relating concentration to flux
     1.2.1.3.3.   log-wind speed profiles
     1.1.1.1.1.   magnetic north, true north, angle of declination.
1.2.2. **Specific software**. To perform regressions and construct graphs it is necessary to reformat tables of numbers and to import and export tables of numbers into various software. The following software can be used to accomplish those tasks. Other software may substitute.
    1.2.2.1.EXCEL - spreadsheet, statistical analysis, some graphics (Microsoft Corporation)
    1.2.2.2.Minitab - spreadsheet and statistical analysis (Minitab Inc)
    1.2.2.3.DOS - operating system (Microsoft Corporation)
    1.2.2.4.NOTEPAD ascii file editor (Microsoft Corporation)
    1.2.2.5.ISCST3 - the USEPA program for estimating air concentrations
    1.2.2.6.WEATH6A - program by B Johnson for summarizing met data (Johnson 2010)
    1.2.2.7.A graphics plotting program.
    1.2.2.8.Google Earth for locating and plotting study fields.
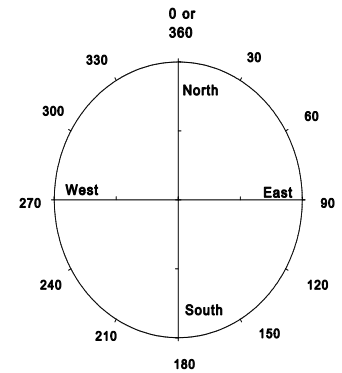
Normally, wind direction is the 'from ' direction. A westerly wind is a wind from the west, from about 270 degrees. ISCST3 requires wind to be in the 'to' direction, 180 degrees offset from the 'from' direction.

1.3. Overview of procedure

1.3.1. **Estimate the flux density**. Most studies measure air concentrations with measurements periods ranging from 2 to 24 hours. A single monitor continuously sampling the air for 8 hours produces a single 8-hour measurement. This measurements represents the average concentration during that time period. During that same 8 hour period meteorological data (e.g. wind speed and direction) are measured at sampling frequencies usually exceeding 60 samples/hour. Part of the analyst′s task is to average meteorological data into appropriate time intervals to match the chemical monitoring periods. The ISCST model estimates air concentrations using meteorological data in conjunction with the geometry of the field, the location of samplers in relation to the field and an initial (nominal) flux. The flux associated with an application is estimated by comparing the model estimated air concentrations to the measured air concentrations. The nominal flux is adjusted so that on average the magnitude of the ISCST estimated air concentrations match the magnitude of the measured air concentrations.

What is flux? The concept quantifies the mass that comes out of the ground and enters the atmosphere per unit area per unit time The units are mass per time per area, typically ug/m^{2}s or lbs/acre-day. The flux is potentially affected by various factors, including atmospheric conditions, soil conditions, application method and application rate.

We assume that flux is proportional to application rate. We have not seen evidence to contradict this assumption. Over the range of practical application rates for fumigants we believe that properties of mass diffusion through the soil and back out into the atmosphere are not affected by the amount of mass being applied either in or on top of the soil.

Flux and flux density. Physical chemists define flux as mass/area-time. Soil physicists use flux to mean mass/time (i.e. flow) and flux density to mean mass/area-time. In this workbook, flux and flux density will be used interchangeable and will mean mass/area-time.

1.3.2. **Proportionality between flux and air concentration**. The Gaussian equation, the kernel of the ISCST3 model, explicitly includes a proportional relationship between flux and concentration. Doubling the flux doubles the concentration. The proportional relationship between flux and concentration is the foundation of the back calculation procedure. As discussed in subsequent sections, the back calculation procedure requires an initial (nominal) flux. This is essentially a guess and does not need to be accurate. The ISCST3 model is first run to obtain estimated air concentrations based upon the nominal flux. The estimated air concentrations are then compared to the measured concentrations. The proportionality property allows a simple adjustment of the nominal flux value to an adjusted flux value that, on average, brings the magnitude of the model estimated air concentrations in line with the magnitude of the measured air concentrations. A typical nominal flux value is 100ug/m^{2}s (0.0001 g/m^{2}s).

$$C = \frac{FK}{2\pi U_s} \int_x \frac{VD}{\sigma_y \sigma_z} \left(\int_y \exp\left[-0.5 \left(\frac{y}{\sigma_y} \right)^2 \right] dy \right) dx$$

$$C = FP$$

The first equation is the full, gaussian equation which relates concentration, C, to flux, F, and meteorology, distance and height. With all meteorology fixed and equal to P, as in the second equation, then the proportionality between C and F is clear.

1.4. **Some useful conversion factors.**

Conversion Factors

To convert from Column 1 to Column 2 multiply Col 1 by Factor1-2

To convert from Column 2 to Column 1, multiply Col 2 by Factor2-1

	Factor1-2	Column 1	Column 2	Factor2-1
1.3.3.				
1.3.4.	0.447	mph	m/s	2.24
1.3.5.	10000	hectares	square meters	0.0001
1.3.6.	0.405	acres	hectares	2.47
1.3.7.	4047	acres	meters	0.000247
1.3.8.	0.305	feet	meters	3.28
1.3.9.	0.112	lbs/acre	g/m^2	8.93
1.3.10.	112000	lbs/acre	ug/m^2	8.93e-6
1.3.11.	1.30e-6	lbs/acre-day	g/m^2s	7.71e5
1.3.12.	1.30	lbs/acre-day	ug/m^2s	0.771
1.3.13.	454	lbs	grams	0.00220
1.3.14.	86400	day	seconds	1.157e-5
1.3.15.	0.01745	degrees	radians	57.3
1.3.16.	0.258	ug/m^3 m.b.	ppb m.b.	3.88*
1.3.17.	0.001	ppb	ppm	1000.

*methyl bromide at 25^oC

Conversions that do not fit into the table:

1) Fahrenheit to Celsius (centigrade), C=(F-32)*5/9 gives Celsius from Fahrenheit
2) Celsius to Fahrenheit, F=(C*9/5)+32 gives Fahrenheit from Celsius
3) Celsius to Kelvin, C+273=K and in the other direction, C=K-273

4) Finally, the conversion from parts per billion (ppb) to ug/m^3 is both temperature and compound specific. At 25 degrees for methyl bromide convert ppb to ug/m^3 by multiplying by 3.88. Conversely, to convert from ug/m^3 to ppb at 25° degrees for methyl bromide, multiply by 0.258. For methyl bromide 815ug/m^3 is equivalent to 210 ppb. Johnson (2001) gives a more general description that can be used for other gases

815ug/m^3 = 210 ppb for methyl bromide at 25° C

1.5 **Example used in this workbook.** The example presented in this workbook was an actual set of calculations to analyze the Seal Beach broadcast tarp application (Johnson and Wofford 1999). The tutorial appended to the Workbook goes into much more point by point methodology for the various techniques described here.

210 ppb = 0.210 ppm

2. **ASSEMBLE DATA** - Various data required for the analysis must be put into a form which can be used by the ISCST3 model.

2.1. **Geographic data** (the geometry of the field and the sampler locations)

2.1.1. **Field location data**. The analysis begins with examining the field map. Determine whether the units of the map are local units of feet, meters, yards or in Geographical Information System (GIS) units such as Universal Transverse Mercator (UTM) Geographic Coordinate System or latitude and longitude (lat/long). If the map is in local units, determine north and whether north is defined as magnetic north or true north.

2.1.2. **Converting local field location to coordinates**. If the map is in local units, use the lower left corner of the field as coordinate 0,0. Arrange the two sides adjacent to this corner so that the vertical side (north/south) is in the Cartesian coordinate system "y" direction and the horizontal (east/west) side in the Cartesian coordinate system "x" direction. Rectangular fields are easily arranged in the Cartesian coordinate system. For fields that area not rectangles, assign the lower left in an

orientation that forms a 90 degree angle. The remaining sides will determine the orientation of remainder of the field. The ISCST3 model allows irregularly shaped polygons. The coordinate of each vertex should be given according to instructions in the ISCST3 user's manual.

For the Seal Beach study, the lower left corner of the field is designated as (0,0), as the origin (Figure 1). The rest of the coordinates follow from the geometry of the field size. The field dimensions are provided in Table 1 of Johnson and Wofford (1999). Section 04 of the tutorial goes into greater detail. A different geometry example which uses multiple polygons to represent a more irregular field can be found in the earlier Workbook version (Johnson et al. 1999 Figures 1,2,3).

2.1.3. **Field location in relation to direction.** The orientation of the field is must be matched correctly to the wind direction frame. Specifically, it must be determined whether north on the field map refers to magnetic north or true north. And later for wind direction, the same determination will be made for truth north or magnetic north. Along the central coast, the difference between magnetic north and true north is about 15 degrees. Thus, a measurement of 15 degrees with respect to true north would be equivalent to 0 degrees magnetic north along the central coast of California. The ISCST3 allows field rotation from north when necessary to adjust for the difference between true and magnetic north when the field measurements and weather data are not on the same basis.. However, it is important to understand the fundamentals behind the necessity for rotation. In this example, both the field directions and the wind directions were measured in relation to magnetic north. Therefore, no rotation or adjustment of any angles was necessary.

The coordinates for each corner of the polygon representing the field input can be checked by plotting the field in Sigmaplot, AutoSketch or an equivalent graphics program. The plotted shape should approximate the map. Compare Figure 1 and Figure 2.

Angle of declination (difference between truth north and magnetic north) can be found at the bottom of the USGS quad maps. The star is true north. MN is magnetic north. In this case, the declination is 14°. The GN is UTM north.
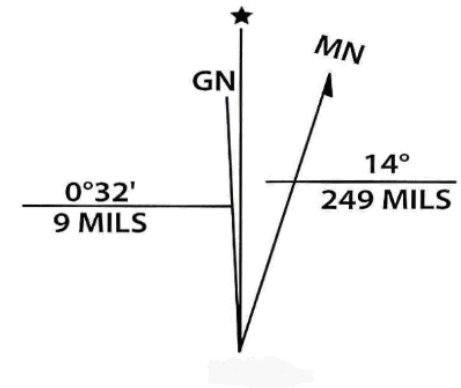
2.1.4. **Air sampler location data**. Each sampler location has a coordinate position. There must be enough information on the original map to determine these coordinates. As with the field coordinates, the sampler locations can be entered and plotted with a graphics program to check against the original study map. Compare Figure 2 and Figure 3. Each sampler will have a sampler height, the distance above ground. This is typically 1.2m Tutorial Section 04 shows how to calculate the monitor locations in order to specify them in the control file.

2.2. **Chemical monitoring data**. Chemicals are typically monitored over periods ranging from 2 to 24 hours. Concentration results from such monitoring are average concentrations over the entire sampling period. During a monitoring period, wind direction shifts,   flux changes, and other conditions change. The instantaneous concentration at a particular location can vary widely during the monitoring period. However, the result of the chemical analysis is a single, average value for the entire sampling period. Average concentrations for the Seal Beach study are shown in Table 1.. Note that the concentration units are ppm (parts per million). If a sampler stops operating during a monitoring period, the general guideline is to use the data if the sampler operated for at least 70% of the time period (Johnson 1999).

In practice, all samplers surrounding a field can not be started at exactly the same time. The field crew travels in a circuit to sampling stations to change the sampling tubes. Use the average of the start and average of the end times to define a sampling period even though sample start times may range over a half an hour. This may be rounded off to the nearest half hour.

2.3. **Meteorological data.** In most cases, onsite meteorological data will have been collected. This data will usually consist of temperature, wind speed and direction, sometimes humidity, precipitation, or standard deviation of wind direction. The Tutorial Section 05 goes into much greater detail on processing meteorology.

2.3.1. **Wind speed**. The ISCST3 program requires wind speed in meters per second.

The WEATH6A program converts wind speed in mph to meters per second.

2.3.2. **Wind direction**. Wind direction is typically recorded as the 'from' direction. A northerly wind means that the wind is blowing from the north to the south. However, the ISCST3 program requires wind direction to be input using the 'to' direction. Thus, if a north wind is measured (0 degrees), then ISCST3 expects a measurement of 180 degrees, indicating that the wind is blowing towards the south. The WEATH6A program will perform conversion of 'from' to 'to' directions. Remember, in addition to this direction conversion, the field orientation and the wind measurement basis MUST BE CONSISTENT WITH EACH OTHER (see section 2.1.3 and Tutorial Section 05 point 8f). Both must be in the same frame of reference. If the field is drawn with respect to magnetic north, then the wind directions must be provided with respect to magnetic north. If the field is true north and the wind directions are magnetic north, then the wind directions must be shifted to align properly with the field. Table 2 presents excerpted meteorological data from the Seal Beach broadcast study.

2.3.3. **Temperature**. ISCST3 requires temperature in degrees Kelvin. The WEATH6A program converts Fahrenheit to Kelvin.

2.3.4. **Time**. The start and stop times must be known for each chemical sampling period in order to process the matching meteorological measurement periods. The meteorological measurements may first require hourly summarization. EM standard practice is to take 12 or more measurements every hour of wind speed, wind direction, temperature. These 12 measurements must be summarized for each hour during the chemical sampling period. WEATH6A performs this summary. In Table 2, measurements for the Seal Beach study were recorded once every two minutes. Times must be reconciled with respect to daylight savings time or standard time. If there are different time frameworks, then decide on a common time framework and convert all time units into that framework.

2.3.5. **Stability class** -- see Section 3.3 on stability class estimation and Tutorial section 05 on estimating stability class.

2.4. **Application data**. Application data does not directly enter into the modeling. However, it is important to know attributes about the application such as depth, start of application, duration of application, type of application, application rate and so on. The first sampling period often includes the application. This can cause difficulties for the regression analysis because the source size and flux are not uniform during the sampling period. Interpreting the regression analysis frequently depends on understanding the application factors

2.5. **Soil data**. As with the application data, soil data does not directly enter into the modeling process. Nevertheless, soil measurements such as bulk density, soil moisture, and organic matter content can sometimes aid the analysis.

2.6. **Nearby obstructions.** It can be important to know about buildings, adjacent crops or orchards which could influence wind patterns around the field. These features may be noted on the field maps, located from photographs, or possibly derived from imagery on the internet such as available in Google Earth.

3. **WEATHER SUMMARY PROCEDURES**

3.1. **Format required by ISCST3.** The fixed format which ISCST3 uses is explained on pages 3-66 to 3-69 of the ISCST3 manual. Units required by ISCST3 must be used (meters/second, Kelvin) and wind direction must be expressed in "to" degrees. The framework for wind direction must be the same as the framework for the field and monitor coordinates, both must be with respect to true north or both with respect to magnetic north.

3.2. **How to get data into ISCST3 format**. The WEATH6A program handles much of the

conversion and formatting required by ISCST3 from raw meteorological data collected by EM. WEATH6A is located on I:\airmodel and can be run by typing into a DOS window: *I:\iscst3\WEATH6A.exe*. The "I:\iscst3\" assumes you have mounted 'dprhq01\air_emergency_proj' as drive I. However, this path and drive assignment are subject to change. Get help if you can't locate the program weath6a.exe.
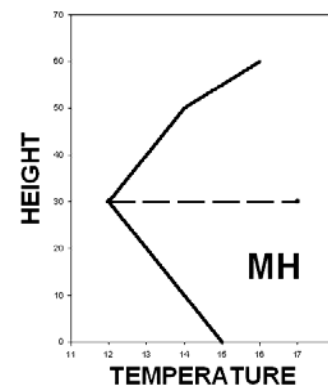
WEATH6A requires two input files, a raw met data file with comma delimited data in a certain order and in certain units (see Tutorial Section 05 and documentation for WEATH6A, Johnson 2010) and a cut file, which contains the date and hour for each time period for which a summary is required.

The prepared raw data file (prepared for WEATH6A) consists of mm,dd,hh,mi,int,at,agt,dir,spd where commas separate values and mm=month, dd=day, mi=minute, int=interval code, at=ambient temperature (F), agt=above ground temperature, dir='from' direction, spd= wind speed (miles per hour). 'Int' and 'agt' are not used, but there must be place holders in the file. The input file must be sorted from oldest to newest. WEATH6A produces output file giving time interval, average ambient air temperature in degrees Kelvin, average wind direction 'to' (mod(180+FROM,360)), scalar average wind speed (meters/second=.447*milesperhour). The data file can usually be prepared for WEATH6A input by using EXCEL and creating a 'CSV' (comma separated values = comma delimited) file, which is comma delimited.

City	Latitude (deg-min)	
Sacramento	38º	34'
San Francisco	37º	46'
Fresno	36º	46'
Monterey	36º	36'
Visalia	36º	20'
Orange	33º	48'

The cut file contains a listing of month, day, hour, minute, each separated by commas for each time period desired to summarize. The cut file can be created using EXCEL or Minitab.

In order to run WEATH6A, you must input the mixing height in meters. You must also know when sunrise and sunset occurs. This can be determined by running a program on the Naval Observatory Web site (*http://aa.usno.navy.mil/AA/*). In order to run these programs, you need to know the latitude of the site and the date. The Navy website has latitude information for most cities..

The output from the WEATH6A program consists of two files: a documentation file and a nearly-ISCST3-ready file. The nearly-ISCST3-ready WEATH6A output file provides the temperature values, wind direction and wind speed values which can be used for ISCST3 modeling. What is missing is the stability class. These are represented as Xs in the output file (see Tutorial Section 05 and WEATH6A documentation). The second output file from WEATH6A is a documentation file showing the time periods and night day designators in addition to the meterological data. The documentation file is useful for determining stability.

3.3. **Stability.** Stability is a critical component of the meteorological input to ISCST3. Stability characterizes the vertical mixing within the boundary layer. During a sunny day, the solar radiation heats up the ground, which heats up the air. This causes parcels of air to become less dense and rise like bubbles through the heavier, cooler air above. In turn, cooler air moves downward to displace the rising parcels. The degree of vertical mixing is captured in a six unit scale, sometimes using letter A through F, or using numbers 1 through 6. The ISCST3 model requires the numerical stability code, but stability discussions and tables often use the letters. The code A (1) denotes maximal vertical mixing that occurs on sunny, summer afternoons. The code F (1) denotes night time stable conditions, characterized by little or no vertical mixing, sometimes combined with a temperature inversion at the surface. A temperature inversion at the surface has the coldest air at the ground surface and warmer air above. Since the coldest air is also the most dense, there is no mixing. Stability condition D (4) is neutral stability, where the temperature remains approximately the same over some vertical distance. This occurs under cloudy conditions, day or night or when it is very windy. The remaining stability classes represent intermediate conditions between A (1) , D (4) and F (6) stability classes. In the Gaussian model, the stability class influences how quickly the downwind plume spreads out in a vertical and horizontal direction. Under F (6) stability, the plume remains concentrated and tight for long distances. Under A (1) stability, the plume readily mixes vertically. and consequently, concentrations tend to decline more quickly down wind. However, very high ground level concentrations can

Idealized temperature profile under convective daytime mixing conditions. MH indicates mixing height at dashed line.

occur when an elevated release plume shows looping behavior under A stability.

3.4. **Determining stability.** There are many procedures for determining stability. For this workbook, the procedure presented is the one used most often in EM for site specific monitoring studies (Budney 1977). It requires knowledge of sunset and sunrise times, and the sun's angle above the horizon on an hourly basis. The sun angle above the horizon (altitude) can be derived from the naval observatory web site [*http://aa.usno.navy.mil/AA/*]. In the latter case, choose under data services, 'Positions of sun and moon', then choose 'altitude and azimuth of the sun or moon during one day', then fill out the online form. Enter the name of a nearby city and the program will give the latitude and longitude, in addition to calculating the angles.

Once you have obtained the sun altitudes, record them for each hour on the WEATH6A output. The WEATH6A program labels the hours night/day, using the user input sunset/sunrise times and also using the EPA rule of hour after and hour before. The Naval Observatory website only reports Standard time.Make sure that the time units are consistent. Do not mix standard time with Pacific Daylight time. All time units need to be in the same time frame. Determine carefully whether times are recorded in Standard or Daylight Savings time.

Use the sun angles of each hour (the Navy website calls these "altitudes") to classify the insolation as strong, moderate or slight solar insolation. If cloud information is available, these categories can be modified. A fully cloudy sky is always D stability. Next start with the first hour. Assign the stability based on night/day, solar insolation (if daytime), and wind speed. Do not change the stability class by more than 1 stability class per hour. For example, if stability class at 2100 hrs is E, then stability class at 2200 hrs can only be F, E or D. Stability classes are not allowed to jump or skip classes from hour to hour.

Under Clear Sky Conditions

Category	*Sun Elevation Angle*
Strong insolation	$SEA > 60^o$
Moderate insolation	$35^o < SEA < 60^o$
Slight insolation	$15^o < SEA < 35^o$

Stability categories

A	*1*	*very unstable*
B	*2*	*unstable*
C	*3*	*unstable*
D	*4*	*neutral*
E	*5*	*stable*
F	*6*	*very stable*

After inputting the stability classes, the weather file is almost ready for use by ISCST3. The weather file will most likely contain all of the periods in the study. So, the particular monitoring period that is going to be simulated needs to be extracted from the ISC-ready weather file and placed in its own file with the appropriate first-line header record.

4. **RUN ISCST3**

4.1. **Overview**. There are two files needed for a basic ISCST3 run: a control file and a meteorological data file. The ISCST3 control file contains the name of the meteorological data file. The control file contains various specifications on how to conduct the simulation. Some important elements are the source geometry (field coordinates), the receptor geometry (in this case, the coordinates of the monitor locations), the source information (sometimes there are multiple sources, for example, to approximate an irregularly shaped field) which includes the flux, the name of the meteorological file, and the name of any output files, as well as other information and controlling parameters. Table 3 presents an annotated control file. The ISCST3 manual gives extensive instructions on how to build the control file. The simplest method of producing a control file is to modify an existing control file from a similar problem.

An alternative method for determining stability class requires the standard deviation of wind direction. Further references and a meta-code for this procedure can be found in Johnson (1998).

TIP: ASCII files can be edited using NOTEPAD

4.2. **Run ISCST3.** To run ISCST3 type in to the DOS command window

I:\ISCST3\iscst3   infile   outfile

where infile is the control file and outfile is the output file. Note that "I:\ISCST3 is a pathname intended to reference a location on a network drive (in fact, on dprhq01\air_emergency_proj). However, this path and drive ("I") assignment are subject to change. Get help if you can't locate

the "iscst3.exe" file.

4.3. **Interpreting error messages**. ISCST3 gives error messages when there are mistakes in the input file. ISCST3 does NOT give an error message if the frame of references for wind direction and field locations are different. However, error messages will be produced if ISCST3 detects inconsistencies in input specifications or missing information. Spend about 15-20 minutes attempting to solve the error messages by the iterative process of reading the manual, modifying the control file and rerunning the simulation. This procedure can be frustrating, but it is critical to learning about the ISCST3 program. The Tutorial (Section 03) explains how to keep a PDF of the ISCST3 manual always available on screen as work through setting up an ISCST3 run and how to search the manual using Acrobat Reader.

TIP: Construct filenames that mean something. SBBP1.IN, SBBP1.OUT, SBBP1.MET might indicate Seal Beach Broadcast study,period 1: control file (IN), output file (OUT) and meteorological file (MET).

4.4. **Checking output**. When starting a series of similar runs, for example, the first period of a 6 measurement period simulation, print and check the output file. Check the met data, the receptor and field coordinates and the source information. Look over the control parameters. The program reprints and interprets the control information from the input control file. Before proceeding, determine that the program is correctly interpreting the input parameters by examining the output.

In most cases, for subsequent periods the only change in the control files is the title and the met data file. Use the title to document the model run: e.g. 'Period 3, Seal Beach.'Always provide sufficient documentation in the control file that the analysis is clear and repeatable by other staff.

5. **COMPARING SIMULATED CONCENTRATIONS TO MEASURED CONCENTRATIONS**. The objective of these simulations is to estimate the flux by the 'back calculation' method.   The flux associated with an application is estimated by comparing the model estimated air concentrations to the measured air concentrations. The

nominal flux is adjusted so that on average the magnitude of the ISCST estimated air concentrations match the magnitude of the measured air concentrations.

5.1. **Units must be consistent**. Make sure that the measured values and the simulated values are in the *same* units. Most often we have used ug/m3 for concentration units.

5.2. **Regression.**

5.2.1. **Linear regression**. The simple linear regression is used to calibrate the model flux to the measured concentrations. The regression is conducted with measured values on the y-axis and the modeled values on the x-axis. Always fit the full simple linear regression model that includes both the slope and the intercept. Tutorial Section 07 gives more details on how to perform these regressions. The Tutorial also explains how to read a 'plt' file into Excel. In the Supplementary material of Tutorial, Example 7 shows the regression of measured on modeled concentrations for period 3, Seal Beach broadcast.

5.2.2. **What do you do with regression.**

5.2.2.1. First step is to determine if the regression slope is significant at the 5% significance level. The question, "Is the slope statistically significant" is equivalent to asking, "Does a 95% confidence interval around the slope include 0?" If the answer is no, then the slope is significant. Otherwise, if the confidence interval includes 0, then the slope is not significant.

5.2.2.2. If the slope is significant, then test whether the intercept is significantly different from 0. The ideal result at this point in the analysis is a statistically significant regression ($p<.05$), a large R^2 value ($>90\%$) and a small and statistically non-significant intercept. The intercept value can be considered unimportant if the intercept is statistically significant, but the magnitude is small relative to the average magnitude of the measured values. If the

intercept is statistically significant and large in relation to the measured values, consult with more experienced staff. Some alternative analysis methods are discussed below.

5.2.2.3. After obtaining the slope, and assuming that the regression has been conducted with the measured values on the y axis and the modeled values on the x axis, then multiply the slope by the nominal flux used in the simulation (usually the nominal flux is 100ug/m2sec). Conducting the simulation using the adjusted flux will give a regression slope close or equal to 1.0. This is the final estimate.

Table 4 shows the period 3 data and regression for the Seal Beach broadcast methyl bromide study. For period 3 the linear regression slope was 0.16. Therefore, the nominal flux of 100ug/m^{2}s is multiplied by the coefficient of 0.16 to obtain a new flux estimate of 16ug/m^{2}s.

A graphical view of this regression is shown in Figure 4.

5.2.2.4. If the slope is not significant, then additional analysis must be performed.

5.3. **What to do when linear regression fails.** It is difficult to set fixed procedures to follow when regression analysis breaks down. First determine reasons for failure of the regression. Common reasons are that first sampling period included the application or that wind speeds were very low (calms). However, often no single factor can be determined. The remainder of this section gives some techniques that have been proposed and/or used when the regression fails.

5.3.1. **Redo simulation using shorter time intervals for the meteorological data.** Weather data averaged on a one hour time step can not reflect changes in wind direction under low wind speeds that may be important in matching the simulated air concentrations to the pattern and magnitude observed in the measured

concentrations. On-site weather data can be summarized over shorter intervals (e.g. 15 minutes) and those finer interval averages can then be used to simulation the entire air concentration sampling interval.

5.3.2. **Sort values and regress again**. Sort the x values and the y values independently, and rerun the regression. Matching of measured air concentrations in both space and time to the simulated air concentration is a very rigorous comparison. Air simulation models that match the magnitude of measured air concentrations during a particular sampling interval are considered to match well. The exact pattern does not have to match. This is the justification supporting the sort and re-regress procedure. Note that if sorting is used, the resulting p-value (significance level) is not a conventional p-value because sorting leads to a much greater frequency of 'significant' regressions, even with randomly generated data.

The p-value from a sorted regression should not be cited as the significance level because it no longer has the conventional meaning.

5.3.3. **Measured/Modeled**. This estimate is obtained by simply summing up the measured values and dividing by the sum of the modeled values. Use that quotient to adjust the modeled flux rate.

5.3.4. **Substitute another period.** When meteorological conditions are similar and concentrations are similar, it may be reasonable to substitute the flux from another period.

5.3.5. **Force the regression through the origin**. Do not force the regression through the origin. This is statistically incorrect and invalid.

6. **TIME WEIGHTED AVERAGE FLUX**. For various reasons, it may be necessary to find the average flux over several monitoring periods. This is similar to determining a time weighted average concentration. Multiply each period flux by the number of hours during the period, add up the products and divide by the total number of hours in all of the periods used. In the Seal Beach study, the 24-hour time weighted average flux was computed based

on intervals 3 and 4 as follows:

$$weighted\ average = \frac{12h \bullet 0.052\,ppm + 12h \bullet 0.045\,ppm}{12h + 12h} = 0.049\,ppm$$

The flux indices from periods 3 and 4 were combined because they gave the highest concentrations.   Sometimes the measured periods do not total to 24 hours. But a total of more than 20 hours is probably sufficient to characterize a 24 hour average concentration

7. **SIMULATION WITH GRIDS.** It is sometimes necessary to simulate an area around a field using a grid of receptor locations. For example, to look for a maximum sized buffer zone for a 24 hour period, the time weighted average flux can be used with 24 hours of meteorological data and the concentrations on a grid around the field can be estimated. These gridded concentrations can be input into a graphics program which has the capability to plot concentration isopleths and in this way, perhaps by repeated simulations to zoom in on the area of interest in order to increase accuracy, the maximum required buffer zone can be determined. See Tutorial Supplementary Material Coarse Grid section. Also see Tutorial Section 02 Slides 11, 12 and 23 for more contour plot examples. These contour plots were all basically produced by using the gridded receptor feature in ISCST3.

8. **EXTRAPOLATING CONCENTRATIONS TO SHORTER OR LONGER TIME INTERVALS (Peak-to-Mean Concepts).** If an average concentration has been determined for a certain time interval, either by measurement or modeling, is there a way to estimate the maximum concentration for a shorter time interval based on the average concentration? The answer is yes. This procedure is sometimes called peak-to-mean and utilizes power functions.   The average concentration during a time period is based on the integral of a complicated wave function, which would be visible if it were possible to measure air concentrations every second. During the measurement period, this wave function will have various peaks and valleys. Because our framework for considering fumigant air

TIP: Use the plot file feature of ISCST3 to create a data file containing the estimated concentrations, together with the x and y coordinates. Get into Sigmaplot, import the data from this file by specifying (1) white space separators (2) start in column 1 and go to column 3 (3) start in row 9 and go to the end. This will put the x,y,c (concentration) values into the first 3 columns of Sigmaplot. Then create a contour plot using those three columns.

concentrations is human health, we are generally interested in maximum concentrations which might occur (as opposed to being interested in minimum concentrations). Barry (2000) summarized research on this topic and presents the following power law which can be used for estimation of peak concentrations:

$$C_p = C_m \left(\frac{t_p}{t_m} \right)^{-\frac{1}{2}}$$

where

Cp= peak concentration over period tp of interest
Cm=mean concentration over measurement period, tm
tp=duration of peak period of interest
tm=duration of mean measurement period

For example, a five hour measurement period yields a concentration of 85 ug/m3. What would the peak concentration for 30 minutes be? Cm=85 ug/m3, tp=0.5 h, tm=5 h, so that Cp=269 ug/m3. When extrapolating from longer to shorter time periods, the expectation is that the shorter time period peak concentration will be greater than the longer period concentration.

9. ISCST3: TOPICS SINCE 1999

9.4. PERFUM

Johnson (2001) investigated the adequacy of the methyl bromide buffer zones by utilizing ISCST3 in conjunction with an automated program for running 24 hour
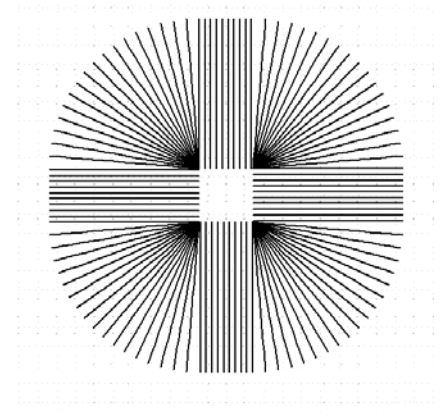
simulations for each day of 20 years of meteorological data and through numerical methods seeking the maximum daily required buffer zone. The software used discrete receptors arranged as spokes radiating away from the edge of the field. He concluded that the DPR methyl bromide buffer zones were adequate more than about 90% of the time.

Reiss and Griffin (2006) utilized these concepts and expanded the approach in a user-friendly software package called PERFUM (Probabilistic Exposure and Risk Model for Fumigants). Whereas Johnson (2001) used a fixed 24-hour flux, Reiss and Griffin (2006) expanded the capability to include a varying flux profile during 24 hours. They also enabled simulation for periods shorter than 24 hours to analyze situations where the reference concentration was based on time periods shorter than 24 hours.

A key concept in these approaches is the use of exceedance probabilities to assess the effectiveness of buffer zones. This concept requires repeated simulations with some variable changing. In Johnson (2001) and Reiss and Griffin (2006), the changing variable was daily meteorology from many weather records. Each day of simulation produced a maximum required bufferzone, which was the maximum distance away from the field where the reference concentration occurred on that simulation day. For methyl bromide, the reference concentration was 815 ug/m3 for 24 hours. These hundreds of estimated distances were sorted and arranged into a cumulative distribution. From this distribution, one can read off the percentile associated with any particular buffer zone distance. In Figure 5 the vertical axis is the cumulative percentile and the horizontal axis is the buffer zone distance. The multiple lines represent cumulative distributions for different application rates. The higher application rates are naturally shifted to the right (i.e. longer required buffer zones). One can use such a diagram in two ways: (1) given a percentile on the y axis, move to the right until the line of interest is intersected, then go straight down to read off the associated buffer zone distance (2) given a buffer zone distance (i.e. position along the x axis) move up vertically until the distribution of interest is intersected, then move to the left to read off the associated percentile on the y-axis.
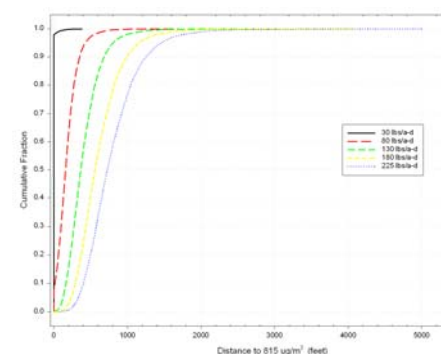
The y-axis above is cumulative fraction. The x axis is distance. The different lines represent increasing application rates (Johnson 2001).

9.5. SOFEA

A different kind of modeling effort led to the development of Soil Fumigant Exposure Assesment System (SOFEA) by Steve Cryer of DowAgrosciences (Cryer 2005). This modeling tool uses a modified version of ISCST3 (Johnson 2001). The original intent of the SOFEA model was to examine how various strategies for allocation of 1,3-dichloropropene might affect long term air concentrations. The simulation domain is roughly a 3x3 township area, though in principal the model area can be expanded. The modeling tool is intended to run over several years and estimate chronic air concentration distributions of 1,3-dichloropropene under user-imposed yearly township limits on 1,3-D use. The tool requires as input (1) cropping patterns (2) field size distributions (3) date of application distributions (4) application rate distributions and other miscellaneous distributions. The model also allows input of a flux profile for two application types: drip and shank applications. In addition, the software allows for input of historical-based section weights to give realistic clumping patterns to the simulated use. These various distributions are all randomly sampled using Crystal Ball software and together with township-level constraints on total pounds applied, a synthetic application database, analogous to the Pesticide Use Report database, is produced which reflects the various distributions and constraints. This synthetic database of applications is then used to create very large control input files (hundreds of pages) for the modified ISCST3. This modeling tool uses years of specially prepared hourly meteorological data, primarily based on CIMIS collected meteorology. A large receptor grid (typically over 11,000 points) covers the 3x3 township area and air concentration estimates are collected during the model run.

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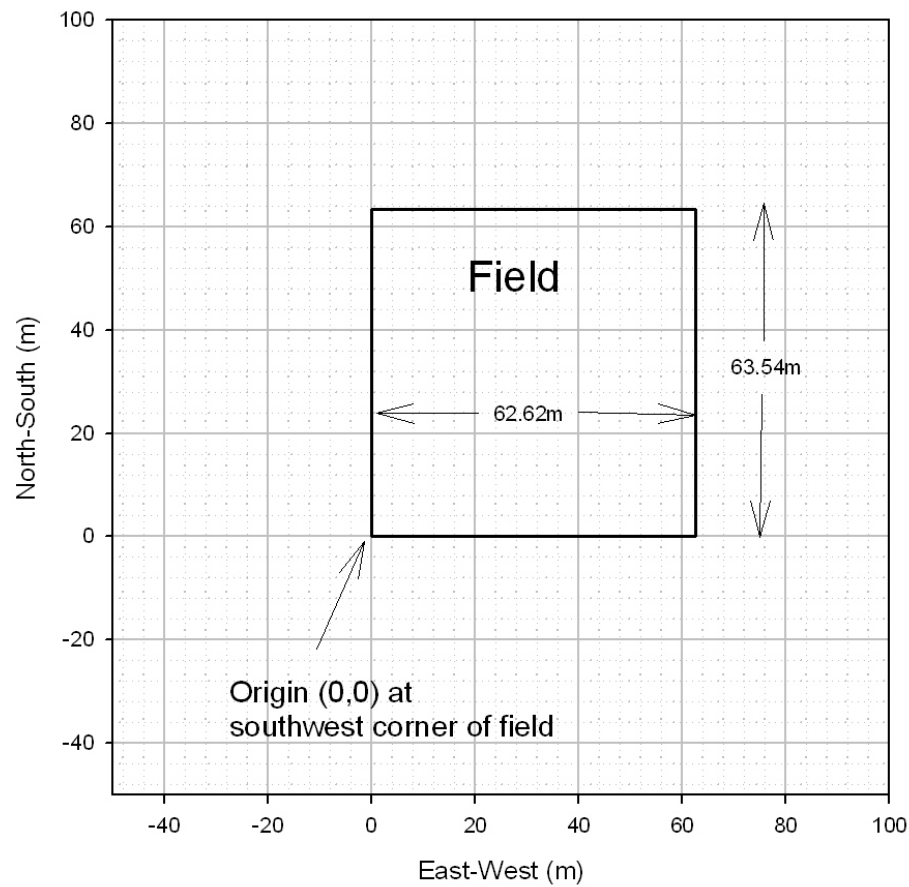
Figure 1. Mapping of Seal Beach broadcast field (Johnson and Wofford 1999).

0.049 ppm

0.016 ppm

N

0.034 ppm

NW

NE

35'

33'

32'

W — 33' —

Application area

— 32' — E

0.005 ppm

0.024 ppm

32'

32'

33'

SW

S

SE

ND

0.011 ppm

0.019 ppm
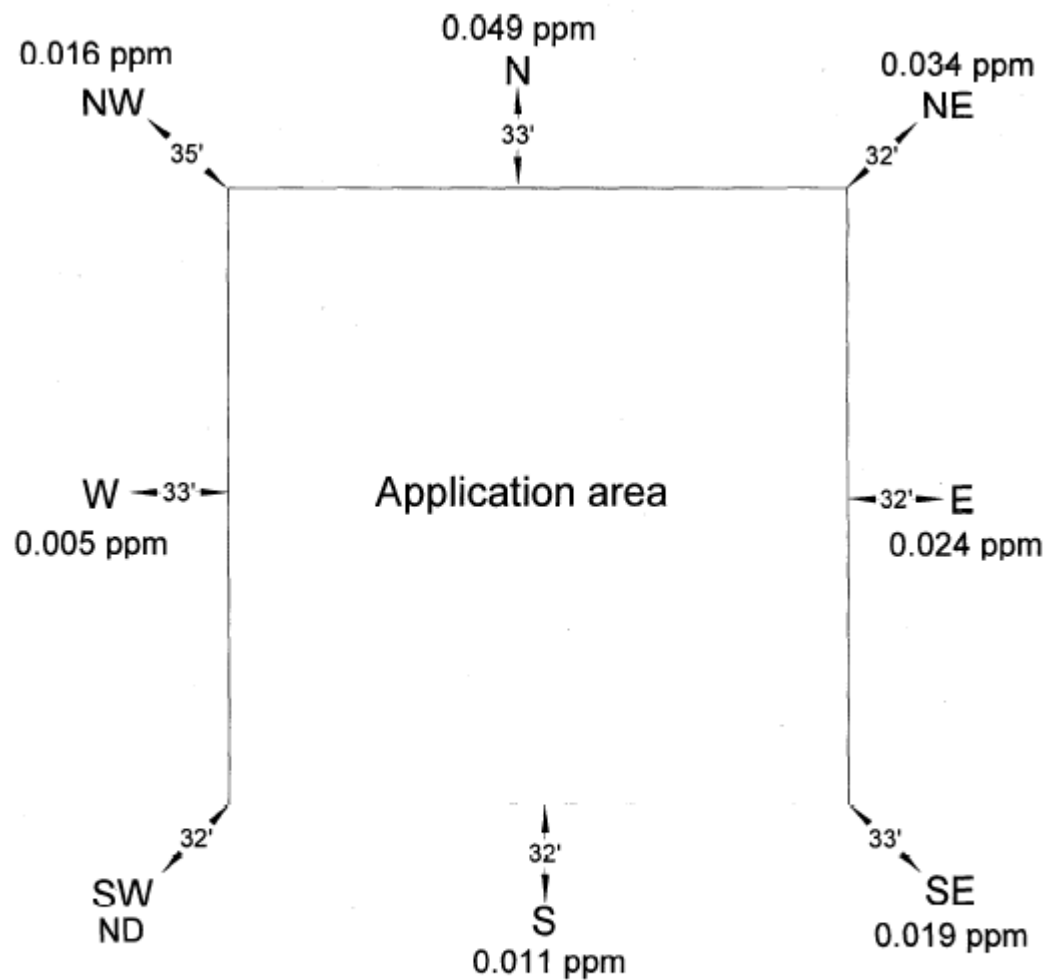
Figure 2. The extracted Figure 3 from Johnson and
Wofford (1999) showing broadcast field treatment,
location of monitors and 24 hour time weighted
methyl bromide concentrations.
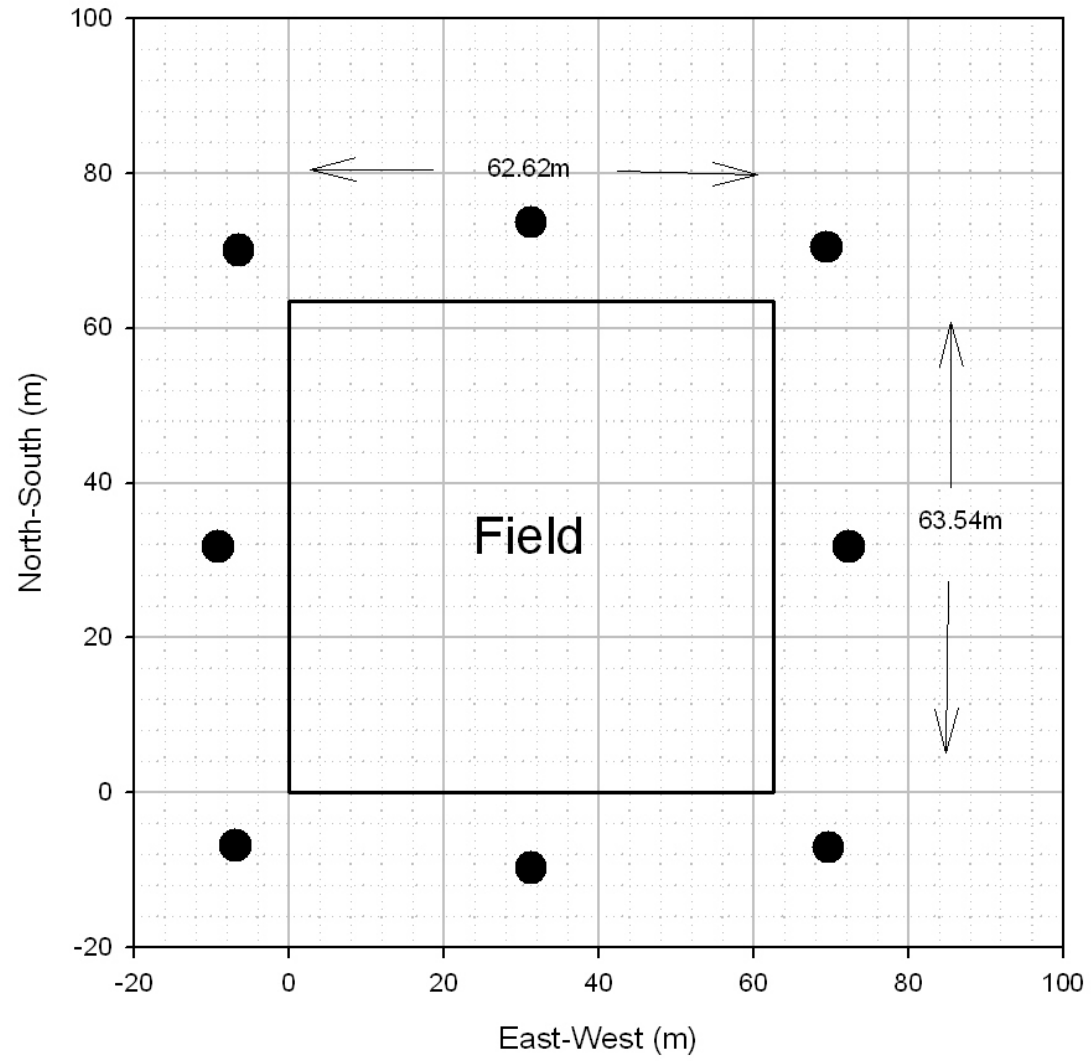
Figure 3. Broadcast Seal Beach field showing monitor locations (Johnson and Wofford 1999).

Page 35
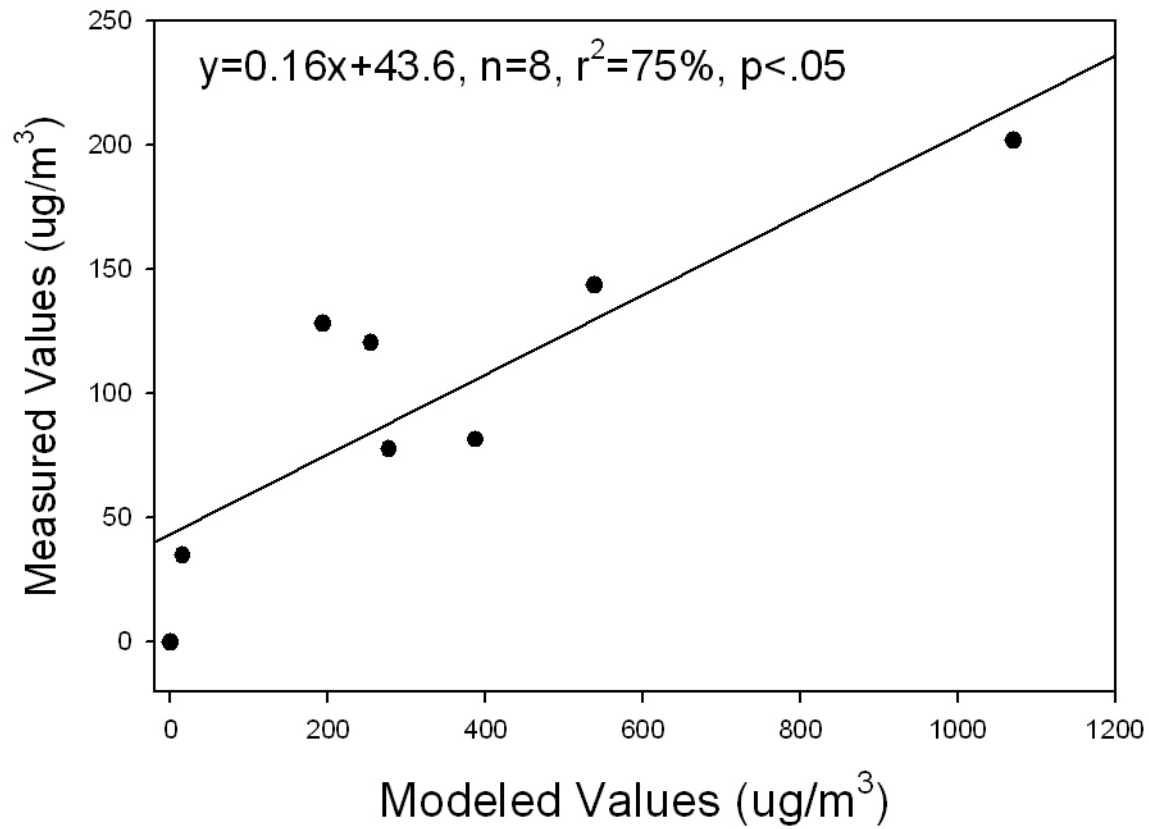
Figure 4. Measured versus modeled regression for third period of Seal Beach methyl bromide study broadcast treatment (Johnson and Wofford 1999).
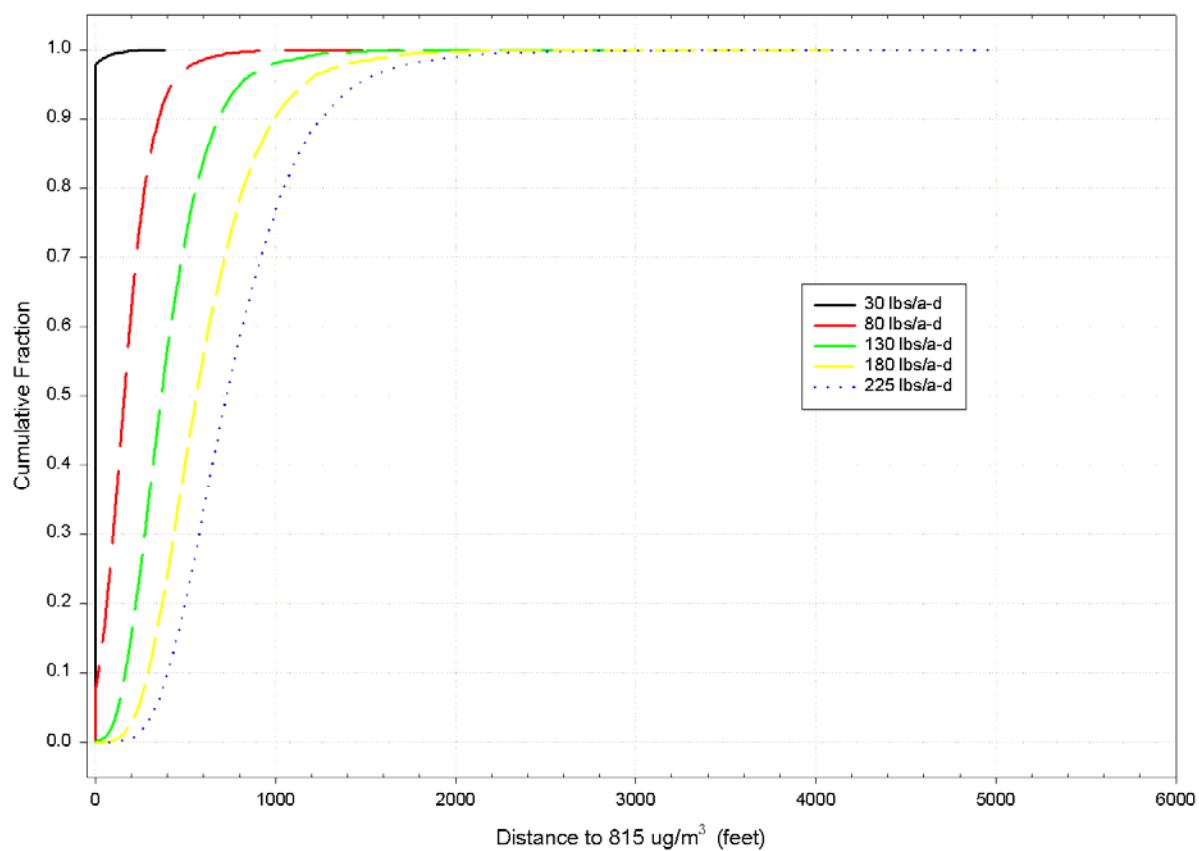
Figure 5.2.2. Cumulative distribution of daily maximum distance to 815 ug/m3 for 10 acre plot.

Figure 5. Cumulative distributions of buffer zone distances for different methyl bromide application rates for 10 acre field at various application rates (Figure 5.2.2 from Johnson 2001).

Table 1. Extract from Johnson and Wofford (1999, Table 3) showing methyl bromide monitoring results for Seal Beach broadcast treatment.

| | Sampler | | Methyl Bromide (ppm) for each Sampling Period | | | | | |
| | | | Interval 1 | Interval 2 | Interval 3 | Interval 4 | Interval 5 | 24-Hour |
Plot	Site	Distance	5 Hour	6 Hour	12 Hour	12 Hour	12 Hour	TWA[1]
Seal	N	33 ft	0.018	0.023	**0.052**	**0.045**	0.050	0.049
Beach	NE	32 ft	0.025	0.054	**0.021**	**0.047**	0.014	0.034
	E	32 ft	0.015	0.052	**0.033**	**0.016**	ND	0.024
	SE	33 ft	ND	0.022	**0.037**	**ND**	ND	0.019
	S	32 ft	ND	ND	**0.020**	**ND**	ND	0.011
	SW	32 ft	ND	ND	**ND**	**ND**	ND	ND
	W	33 ft	ND	ND	**0.009**	**ND**	0.012	0.005
	NW	35 ft	ND	ND	**0.031**	**ND**	0.042	0.016

Table 2. Excerpted meteorological data from data logger for Seal Beach broadcast study (Johnson and Wofford 1999).

Microsoft Excel - sealbeachmet.xls

File Edit View Insert Format Tools Data Window Cell Run CBTools Help Adobe PDF

A1

	A	B	C	D	I	J	K	L	M	N	O	P
1					Maximum	Maximum	Average	Average	Average	Average Resultant		
2			Julian		RH	Wind Speed	Air Temp.	RH	Wind Speed	Wind Speed	Resultant	Standard Deviation
3	Array	Year	Date	Time	%	m/s	°C	%	m/s	m/s	Wind Direction	Wind Direction
5	11	1999	174	1420	56.33	5.919	23.63	55.82	5.684	5.676	202.4	3.117
6	11	1999	174	1422	59.98	5.782	23.09	57.32	4.972	4.887	207	10.6
7	11	1999	174	1424	59.75	5.037	23.04	57.49	4.028	3.916	218.5	13.5
8	11	1999	174	1426	62.68	5.821	22.89	58.44	4.804	4.689	220.3	12.49
9	11	1999	174	1428	60.33	5.645	22.63	58.5	4.657	4.586	230.4	10.05
10	11	1999	174	1430	62.24	5.645	22.55	59.16	4.602	4.38	219.2	17.8
11	11	1999	174	1432	60.83	5.253	22.81	57.77	4.678	4.638	236.8	7.49
12	11	1999	174	1434	60.26	5.449	22.71	58.78	4.57	4.528	237.1	7.8
13	11	1999	174	1436	60.59	5.566	22.58	58.48	4.965	4.933	232.3	6.486
14	11	1999	174	1438	61.34	5.586	22.33	59.28	4.839	4.813	230.8	5.864
15	11	1999	174	1440	60.33	5.37	22.39	58.86	4.631	4.579	221	8.65
16	11	1999	174	1442	61.03	5.429	22.66	58.1	4.837	4.764	226.3	9.94
17	11	1999	174	1444	60.19	5.312	22.67	58.22	4.662	4.629	223.7	6.876
18	11	1999	174	1446	61.03	5.566	22.72	58.71	4.828	4.735	235.9	11.23
19	11	1999	174	1448	60.36	5.468	22.6	58.66	4.805	4.77	233.1	6.899
20	11	1999	174	1450	60.36	5.684	22.61	57.96	4.907	4.874	233.6	6.597
21	11	1999	174	1452	59.26	5.018	22.67	57.47	4.204	4.146	228	9.56
22	11	1999	174	1454	59.74	5.821	22.75	58.19	4.809	4.786	235.8	5.565
23	11	1999	174	1456	60.34	5.292	22.68	57.92	4.575	4.55	234.8	5.943
24	11	1999	174	1458	59	5.194	22.92	57.19	4.482	4.436	236.9	8.21
25	11	1999	174	1500	57.73	5.508	23.24	56.01	4.23	4.174	239.1	9.27
26	12	1999	174	1500	62.68	5.919	22.73	58.11	4.663	4.548	228.8	10.28
27	11	1999	174	1502	58.26	4.998	23.27	56.26	4.377	4.36	228.4	4.999
28	11	1999	174	1504	58.38	5.723	23.01	56.52	4.502	4.476	221.8	6.228

Table 3. Annotated control file.

```
                                              Rural setting
                                                    SBBRP1.IN
CONTROL {
  CO STARTING
  CO TITLEONE  Seal Beach Broadcast Tarp June 24-26 1999    no calms processing
  CO MODELOPT  CONC  (RURAL)              NOSTD  NOBID  (NOCALM)
  CO AVERTIME  period
  CO POLLUTID  OTHER
  CO DCAYCOEF  .000000           error output
  CO RUNORNOT  RUN                      File
  CO ERRORFIL  ERRORS.OUT → error output File
  CO FLAGPOLE  1.2  ←—— DEFAULT RECEPTOR HEIGHT (m)
  CO FINISHED
}

SOURCES {
  SO STARTING
                                Comment lines (**)        lower left corner of source
  ** Source Location Cards:  ←—— Comment lines (**)
  **              SRCID SRCTYP        XS    x      YS   y       ZS
                   name
  SO LOCATION  (acre1)(AREA)        (0.00)      (0.00)         .0000
                         source type
  ** Source Parameter Cards:
  ** POINT:   SRCID     QS            HS        TS        VS      DS
  ** VOLUME:  SRCID     QS            HS        SYINIT    SZINIT
  ** AREA:    SRCID     QS            HS        XINIT     YINIT   xinit = length of source
                                                                          x-direction
  SO SRCPARAM (acre1)  (.10000000E-03)   .0000  (62.62)   (63.54)  yinit = length of source
                                                                          y-direction
  SO EMISUNIT (.100000E+07)(GRAMS/SEC)        (MICROGRAMS/CUBIC-METER)
  SO SRCGROUP ALL
  SO FINISHED
}
                    factor converts          user-specified flux
                     g/s → µg/m³              g/m²-s, in this case
                                                 0.0001 g/m²-s

RECEPTORS {
  RE STARTING
  RE DISCCART 29.49 73.57
  RE DISCCART 69.62 70.53
  RE DISCCART 72.35 31.62
  RE DISCCART 69.92 -6.99
  RE DISCCART (31.92 -9.73)  ← x,y location of receptor
  RE DISCCART -6.99 -6.99
  RE DISCCART -10.03 31.92
  RE (DISCCART) -7.9 70.53  —— DISCRETE CARTESIAN RECEPTORS
  RE FINISHED
}
                          contains met data

METEOROLOGY {
  ME STARTING
  ME INPUTFIL  SBP1.MET (4I2,2F9.0,F6.1,I2,2F7.1)
  ME ANEMHGHT  10.000 METERS
  ME SURFDATA  (99999) 1999          SURFNAME
  ME UAIRDATA  (99999) 1999          UAIRNAME
  ME WINDCATS   1.54   3.09    5.14    8.23   10.80
  ME FINISHED
                         must match codes in first line of met file
}

OUTPUT {
  OU STARTING
  OU PLOTFILE  PERIOD ALL SBBRP1.PLT
  OU FINISHED
                  concentration output file - easier to use
                  this output file for plotting
}
```

Table 4. Regression for period 3 of Seal Beach broadcast methyl bromide study. First column is the modeled values based on a flux of 100ug/m2s.
Second column contains the measured values at each monitor in ug/m3. The regression analysis shows a highly significant regression (p<.0056) with an almost significant intercept shown in the "P-value" column (p<.0506). The statistical significance of the multiplicative coefficient is the same as the regression statistical significance. The multiplicative coefficient is 0.160168 (extra decimals for clarity). The flux is estimated by multiplying 100*0.16=16ug/m2s.

1071.348	201.76	SUMMARY OUTPUT									
386.9707	81.48										
193.9631	128.04	*Regression Statistics*									
538.7434	143.56	Multiple R	0.864195								
277.3964	77.6	R Square	0.746833								
0	0	Adjusted R	0.704639								
15.386	34.92	Standard E	34.68447								
254.748	120.28	Observatio	8								
modeled	msrd	ANOVA									
ug/m3	ug/m3		*df*	*SS*	*MS*	*F*	*ignificance F*				
		Regression	1	21293.08	21293.08	17.6998	0.005641				
		Residual	6	7218.073	1203.012						
		Total	7	28511.15							
			Coefficients	*standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
		Intercept	43.6265	17.89464	2.437964	0.050612	-0.160116	87.41311	-0.160116	87.41311
		X Variable	0.160168	0.038071	4.207113	0.005641	0.067012	0.253323	0.067012	0.253323

Tutorial for Preparing and Running ISCST3 Model

This tutorial is derived from materials used to teach a one-day course in using ISCST3. The course was taught by Bruce Johnson and Terrell Barry on April 13, 2010.

California Environmental Protection Agency
**Department of Pesticide Regulation**
Environmental Monitoring Branch

Section 01. Set up to run ISCST3 (these instructions will give you the ability to run ISCST3 at your work station at your regular desk and create a DOS icon on your desktop – see Part 4 for workstation instructions)
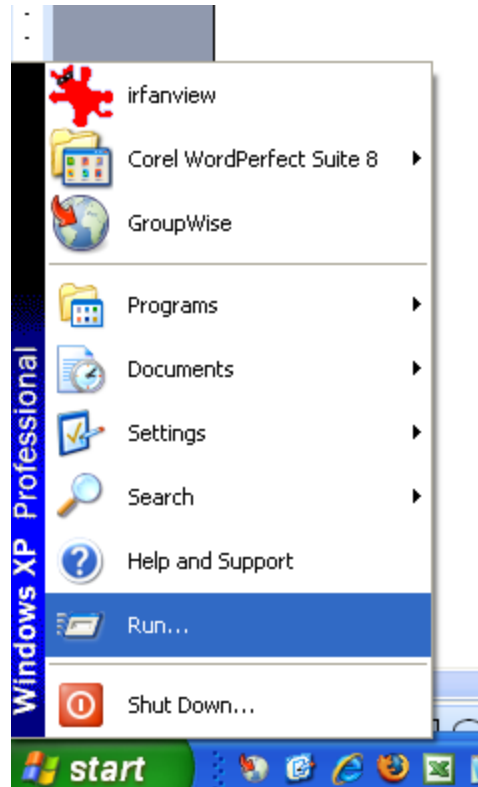

Part 1. Create ISCDIR subdirectory on your home network drive and assign drive letter T to \\dpr_home\username$\ISCDIR

1. Insert CD
2. Left click on START

3. Left click on RUN
4. Type in \\dpr_homedir\username$ (note: username is your username, for example, mine is bjohnson, so I would type in "\dpr_homedir\bjohnson$" without the quotes
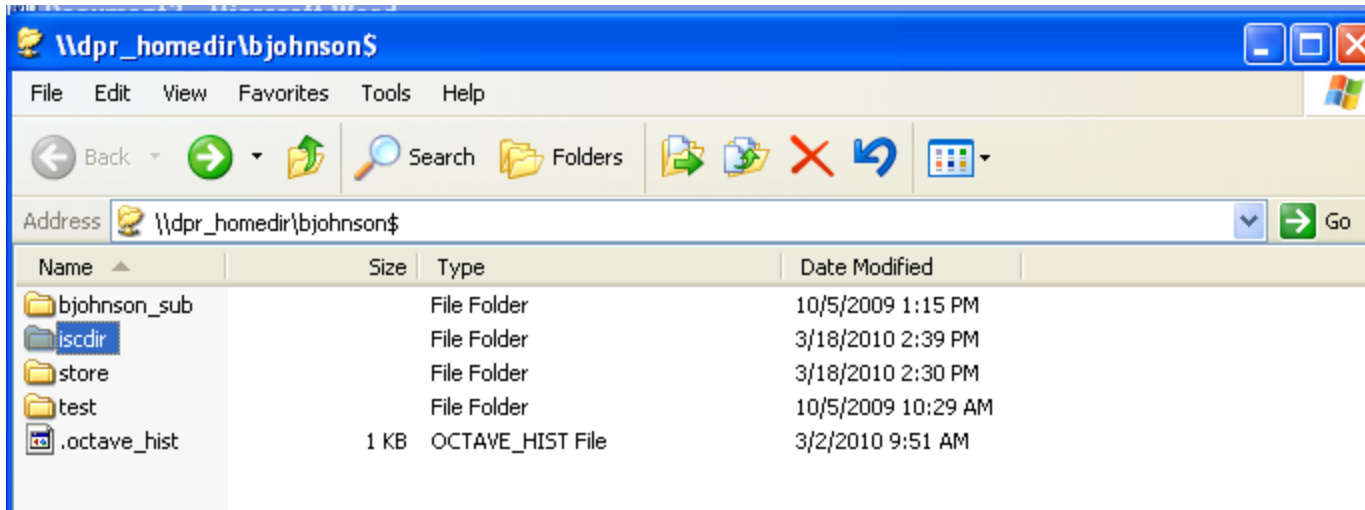
5. You should now see a window showing directories and files on your home network drive.

6. Create a folder called ISCDIR (File, New, type in ISCDIR,)
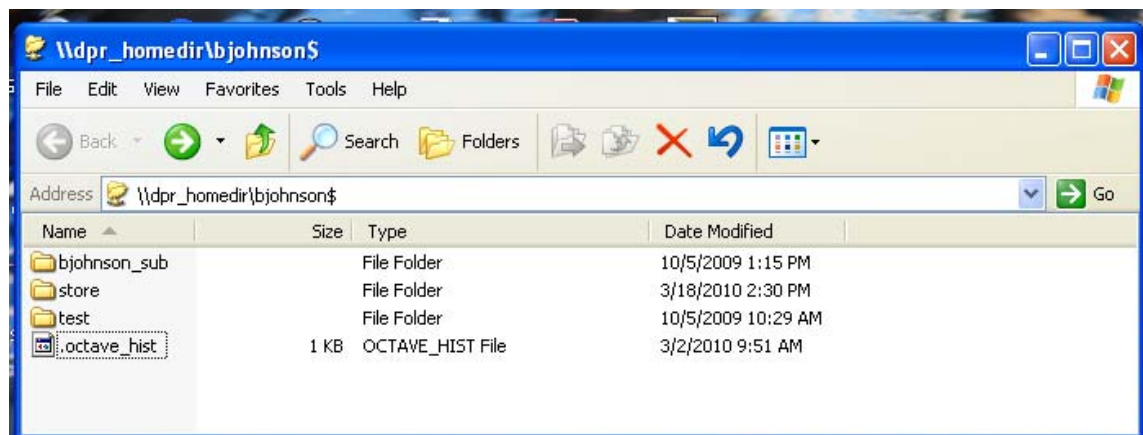
7. In the window above, click on Tools, Map Network Drive, and obtain the window below called "Map Network Drive".

8. In the **Drive:** field, click on the down arrow to select the letter "T".

9. In the **Folder:** field, type in exactly: \\dpr_homedir\username$\iscdir (where username is your username).

10. Click on finish

11. You should now have the drive letter "T" assigned to \\dpr_homedir\username$\iscdir
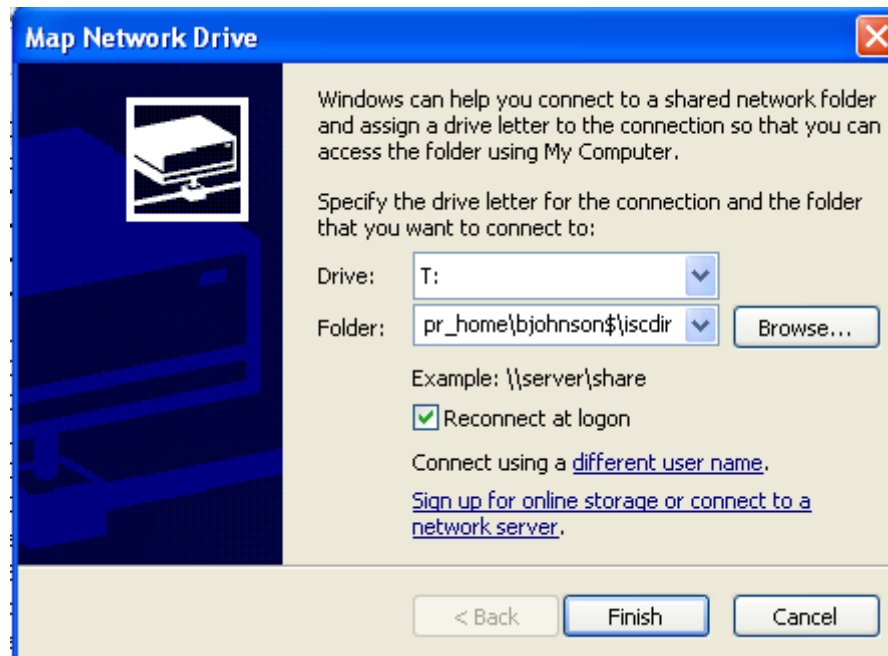
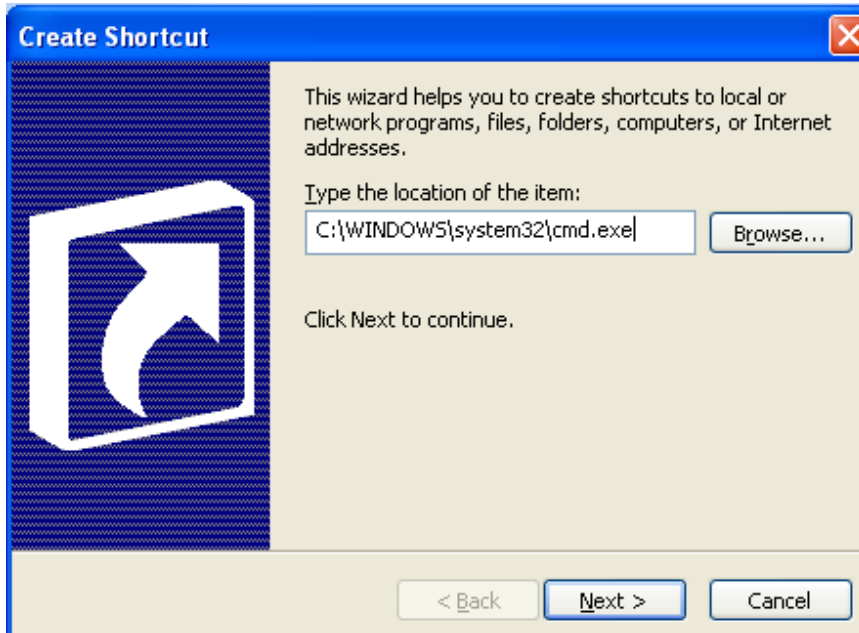**Part 2. Copy the files and subdirectories from the CD to ISCDIR.**

1. Use Windows Explorer to copy all of the files and directories from the CD to ISCDIR.

Part 3. Create an icon on the desktop for CMD.EXE.

1. Right click on an empty place on the desktop.
2. Click on "new"
3. Click on "shortcut"
4. In the field "Type the location of the item:" , type in the following text

        C:\WINDOWS\system32\cmd.exe

Click "next", click "finish".

5. You should now have an icon on your desktop labeled 'cmd' or 'cmd.exe'.

6. Double click on the new icon and type in "T:" without the quotes, hit return.

7. You should now see a window with the prompt at the end of a four character line: "T:\>". *If this is not the case, get help before proceeding*. The "T:" drive actually stands for \\dpr_home\username$\ISCDIR and all of the files and directories from the CD should be here.
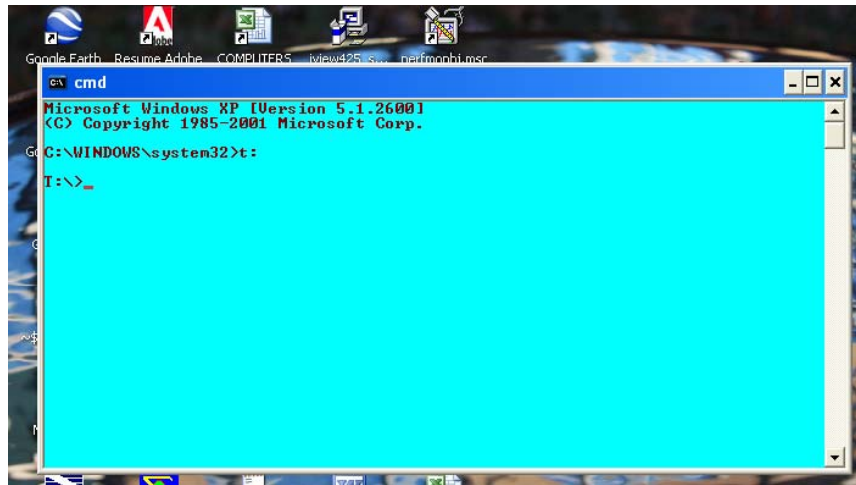
8. In the 'cmd' window shown above, type in the following command and hit return ATTRIB –R *.* /S /D (allows you to modify the files on T:)
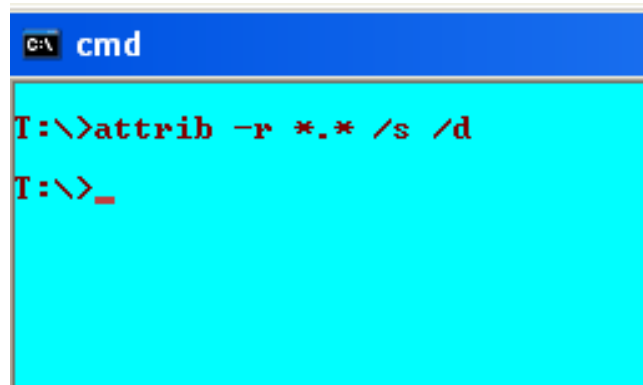
9. Some quick and dirty "DOS" commands (not case sensitive):
    a. DIR lists the current directory contents
    b. DIR *.out lists all of the files with the 'out' extension
    c. TREE shows the current and subdirectory structure
    d. DEL *filename* deletes the file called *filename*
    e. CD.. moves up one directory level
    f. CD *subdirectory* moves down one level to *subdirectory*
    g. COPY *filename1 filename2* makes a copy of *filename1*
    h. If ISCST3 is in the parent directory, one level above where you're currently located, you can run it by typing ..\ISCST3.exe
    i. NOTEPAD *filename* runs the NOTEPAD text editor on *filename*
    j. MKDIR *subdirectory* creates a subdirectory
    k. ..\ISCST3 runs isc when the ISCST3.EXE file is in the parent directory
    l. ISCST3 runs isc when you are currently in the directory containing ISCST3.EXE
    m. ..\ISCST3 *controlfile.in outputfile.out* runs isc with the control file and puts the output into the output file (there may be additional output files listed in the control file, and there may be additional input files, such as meteorology, that are named in the control file but not shown in the command line)
    n. HELP DIR gets help for the command DIR (or other DOS commands)

Example of moving location from PROBLEM1 to PROBLEM2 subdirectory. Note in this example the parent directory does not really have a name. It is the T: drive. The two subdirectories to T:\ are problem1 and problem2 (or T:\problem1 and T:\problem2).

Part 4. At your workstation at your cubicle (use these instructions to be able to run ISCST3 at your cubicle).

1. Follow Part 1, Steps 7 through 11, to assign the drive letter "T:" to the iscdir subdirectory on your network drive. It is unlikely, but if you already have the letter T assigned to something, then use a different available letter. But you will have to adjust all of the instructions accordingly (i.e. if you use "M:", then substitute "M:" for "T:").
2. Follow Part 3, Steps 1 through 6, to create the CMD.EXE icon on your desktop.

Section 02 Introduction and Overview of Gaussian plume method. (slides)
Slide 1

Slide 2

Slide 3

Background

- Fumigants are highly volatile pesticides injected into soil at high rates, compared to other pesticides
- Fumigants can volatilize from soil and move offsite, causing potential public health impacts
- Four commonly used fumigants
  - 1,3-Dichloropropene
  - Chloropicrin
  - Methyl Bromide
  - Metam-Sodium and other MITC generators

3

Slide 4

Slide 5

Slide 6

Slide 7

Table 7 lists sampler distances for all off-site monitoring associated with soil fumigations.

Beard, K.K., Murphy, P.G., Fontaine, D.D. and Weinberg, J.T. 1996. Monitoring of Potential Worker Exposure, Field Flux, and Off-Site Air Concentration During Chloropicrin Field Application. Lab Project Number: HEH 160. Unpublished study submitted by Chloropicrin Manufacturers Task Force. DPR Data Volume 199-073.

Slide 8

Slide 9

dpr
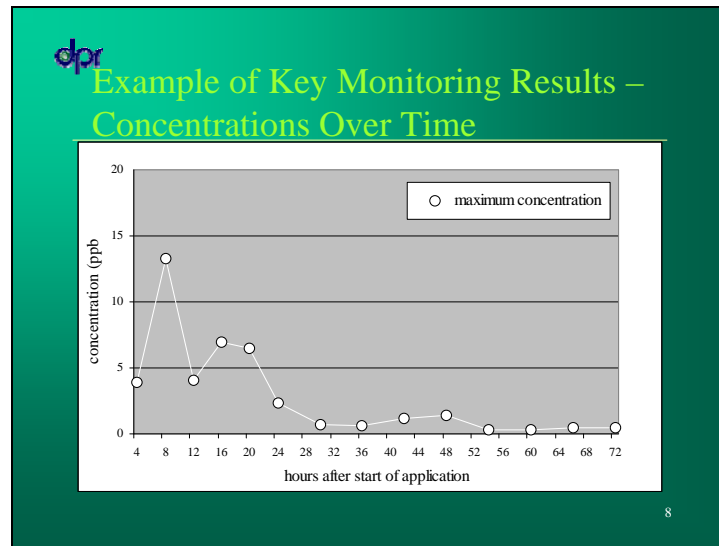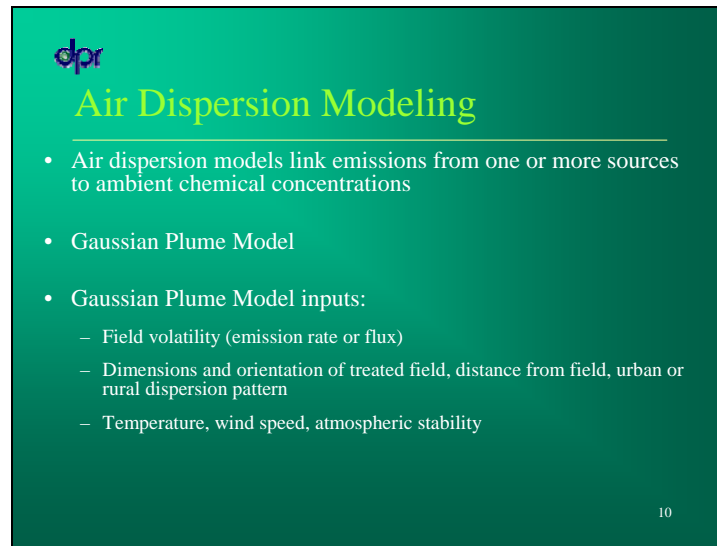
Air Monitoring Data

- Air concentrations vary with many factors, such as distance from field, amount of pesticide applied, time, application method, weather
- Monitoring provides a snapshot of concentrations and represents specific fields and conditions
- DPR supplements air monitoring data with computer modeling to
  - Estimate air concentrations for different situations
  - Develop measures to control exposure (buffer zones)

9

Slide 10

Temperature, wind speed, and other meteorological conditions (e.g., stability class).

Slide 11

Modeling analysis of a chloropicrin incident near Mettler, California.

This incident occurred over two nights and was associated with the application of chloropicrin to the field shown here.

Wind direction aligned with the long dimension of the rectangular application and the apt. buildings directly west of the application area.

The shape of the concentration isopleths illustrates the typical Gaussian plume form.

Slide 12
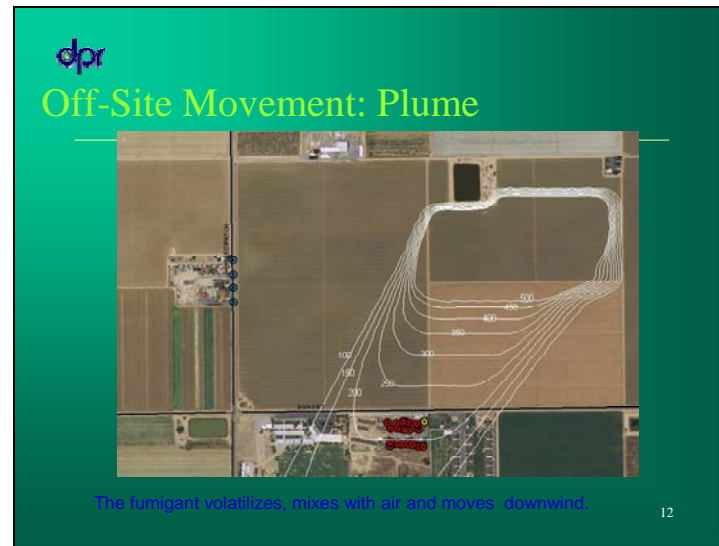
This figure shows the plume form the second night of the set of incidents.

The application encompassed both the rectangle shown in the previous figure and the area of the field immediately to the north.
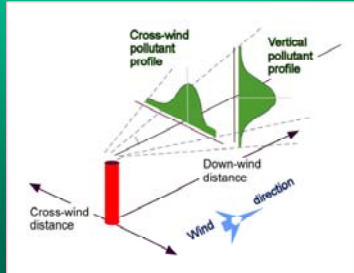
As shown here, the wind direction changed, resulting in a broader cross-wind direction Gaussian plume moving off the site.

Slide 13

Plume diagram from the University of Colorado website:

http://www.colorado.edu/geography/babs/empact%20draft%20web%2018apr%2004/about%20aermod.htm

Slide 14

Slide 15
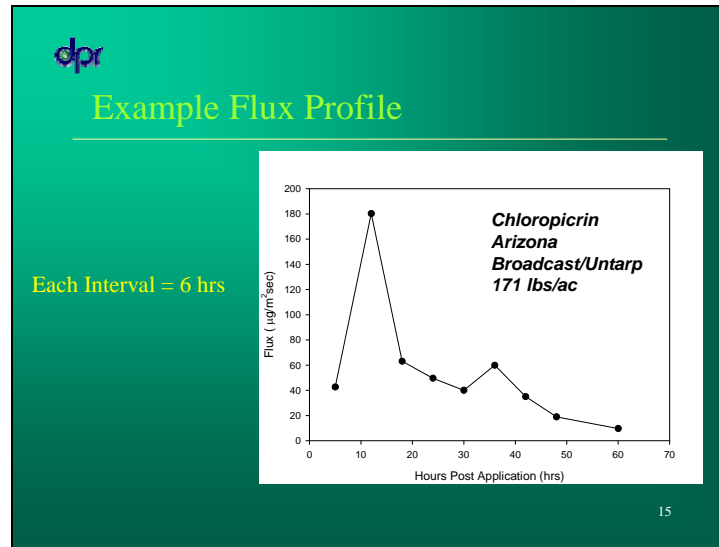
This flux profile shows how the flux changes over time following an application.

This particular flux profile is for the AZ broadcast untarp application method that was used in the chloropicrin exposure appraisal.
The peak 6hr flux of 180.3 ug/m2sec was used as the screening flux.

Slide 16

Slide 17

Slide 18

dpr

Atmospheric Stability

- Atmospheric stability quantifies the level of turbulence in the atmosphere
- Turbulence is the degree of mixing in the atmosphere The amount of turbulence in the atmosphere has a major influence on a pollutant plume
- Turbulence reduces the concentrations in the pollutant plume by increasing the amount of unpolluted air mixing into the plume

18

Slide 19

Meteorological conditions defining Pasquill stability classes

Surface windspeed	Daytime incoming solar radiation			Nighttime cloud cover	
m/s	Strong	Moderate	Slight	> 50%	< 50%
< 2	A	A – B	B	E	F
2 – 3	A – B	B	C	E	F
3 – 5	B	B – C	C	D	E
5 – 6	C	C – D	D	D	D
> 6	C	D	D	D	D

Note: Class D applies to heavily overcast skies, at any windspeed day or night

19

Slide 20

dpr
Using ISCST3 to Determine
Regulatory Requirements

- Input: flux from monitoring studies
- Input: meteorological conditions
  - Example of *screening conditions* (methyl bromide): 1.4 m/s wind speed; constant wind direction; C stability
  - Example of *historical conditions*: hourly data for 5 years from a single meteorological station
- Output: distance to target concentration
  - buffer zone

20

Slide 21
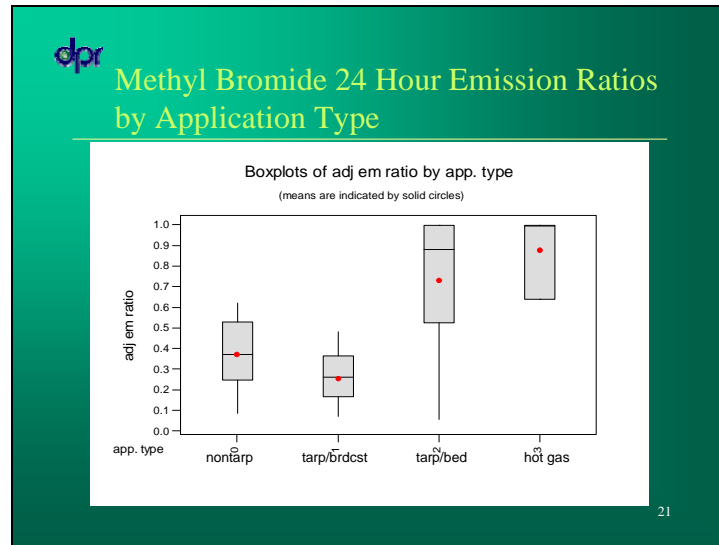
Slide 22

dpr

Example of Regulatory Requirements:
Methyl Bromide

- Specify method of fumigation, based on methods monitored
- Specify emission ratio, based on flux data and target concentration

Fumigation Method	Emission Ratio (fraction volatilized/day)
Shallow injection to flat field using "Nobel plow" shank and tarp	0.25
Shallow injection to bedded field using straight shank and tarp	0.80
Deep injection to flat field using straight shank without a tarp	0.40

22

Slide 23

Slide 24

dpr
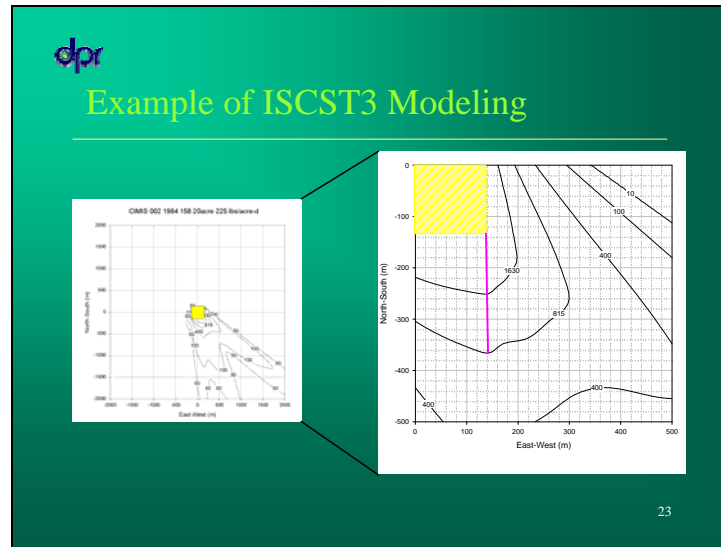
Example of Regulatory Requirements:
Methyl Bromide

- Buffer zone distance ranges from 50 to 4600 feet
  (15 to 1400 meters) depending on
  - Flux (application rate x emission ratio)
  - Area treated (number of acres)
- Buffer zone duration ranges from 36 to 84 hours
- Limits on application rate and area treated
- Separation requirements between applications
  - 1300 feet (1/4 mile, 400 meters)
  - 36 hours

24

Slide 25

dpr

Effectiveness of Methyl Bromide Buffer Zones

- Compared regulatory buffer zone distance vs. distance to target concentration (210 ppb, 815 ug/m^3) for 34 monitoring studies
  - Regulatory distance longer than distance to 210 ppb for 33 of 34 studies
- Compared regulatory buffer zones using screening weather conditions vs. historical weather data
  - Compared 25 combinations of flux and acreage, using 5 yrs of historical weather data from 4 counties
  - Screening weather conditions had longer buffers than historical weather conditions 89 – 100% of the time

25

Slide 26

dpr

Key Points

- DPR uses air monitoring and computer modeling to determine if exposures exceed its target concentration and to develop control measures
- Target concentration and flux are key factors in determining need for and size of buffer zones
- Buffer zone size, duration, and other requirements vary with flux, area treated, and method of application

26

Section 03 Keep ISC Manual on screen and ready to search

1. Using Windows Explorer, double click on T:\docs\ISC-V1.PDF
2. This should bring up the ISC manual using Adobe Reader.
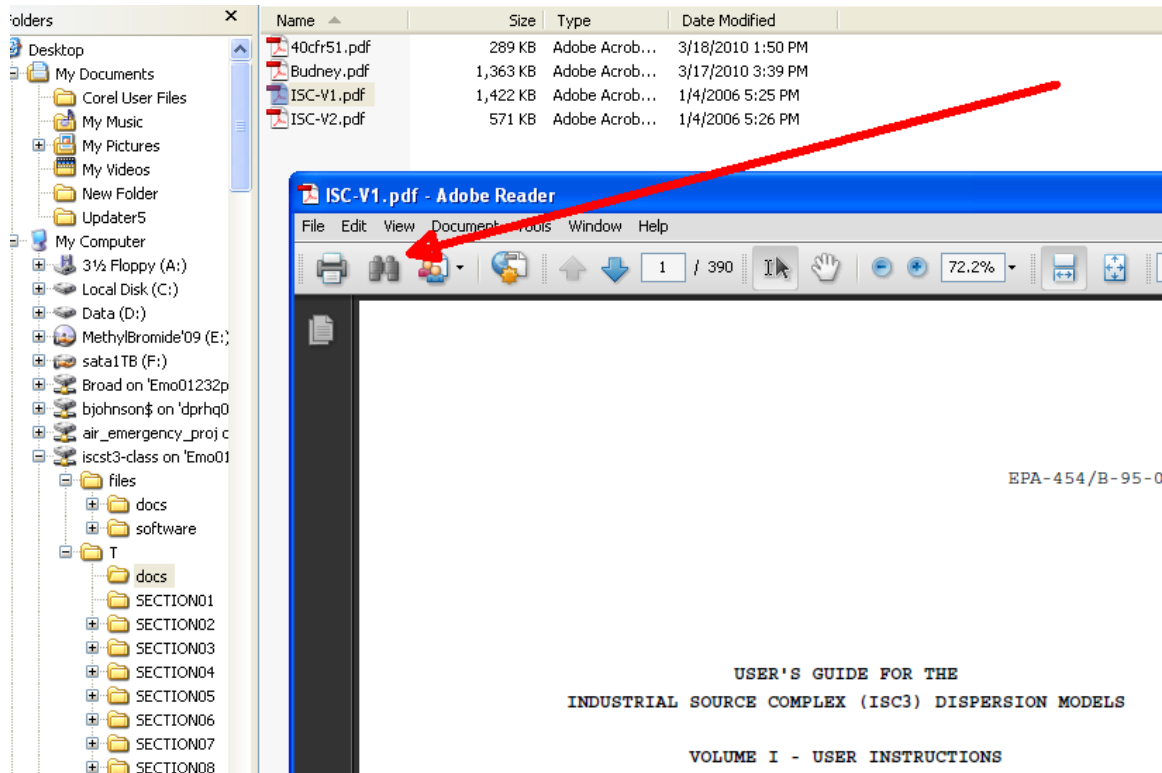
3. You NEED to have the binoculars icon in the toolbar
   a. If it's not there, here's how to get it there.
      i. Click on Tools, Customize Toolbars
      ii. Scroll down to the section "File Toolbar" and put a checkmark next to the binoculars "Search" icon
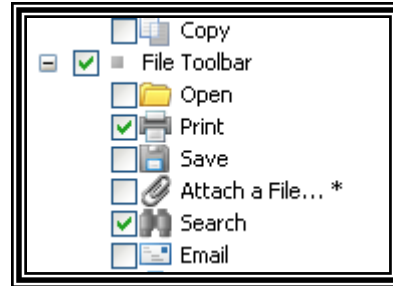
iii. Click on OK.

4. With the "USER'S GUIDE …" on the screen, click on the binocular icon. A "Search" window will pop up, click on the "Arrange Windows" icon. You should now have your windows arranged with the document on the right and a search menu window to the left.
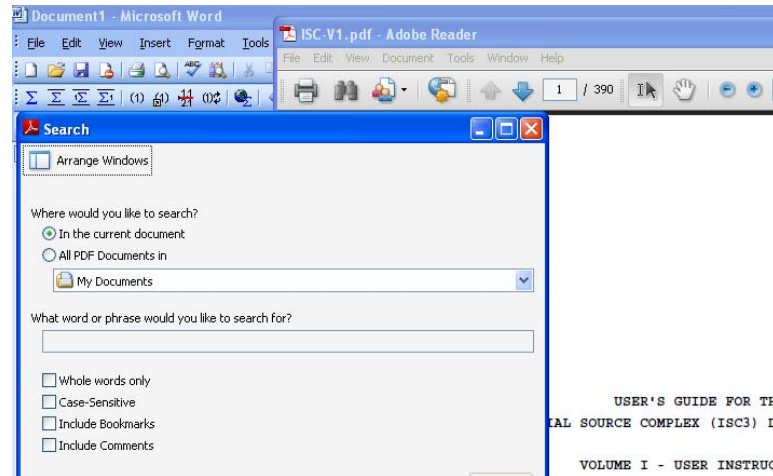
5. Type the word "control" into the search field and click on search.

6. On the left, the search panel will show all of the instances where the word 'control' appears in the document and on the right it shows the first appearance of the word in the document with the word highlighted. If you click on different lines on the left, the document on the right reflects your new location where the word 'control' appears. Use this procedure to get answers to questions you may have in designing ISCST3 control files. I almost always have the manual up on the screen ready to access when I'm running ISCST3 because I can't remember all of the little details that arise when working on control files.
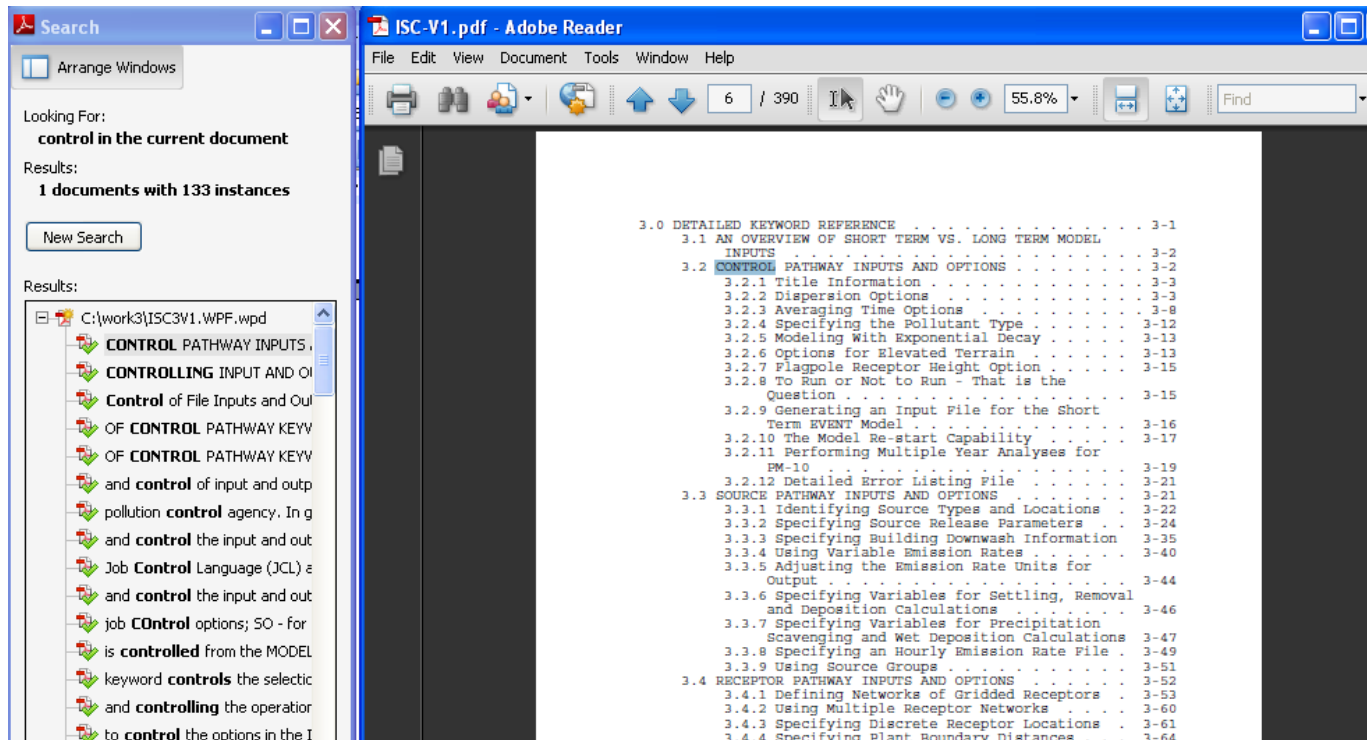
Section 03 Overview of control file pathways (control file sections).

1. The input file (input runstream file) has five basic sections: CONTROL, SOURCES, RECEPTORS, METEOROLOGICAL, OUTPUT.

```
SBSAP5.IN - Notepad
File   Edit   Format   View   Help

CO STARTING
CO TITLEONE Seal Beach Bedded Shank Ahead Tarp June 24-26 1999
CO MODELOPT CONC    RURAL            NOSTD   NOBID   NOCALM
CO AVERTIME   period
CO POLLUTID OTHER
CO DCAYCOEF    .000000
CO RUNORNOT RUN
CO ERRORFIL ERRORS.OUT
CO FLAGPOLE 1.2
CO FINISHED

SO STARTING
** Source Location Cards:
**           SRCID SRCTYP        XS            YS            ZS

SO LOCATION   acre1 AREA         0.00       -0.60         .0000

** Source Parameter Cards:
** POINT:   SRCID        QS            HS         TS         VS          DS
** VOLUME:  SRCID        QS            HS         SYINIT     SZINIT
** AREA:    SRCID        QS            HS         XINIT      YINIT

SO SRCPARAM  acre1    .10000000E-03    .0000    63.84       64.91

SO EMISUNIT   .100000E+07 (GRAMS/SEC)            (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED

RE STARTING
RE DISCCART 31.62 73.87
RE DISCCART 70.22 70.53
RE DISCCART 73.26 33.14
RE DISCCART 70.53 -6.99
RE DISCCART 31.62 -8.82
RE DISCCART -6.99 -5.78
RE DISCCART -9.12 33.14
RE DISCCART -6.7 71.74
RE FINISHED

ME STARTING
ME INPUTFIL SBP5.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT   10.000 METERS
ME SURFDATA  99999  1999            SURFNAME
ME UAIRDATA  99999  1999            UAIRNAME
ME WINDCATS   1.54    3.09    5.14    8.23   10.80
ME FINISHED

OU STARTING
OU PLOTFILE PERIOD ALL SBSAP5.PLT
OU FINISHED
```

2. The control file 'pathways' (or paragraphs, or sections)

3. (Can use <alt><tab> to switch between programs) Switch over to ISC-V1.PDF, look at the contents (Adobe pg 6) showing the input file sections. At the top "DETAILED KEYWORD REFERENCE"
4. Note the line in the Control (CO) pathway CO ERRORFIL (in this example the filename 'ERRORS.OUT' is listed) If there are errors in the file, ISC will list the errors in this file and it can be helpful to diagnose what's wrong.

5. Switch over to ISC manual and search for 'error' keyword, go to 2-26, (Adobe pg 53) review the highlights such as the different kinds of error messages and the structure of an error message.
6. Do a new search for 'Appendix E'
7. Scroll through and show the error message listings.
    a. Notice that errors with specific numbers have paragraphs written up which provide more explanation for the error. Therefore, if there is an error message in your run, you can to to Appendix E and find out more about the error.
8. **For the most part, the easiest way to start building input file is to start with existing input file and modify it for your needs.**
9. The 1999 Workbook has annotated file listing. See 1999 Workbook Table 11 and 13. (adobe pages 43 and 45). Below is another example.

rural setting

```
                                        SBBRP1.IN
CO STARTING
CO TITLEONE Seal Beach Broadcast Tarp June 24-26 1999
CO MODELOPT CONC   RURAL          NOSTD  NOBID  NOCALM      no calms processing
CO AVERTIME  period
CO POLLUTID OTHER
CO DCAYCOEF    .000000
CO RUNORNOT RUN                  error output file
CO ERRORFIL ERRORS.OUT
CO FLAGPOLE 1.2        DEFAULT RECEPTOR HEIGHT (m)
CO FINISHED
```

```
SO STARTING
                                        Comment lines (**)
** Source Location Cards:                    lower left corner of source
**          SRCID SRCTYP        XS    X    YS   y      ZS
            name
SO LOCATION  acrel AREA        0.00      0.00        .0000
              source type
** Source Parameter Cards:
** POINT:   SRCID     QS           HS     TS      VS      DS
** VOLUME:  SRCID     QS           HS     SYINIT  SZINIT
** AREA:    SRCID     QS           HS     XINIT   YINIT     Xinit = length of source
                                                            x-direction
SO SRCPARAM acrel   .10000000E-03   .0000   62.62   63.54   yinit = length of source
                                                            y-direction
SO EMISUNIT  .100000E+07 (GRAMS/SEC)         (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED     factor converts
                 g/s → µg/m3
```

user-specified flux
g/m^2-s, in this case
0.0001 g/m^2-s

```
RE STARTING
RE DISCCART 29.49 73.57
RE DISCCART 69.62 70.53
RE DISCCART 72.35 31.62
RE DISCCART 69.92 -6.99
RE DISCCART 31.92 -9.73      x,y location
RE DISCCART -6.99 -6.99       of receptor
RE DISCCART -10.03 31.92
RE DISCCART -7.9 70.53      DISCRETE CARTESIAN RECEPTORS
RE FINISHED
```

```
                          contains met data
ME STARTING
ME INPUTFIL SBP1.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT   10.000 METERS
ME SURFDATA  99999  1999          SURFNAME
ME UAIRDATA  99999  1999          UAIRNAME
ME WINDCATS   1.54   3.09   5.14   8.23   10.80
ME FINISHED
              must match codes in first line of met file
```

```
OU STARTING
OU PLOTFILE PERIOD ALL SBBRP1.PLT
OU FINISHED
          concentration output file - easier to use
          this output file for plotting
```

CONTROL
SOURCES
RECEPTORS
METEOROLOGY
OUTPUT

Section 04 Encoding the geometry into the ISCST3 control file. The field (source) and monitoring locations (receptors) must be described geometrically and the coordinates and distances input into the ISCST3 control file.

1. The yellowed lines are where the geometrical information describing the source and receptors is located.

```
CO STARTING
CO TITLEONE geometry example
CO MODELOPT CONC   RURAL          NOSTD  NOBID  NOCALM
CO AVERTIME  period
CO POLLUTID OTHER
CO DCAYCOEF    .000000
CO RUNORNOT RUN
CO ERRORFIL ERRORS.OUT
CO FLAGPOLE 1.2
CO FINISHED


SO STARTING

** Source Location Cards:
**           SRCID SRCTYP       XS           YS           ZS

SO LOCATION   acrel AREA         0.00         0.00         .0000

** Source Parameter Cards:
** POINT:    SRCID      QS          HS       TS        VS        DS
** VOLUME:   SRCID      QS          HS     SYINIT    SZINIT
** AREA:     SRCID      QS          HS      XINIT     YINIT

SO SRCPARAM  acrel    .10000000E-02     .0000      100.       100.

SO EMISUNIT    .100000E+07 (GRAMS/SEC)          (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED


RE STARTING
RE DISCCART 500.9 273.57
RE DISCCART 691.62 170.52
RE DISCCART 722.35 313.62
RE FINISHED


ME STARTING
ME INPUTFIL PERIOD3.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT   10.000 METERS
ME SURFDATA  99999  1999          SURFNAME
ME UAIRDATA  99999  1999          UAIRNAME
ME WINDCATS   1.54    2.09    5.14    8.23   10.80
ME FINISHED


OU STARTING
OU PLOTFILE PERIOD ALL PERIOD3.PLT
OU FINISHED
```

2. The coordinate framework is determined usually by setting the southwest corner of the field to (0,0) as the origin with north going up and east going to the right.
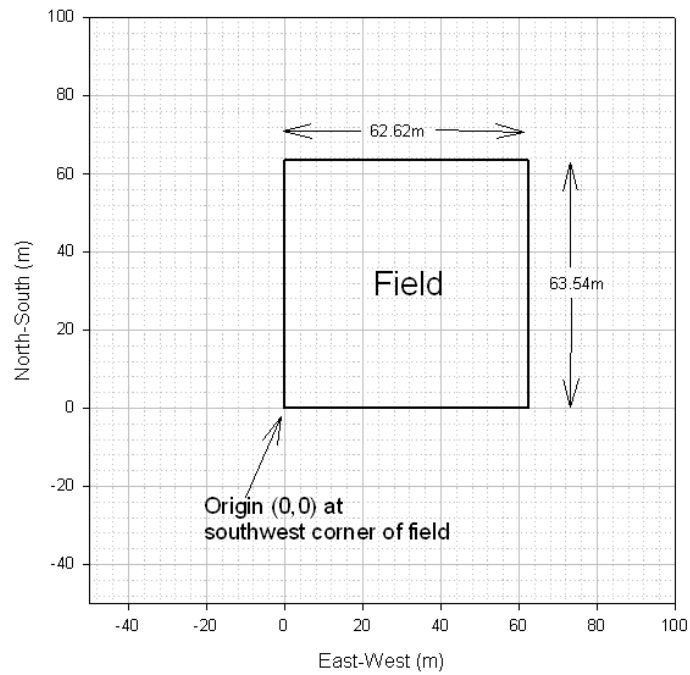
3. Look up "location keyword" in the ISC Manual, read that first paragraph which shows what's on the line (bottom Adobe pg 97).

```
**              SRCID SRCTYP        XS              YS              ZS

SO LOCATION    acre1 AREA          0.00            0.00           .0000

** Source Parameter Cards:
** POINT:    SRCID       QS              HS          TS          VS
```

4. Look up "srcparam card" and go to the entry "the SRCPARAM card, which is a mandatory keyword for each source being modeled. Since" Note the use of the word "card" to refer to a line in the control file. Extra credit if you can explain why the word "card" is used to stand for a line in the control file. Read down through this section and notice that the syntax and variables on the SRCPARAM card line depend on the kind of source (point, volume, area). We are most interested in area sources. Read that section. In particular see that XINIT and YINIT give the x and y lengths of the rectangular source.

```
** AREA:    SRCID       QS              HS          XINIT       YINIT

SO SRCPARAM acre1    .10000000E-03      .0000       100.        100.

SO EMISUNIT     .100000E+07  (GRAMS/SEC)       (MICROGRAMS/CUBIC-METER)
```

5. Look up "DISCCART" in the ISC Manual. Read about discrete receptors and how they are described.

```
RE  STARTING
RE  DISCCART  500.9 273.57
RE  DISCCART  691.62 170.53
RE  DISCCART  722.35 313.62
RE  FINISHED
```

6. Get "mebr-study.pdf" up on the screen and use Table 1 to obtain the field dimensions for Seal Beach Broadcast. Write these dimensions down. Use Figure 3 and a calculator or Excel to determine the coordinates of the monitors. Make the southwest corner of this field 0,0. Once you have these numbers, complete the SO LOCATION, SO SRCPARAM AND RE DISCCART lines in the file called EX04.TXT. Use Notepad to enter the changes to EX04.TXT. You should create eight DISCCART lines. Hint: 3.28 feet = 1 meter and a right triangle with angles 45,45,90 has the ratio of sides as 1:1:1.41 (i.e. if the sides are 1 and 1, the hypotenuse is 1.414). Also, it is a good practice to start with a single monitor and work around the field either clockwise or counterclockwise.

-6.47	70.01			31.31	73.60			69.52	70.44
		0.00	63.54			62.62	63.54		
-9.15	31.77							72.38	31.77
		0.00	0.00			62.62	0.00		
-6.90	-6.90			31.31	-9.76			69.73	-7.11

Encoding geometry.

Step 1. Determine the corners of the field. These come from the methyl bromide memo Table 1, Seal Beach Broadcast

Step 2. Convert the feet to meters (3.28'=1m)

Step 3. Start at a receptor and work, say clockwise around.

Step 4. For corners, use trig to convert the hypotenuse into x,y components and adjust the corner x,y location accordingly. For sides, use the midpoint of the edge etc etc.

Step 5. Insert the SW corner location and length/width of field into appropriate places in SOURCE pathway of control file.

Step 6. Insert the monitoring locations (receptors) into the RECEPTOR pathway of the control file using the discrete receptor syntax.

$\sqrt{2}$ = 1.414

Plot Areas

	Length (m) E-W	N-S	Area (m2)	Acres
Seal Beach				
Broadcast	62.62	63.54	3978.9	0.98
Shank In	65.06	65.06	4232.8	1.05
Shank Ahead	63.84	64.91	4143.9	1.02
Santa Maria				
Broadcast	64.01	62.48	3999.3	0.99
Shank In	64.92	64.01	4155.5	1.03
Shank Ahead	64.62	64.01	4136.3	1.02
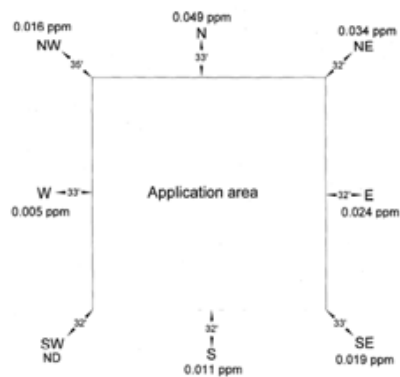
Figure 3. Seal Beach broadcast application plot and 24-hour time weighted

Determining the field and receptor coordinates for Seal Beach Broadcast study (Johnson and Wofford 1999).

Section 05. Meteorology, consistency in directions,WEATH6A, stability, from/to directions, Pasquill, declination, creating met file, sun angle, exercise creating met file

```
RE DISCCART -6.47 70.01
RE FINISHED


ME STARTING
ME INPUTFIL SBP1.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT    10.000 METERS
ME SURFDATA  99999  1999              SURFNAME
ME UAIRDATA  99999  1999              UAIRNAME
ME WINDCATS     1.54     3.09     5.14     8.23    10.80
ME FINISHED
```

1. Meteorology file is referenced in "ME" pathway (or paragraph) or input control file.
2. Filename, FORTRAN format in INPUTFIL line.
3. SURFDATA and UAIRDATA must have station ID, year consistent with first line in meteorological data file. Can use arbitrary ID numbers for custom situations. Just make sure they match and make sure year matches.

```
ME STARTING
ME INPUTFIL SBP1.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT    10.000 METERS
ME SURFDATA  99999  1999              SURFNAME
ME UAIRDATA  99999  1999              UAIRNAME
```

SBP1.MET - Notepad

File   Edit   Format   View   Help

```
    99999        99    99999        99
99 624 9   68.6439    0.7367 292.7 2   300.0   300.0
99 62410   36.0762    3.5957 292.6 2   300.0   300.0
99 62411   49.7803    4.1236 292.9 2   300.0   300.0
99 62412   55.6602    4.5357 293.0 2   300.0   300.0
99 62413   48.5289    4.6531 294.4 2   300.0   300.0
```

4. Look up ME INPUTFIL in ISC Manual. (go to Adobe page 150).
   a. Note the station numbers and years in the input control file must match the station numbers and years in the meteorological data file.
   b. Note the table on page 3-80 (Adobe page 152) giving the format and variable definitions.
   c. IMPORTANT NOTE: THE WIND DIRECTION IS THE "TO" DIRECTION.
   d. IMPORTANT NOTE: THE WIND DIRECTION IS THE "TO" DIRECTION. (Stated twice for emphasis).
   e. Question: In the meteorological data file for ISC, is the wind direction the "from" or "to" direction?
   f. The "to" direction means the direction that the wind is blowing toward. An easterly wind (in conventional meteorological language) would mean a wind that is blowing "from the east" and would be described as a wind with an angle of 90° (in conventional meteorological language). This conventional description is 180° different from what ISC uses for wind direction. For ISC, such a wind would have to be adjusted to 270° in order to represent it blowing towards the west. That is probably why instead of referring to the wind direction, the ISC Manual calls it the "flow vector".
   g. Note the units from Manual (Adobe pg152) that wind speed is m/s, temperature is Kelvin and stability class is an integer 1, 2, 3, 4, 5, or 6.
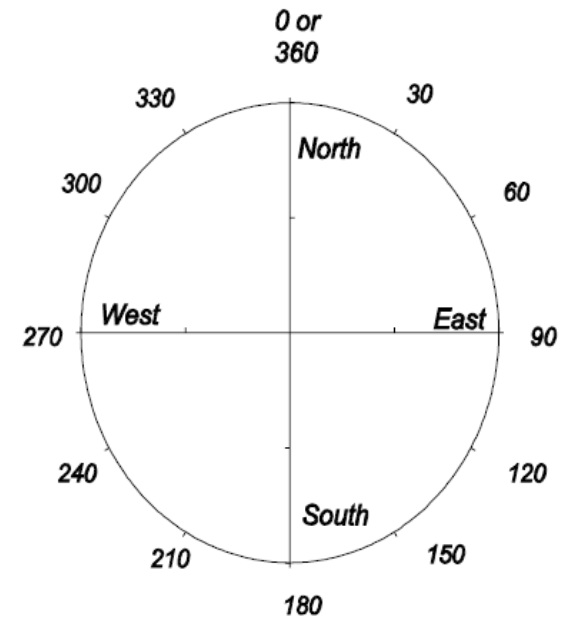
Section 05 Processing meteorological data with WEATH6A. The purpose of this section is to take an Excel file containing data from a data logger and process it into a text file that will contain ISC –compatible meteorological data. This section will basically outline the use of WEATH6 and an associated cutfile. There will be a separate section on determining stability. Separate documentation for WEATH6A is available in DOCS.

1. Meteorological data typically comes in electronic spreadsheets and consists of many measurements each hour of wind speed, wind direction, temperature, humidity, time/date stamps, precipitation and other variables.
2. Sometimes there are additional summary records included in the data sets. Watch out for these because they shouldn't be included in the analysis.
3. This particular data set for Seal Beach study includes an hourly summary (record array #12, see row 26 in figure above), relatively humidity, 'resultant' wind speed in addition to 'average' wind speed. The difference is resultant=vector average, average=scalar average. ISC typically uses scalar average (ie not resultant).

Microsoft Excel - sealbeachmet.xls

File Edit View Insert Format Tools Data Window Cell Run CBTools Help Adobe PDF

A1

	A	B	C	D	I	J	K	L	M	N	O	P
1					Maximum	Maximum	Average	Average	Average	Average Resultant		
2			Julian		RH	Wind Speed	Air Temp.	RH	Wind Speed	Wind Speed	Resultant	Standard Deviation
3	Array	Year	Date	Time	%	m/s	°C	%	m/s	m/s	Wind Direction	Wind Direction
5	11	1999	174	1420	56.33	5.919	23.63	55.82	5.684	5.676	202.4	3.117
6	11	1999	174	1422	59.98	5.782	23.09	57.32	4.972	4.887	207	10.6
7	11	1999	174	1424	59.75	5.037	23.04	57.49	4.028	3.916	218.5	13.5
8	11	1999	174	1426	62.68	5.821	22.89	58.44	4.804	4.689	220.3	12.49
9	11	1999	174	1428	60.33	5.645	22.63	58.5	4.657	4.586	230.4	10.05
10	11	1999	174	1430	62.24	5.645	22.55	59.16	4.602	4.38	219.2	17.8
11	11	1999	174	1432	60.83	5.253	22.81	57.77	4.678	4.638	236.8	7.49
12	11	1999	174	1434	60.26	5.449	22.71	58.78	4.57	4.528	237.1	7.8
13	11	1999	174	1436	60.59	5.566	22.58	58.48	4.965	4.933	232.3	6.486
14	11	1999	174	1438	61.34	5.586	22.33	59.28	4.839	4.813	230.8	5.864
15	11	1999	174	1440	60.33	5.37	22.39	58.86	4.631	4.579	221	8.65
16	11	1999	174	1442	61.03	5.429	22.66	58.1	4.837	4.764	226.3	9.94
17	11	1999	174	1444	60.19	5.312	22.67	58.22	4.662	4.629	223.7	6.876
18	11	1999	174	1446	61.03	5.566	22.72	58.71	4.828	4.735	235.9	11.23
19	11	1999	174	1448	60.36	5.468	22.6	58.66	4.805	4.77	233.1	6.899
20	11	1999	174	1450	60.36	5.684	22.61	57.96	4.907	4.874	233.6	6.597
21	11	1999	174	1452	59.26	5.018	22.67	57.47	4.204	4.146	228	9.56
22	11	1999	174	1454	59.74	5.821	22.75	58.19	4.809	4.786	235.8	5.565
23	11	1999	174	1456	60.34	5.292	22.68	57.92	4.575	4.55	234.8	5.943
24	11	1999	174	1458	59	5.194	22.92	57.19	4.482	4.436	236.9	8.21
25	11	1999	174	1500	57.73	5.508	23.24	56.01	4.23	4.174	239.1	9.27
26	12	1999	174	1500	62.68	5.919	22.73	58.11	4.663	4.548	228.8	10.28
27	11	1999	174	1502	58.26	4.998	23.27	56.26	4.377	4.36	228.4	4.999
28	11	1999	174	1504	58.38	5.723	23.01	56.52	4.502	4.476	221.8	6.228

4. This data set also includes array#13 which is 24 hour summary at the end of each 24h day.

	Microsoft Excel - sealbeachmet.xls

File   Edit   View   Insert   Format   Tools   Data   Window   Cell   Run   CBTools   Help

I18   *fx* 61.03

	A	B	C	D	I	J	K	L	
1					Maximum	Maximum	Average	Average	Ave
2			Julian		RH	Wind Speed	Air Temp.	RH	Wind
3	Array	Year	Date	Time	%	m/s	°C	%	n
301	11	1999	174	2354	91.5	1.666	16.43	91.2	1.
302	11	1999	174	2356	91.4	1.627	16.43	91.1	1.
303	11	1999	174	2358	91.4	1.686	16.41	91.1	1.
304	11	1999	174	2400	91.5	1.725	16.38	91.3	1.
305	12	1999	174	2400	92	2.646	16.5	90.4	1.
306	13	1999	174	2400	92	7.19	19.9	72.4	3.
307	11	1999	175	2	91.7	2.038	16.35	91.4	1.
308	11	1999	175	4	91.8	1.901	16.33	91.5	1.
309	11	1999	175	6	91.8	1.725	16.32	91.6	1.

5. To save time, I have already converted the Seal Beach met file into a CSV file ready for input into WEATH6A.EXE. Here is what the SEALMET.CSV file looks like when it's opened with Notepad. There are some important features to preparing the data for input into WEATH6A.EXE which will be discussed below.

SEALMET.CSV - Notepad

File   Edit   Format   View   Help

```
6,23,14,20,1,74.53,1,216.40,12.72
6,23,14,22,1,73.56,1,221.00,11.12
6,23,14,24,1,73.47,1,232.50,9.01
6,23,14,26,1,73.20,1,234.30,10.75
6,23,14,28,1,72.73,1,244.40,10.42
6,23,14,30,1,72.59,1,233.20,10.30
6,23,14,32,1,73.06,1,250.80,10.47
6,23,14,34,1,72.88,1,251.10,10.22
6,23,14,36,1,72.64,1,246.30,11.11
6,23,14,38,1,72.19,1,244.80,10.83
6,23,14,40,1,72.30,1,235.00,10.36
```

6. Here is what SEALMET.CSV looks like when opened up in Excel.

Microsoft Excel - SEALMET.CSV

File   Edit   View   Insert   Format   Tools   Data   Window   Cell   Run   CBTools   Help   Adobe PDF

A1 f_x 6
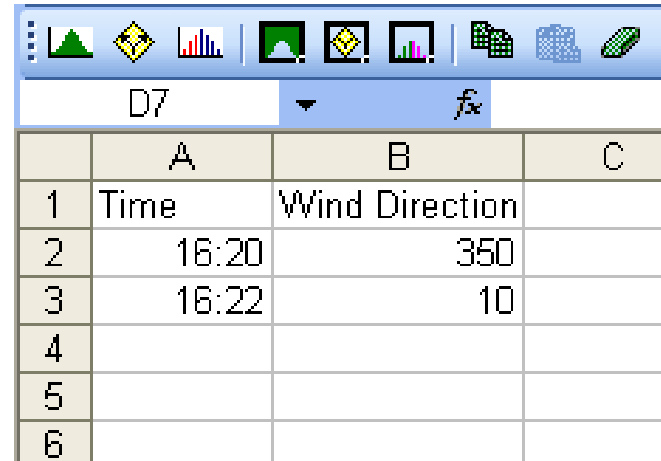
	A	B	C	D	E	F	G	H	I
1	6	23	14	20	1	74.53	1	216.4	12.72
2	6	23	14	22	1	73.56	1	221	11.12
3	6	23	14	24	1	73.47	1	232.5	9.01
4	6	23	14	26	1	73.2	1	234.3	10.75
5	6	23	14	28	1	72.73	1	244.4	10.42
6	6	23	14	30	1	72.59	1	233.2	10.3
7	6	23	14	32	1	73.06	1	250.8	10.47

7. Compare the CSV file above to the corresponding part of the original data logger excel file below. I have hidden non-essential columns.

Microsoft Excel - sealbeachmet.xls

File   Edit   View   Insert   Format   Tools   Data   Window

P1 f_x

	C	D	K	M	O
1			Average	Average	
2	Julian		Air Temp.	Wind Speed	Resultant
3	Date	Time	°C	m/s	Wind Direction
5	174	1420	23.63	5.684	202.4
6	174	1422	23.09	4.972	207
7	174	1424	23.04	4.028	218.5
8	174	1426	22.89	4.804	220.3
9	174	1428	22.63	4.657	230.4
10	174	1430	22.55	4.602	219.2
11	174	1432	22.81	4.678	236.8

8. Important features in comparing the data logger data to the data prepared for WEATH6A at this phase of preparation:

    a. Julian date has been converted to month, day of month (174 Julian date is June 23)
    b. Time went from hhmm to separate columns for hour and minute
    c. Column E and Column G consist entirely of 1's have been added (these are placeholders for now).
    d. Wind speed was originally in m/s and has been converted to miles per hour (column I in SEALMET.CSV, 12.72=5.684/0.447).
    e. Temperature in the original sealbeach.XLS data was in Centigrade and has been converted to Fahrenheit [column F in SEALMET.CSV, 74.53=(9/5)23.63+32].
    f. The wind directions in SEALBEACHMET.XLS appear to be 14° less than the corresponding wind directions in SEALMET.CSV. This is the adjustment for converting from magnetic north measurements to true north measurements. You must always establish **(1) are the geometric diagrams using magnetic north or true north (2) is the data logger which measures wind direction using magnetic north or true north**. What is critical is that both measurements are adjusted (if necessary) to be consistent with each other. They're both either magnetic north or both true north.
    g. Another feature which comes up sometimes is the definition of hour. You must worry about daylight savings time versus standard time. Later on, you will need astronomical information which will most likely be in standard time. If the data logger has used daylight savings time, then the astronomical information and data logger information must be properly aligned so that the actual corresponding hours are used. Another wrinkle is whether in hourly summaries the hour represents the beginning of each hour or the end of each hour. CIMIS data uses hours from 1 to 24, standard time. For downloaded CIMIS data, the hour is always in standard time and it always represents the time at the end of each hour. In other words, 23 represents a summary from 10:01PM to 11:00PM. Note that the hour as used in the files above stand for the hour at the beginning of each time period.

h. I don't want to use WEATH6A.EXE, why can't I just take the average of these values for each hour myself? The procedures, especially for finding the average wind direction, are not so easy. Consider the following data:

     i. What is the average wind direction for these 2 measurements?

    ii. ½*(350+10)=180? Is this correct?

	A	B	C
	D7		f_x
1	Time	Wind Direction	
2	16:20	350	
3	16:22	10	
4			
5			
6			

9. Summary of preparing file in preparation for processing by WEATH6A.
    a. Create CSV delimited file (Excel, File, Save AS, Save as Type, select CSV)
    b. Variables are
         i. Month
        ii. day
       iii. hour
       iv. minute
        v. dummy
       vi. temperature F
      vii. dummy
     viii. wind direction (degrees and direction consistent with field orientation)
       ix. wind speed (miles per hour)

10. Example
    a. Use the DOS window
    b. Go to Section 5
    c. Use the DIR command to verify that SEALMET.CSV and CUTHOUR.IN are there
    d. Run WEATH6A (..\weath6a)
    e. For output filenames pick what you think is reasonable
    f. Get sunrise sunset times from http://aa.usno.navy.mil/
        i. Seal Beach, California June 24 (be sure that these times are consistent with daylight savings time which is what the Seal Beach data set is in)
    g. Wind speed threshold is 2.2 miles per hour
    h. Use "cuthour.in" for the cutpoint file.
    i. Use 99,6,24,9 for starting hour (year 1999, June 24, 9AM)
    j. Use 300-350 for the mixing height (300-350 meters).
    k. This should produce 2 new files in the directory, one which contains the prep file for ISC input and the other is a document file which provides a little more info on what the calculations were based on.
    l. Use Notepad to examine these two output files.

Section 05 Running WEATH6A

This is covered in a separate document (Johnson 2010). The example used is the Seal Beach broadcast study from the same study as the example used in this tutorial**.**

Section 05 Stability Class Determination. This section presumes that you have successfully run WEATH6A. We will use with the document file output from WEATH6A to fill in the stability classes for the Seal Beach data set.

1. The meteorological file is almost ready to use for simulation. Look at sbisc.met. This file is the nearly-ISC-ready meteorological data file (the other file is the WEATH6A document output file, which will be shown further below). In the sbisc.met file there are a column of Xs. The remaining work is to fill in the column of Xs with stability classes. Stability classes were devised to describe the degree of atmospheric stability. The pre-class homework covered stability. Briefly, sun-heated soil in turn heats up the air near the soil, which becomes less dense, rises and creates vertical mixing of the atmosphere. Summer clear sky afternoons are prime unstable periods. The most unstable period is described with the number 1 (will also see the letter 'A'). At the opposite end, most stable conditions occur during late night/early morning under clear skies when radiative cooling

causes the ground to become colder than the air. The ground in turn keeps the air cool, which because of higher density continues to hug the ground and vertical mixing is suppressed. The most stable period receives a number 6 (will also see the letter 'F').

2. The task is to assign the stability numbers 1-6 to each hour (where the Xs are) in a systematic and reproducible way. For the ISC met file, the stability classes must be numbers 1-6, not the letters A-F.

azimuth.

_____

Form A - U.S. Cities or Towns

3. A required piece of information for determining stability is the solar elevation angle. Go to http://aa.usno.navy.mil/data/, click on

   Altitude and Azimuth of the Sun or Moon During One Day

   Fill in the fields for 1999, June 24, 30 minutes, California, Seal Beach, then click on Compute Table.

Object:
⊙ Sun ○ Moon

Year: 1999   **Month:** June ▾   **Day:** 24

Tabular Interval: 30   minutes   (range 1-120 minutes)

State or Territory: California ▾

City or Town Name: Seal Beach

The place name you enter above must be a city or town in the U.S. The place's location will be retrieved from a file with over 22,000 places listed. Either upper- or lower-case letters or a combination can be used. Spell out place name prefixes, as in "East Orange", "Fort Lauderdale", "Mount Vernon", etc. The only exception is "St.", which is entered as an abbreviation with a period, as in "St. Louis". You need only enter as many characters as will unambiguously identify the place.

[Compute Table]   [Clear all fields]

Since the sun altitude is given for standard time and since the Seal Beach data is Pacific Daylight time, the h m values must be increased by 1 hour in order to match up with the SB data.

After getting the time aligned properly with the monitoring period times, pull out a hard copy of the documentation WEATH6A output file (shown below as WEATH6A.OUT) and write the sun altitude times next to each corresponding period on the hardcopy WEATH6A output file. These sun altitudes will be used to gauge the degree of solar insolation, which in turn will be used to estimate the stability class. The table below is excerpted from Budney.

```
Pacific Standard Time

                    Altitude        Azimuth
                                    (E of N)
                  Daylight
 h   m            Time              o
 04:00   5         -8.3             54.5        Sunrise
 04:30             -3.1             59.0        was
 05:00   6          2.6             63.2
 05:30              8.1             67.1
 06:00   7         13.9             70.9        5:43
 06:30             19.8             74.5
 07:00   8         25.8             78.0        P.D.T.
 07:30             32.0             81.6
 08:00             38.2             85.3
 08:30             44.4             89.2
 09:00             50.6             93.5
 09:30             56.8             98.6
 10:00             62.9            104.9
 10:30             68.8            113.7
```

Sky Cover	Solar Elevation Angle > 60°	Solar Elevation Angle ≤ 60° But >35°	Solar Elevation Angle ≤ 35° But > 15°
4/8 or Less or Any Amount of High Thin Clouds	Strong	Moderate	Slight
5/8 to 7/8 Middle Clouds (7000 feet to 16,000 foot base)	Moderate	Slight	Slight
5/8 to 7/8 Low Clouds (less than 7000 foot base)	Slight	Slight	Slight

4. Locate Adobe pg 42 in the 1999 Workbook (Table 10). The same table is also in Budney, Adobe page 18, Table 3-2 "Key to Stability Categories". Cloud cover plays a role both during the day and night. As a practical matter, we frequently do not have cloud cover information and this refinement is not used. If there is no cloud cover data, assume clear skies. Using the categories of degree of solar insolation, classify each daytime hour as strong, moderate or slight and write the classification down on the WEATH6A.OUT hardcopy. WEATH6A uses the user-input sunset/sunrise times to determine day and night categories for each hour.

5. Based on the user-entered sunrise/sunset hours, WEATH6A has classified each hour as day or night. Also, the scalar wind

Table 3-2. KEY TO STABILITY CATEGORIES
Table modified from Budney (1977)

Surface Wind Speed at a Height of 10m (m/sec)	Day Incoming Solar Radiation* (Insolation)			Night Thinly Overcast or $\geq$ 4/8 Low Cloud Cover	$\leq$ 3/8 Cloud Cover
	Strong	Moderate	Slight		
< 2	A	A-B	B	F	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	C	D	D	D	D

The neutral class (D) should be assumed for all overcast conditions during day or night.

speed (m/s) is listed along with other information. For wind speed categories less than 2 m/s at night, the category is F (=6). As you can see the stability categories depend on night vs day, wind speed, and during the day on solar insolation.

6. We will use the stability classification scheme, together with the degree of solar insolation to classify each hour for stability. Since starting at the first hour of the file can lead to ambiguous assignments, it is best to start in the middle of the night by locating an F stability hour. In this case, 2AM to 3AM on June 25th is clearly F stability since the wind speed is less than 3 m/s. Work backwards and forwards with the following additional rule:

The stability class can not change by more than 1 from one hour to the next.

Therefore, if the current hour is class 3, there are 3 possibilities for the next and preceding hours: 2,3,4. If the current hour is 6, there are 2 possibilities: 5,6.

For the daytime conditions, it's helpful to write in the sun angle using the midpoint sunangle as a kind of average between the beginning and ending of the hour.   Here below is an excerpt from my worksheet showing the sun altitude, solar insolation and stability that I've written down for each hour.

```
                                  SCA AVG     180+AVG   SCA AVG    NUMBER OF
     .......TIME PERIOD........    TEMPERA K   DIRECTI   SPD M/S    RECORDS      N/D
 6/24  9: 0 TO   6/24 10: 0       292.698     68.644    0.737      ( 30) ʌ3     DAY  ᵾᵾ.ᵾ M
 6/24 10: 0 TO   6/24 11: 0       292.607     36.076    3.596      ( 30) /3     DAY  5ᴂ M
 6/24 11: 0 TO   6/24 12: 0       292.893     49.780    4.124      ( 30) ᒻ      DAY  ⸅9 STL
 6/24 12: 0 TO   6/24 13: 0       293.001     55.660    4.536      ( 30) ⸊      DAY  ⸅8 STL
```
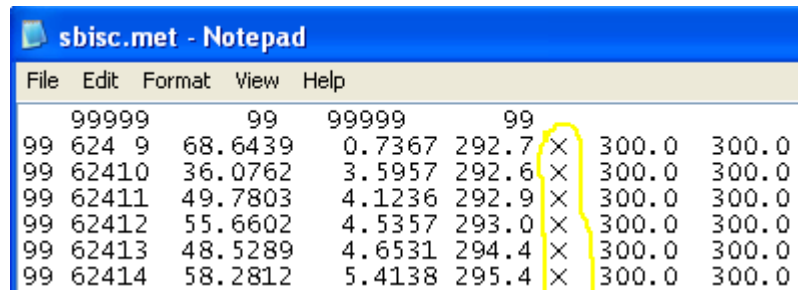
Here is the larger page from which the excerpt above was taken.

```
                                        weath6a.out
WEATHER INPUT FILE: sealmet.csv
class example
USER DEFINED VALUES: SUNRISE@ 5:43, SUNSET@20: 7
     NOTE THAT DAY STARTS 1 HR AFTER SUNRISE AND
     ENDS 1 HR BEFORE SUNSET FOR STABILITY CALCS
TODAY'S DATE: MAR 26 2010
        TIME: 10:06
   WEATH6A: LAST MODIFIED 12/17/2009. SCALER WIND SPEED,
      INCLUDES ALL WIND MSMNTS AND AVERAGE DIRECTION BASED
      ONLY ON MSMNTS WHERE SPEED> 2.2000MPH  (0.9834M/S).
-------------------------------------------------------------
NAME OF ISCST3 MET DATA FILE: sbcisc.met

-------------------------------------------------------------

                            SCA AVG   180+AVG   SCA AVG   NUMBER OF
.......TIME PERIOD........   TEMPERA K  DIRECTI   SPD M/S   RECORDS    N/D
6/24  9: 0 TO  6/24 10: 0    292.698    68.644    0.737    ( 30)      DAY
6/24 10: 0 TO  6/24 11: 0    292.607    36.076    3.596    ( 30)      DAY
6/24 11: 0 TO  6/24 12: 0    292.893    49.780    4.124    ( 30)      DAY
6/24 12: 0 TO  6/24 13: 0    293.001    55.660    4.536    ( 30)      DAY
6/24 13: 0 TO  6/24 14: 0    294.423    48.529    4.653    ( 30)      DAY
6/24 14: 0 TO  6/24 15: 0    295.390    58.281    5.414    ( 30)      DAY
6/24 15: 0 TO  6/24 16: 0    296.229    60.932    5.197    ( 30)      DAY
6/24 16: 0 TO  6/24 17: 0    294.826    64.187    6.178    ( 30)      DAY
6/24 17: 0 TO  6/24 18: 0    294.535    63.993    4.595    ( 30)      DAY
6/24 18: 0 TO  6/24 19: 0    295.987   118.166    3.533    ( 30)      DAY
6/24 19: 0 TO  6/24 20: 0    293.402   132.464    3.756    ( 30)      NIGHT
6/24 20: 0 TO  6/24 21: 0    290.648   131.146    2.859    ( 30)      NIGHT
6/24 21: 0 TO  6/24 22: 0    289.615   137.831    2.267    ( 30)      NIGHT
6/24 22: 0 TO  6/24 23: 0    289.174   143.431    2.386    ( 30)      NIGHT
6/24 23: 0 TO  6/24 24: 0    288.967   146.088    2.497    ( 30)      NIGHT
6/24 24: 0 TO  6/25  1: 0    288.701   145.964    1.065    ( 30)      NIGHT
6/25  1: 0 TO  6/25  2: 0    288.292   339.684    0.785    ( 30)      NIGHT
6/25  2: 0 TO  6/25  3: 0    288.879    14.368    0.749    ( 30)      NIGHT
6/25  3: 0 TO  6/25  4: 0    288.965     2.067    0.979    ( 30)      NIGHT
6/25  4: 0 TO  6/25  5: 0    288.803   346.987    1.253    ( 30)      NIGHT
6/25  5: 0 TO  6/25  6: 0    288.634    10.897    1.612    ( 30)      NIGHT
6/25  6: 0 TO  6/25  7: 0    288.684     6.764    1.460    ( 30)      NIGHT
6/25  7: 0 TO  6/25  8: 0    288.989    21.844    1.059    ( 30)      DAY
6/25  8: 0 TO  6/25  9: 0    289.421     5.326    1.731    ( 30)      DAY
6/25  9: 0 TO  6/25 10: 0    290.263    49.704    1.519    ( 30)      DAY
6/25 10: 0 TO  6/25 11: 0    291.852    25.595    1.801    ( 30)      DAY
6/25 11: 0 TO  6/25 12: 0    291.728    24.988    3.584    ( 30)      DAY
6/25 12: 0 TO  6/25 13: 0    292.109    38.963    3.572    ( 30)      DAY
6/25 13: 0 TO  6/25 14: 0    292.200    28.783    4.599    ( 30)      DAY
6/25 14: 0 TO  6/25 15: 0    291.899    27.322    4.800    ( 30)      DAY
6/25 15: 0 TO  6/25 16: 0    292.320    34.434    4.458    ( 30)      DAY
6/25 16: 0 TO  6/25 17: 0    291.810    38.397    5.138    ( 30)      DAY
6/25 17: 0 TO  6/25 18: 0    291.784    45.756    4.802    ( 30)      DAY
6/25 18: 0 TO  6/25 19: 0    292.764    41.843    3.244    ( 30)      DAY
6/25 19: 0 TO  6/25 20: 0    292.301    27.356    2.762    ( 30)      NIGHT
6/25 20: 0 TO  6/25 21: 0    290.468    31.319    3.016    ( 30)      NIGHT
6/25 21: 0 TO  6/25 22: 0    289.843    33.365    2.345    ( 30)      NIGHT
6/25 22: 0 TO  6/25 23: 0    289.410    15.884    1.734    ( 30)      NIGHT
6/25 23: 0 TO  6/25 24: 0    288.771   359.712    1.861    ( 30)      NIGHT
6/25 24: 0 TO  6/26  1: 0    288.878    27.709    1.849    ( 30)      NIGHT
6/26  1: 0 TO  6/26  2: 0    289.328    21.831    1.910    ( 30)      NIGHT
6/26  2: 0 TO  6/26  3: 0    289.541   345.974    1.483    ( 30)      NIGHT
6/26  3: 0 TO  6/26  4: 0    289.541   345.876    1.553    ( 30)      NIGHT
6/26  4: 0 TO  6/26  5: 0    289.229   339.714    2.623    ( 30)      NIGHT
6/26  5: 0 TO  6/26  6: 0    288.984   320.859    1.945    ( 30)      NIGHT
6/26  6: 0 TO  6/26  7: 0    289.091   295.512    2.342    ( 30)      NIGHT
                            Page 1
```

7. After making the written stability determinations on the WEATH6A.OUT sheet, use these stability classes to replace the Xs on the SBCISC.MET file using Notepad. Do not change the position of the character.
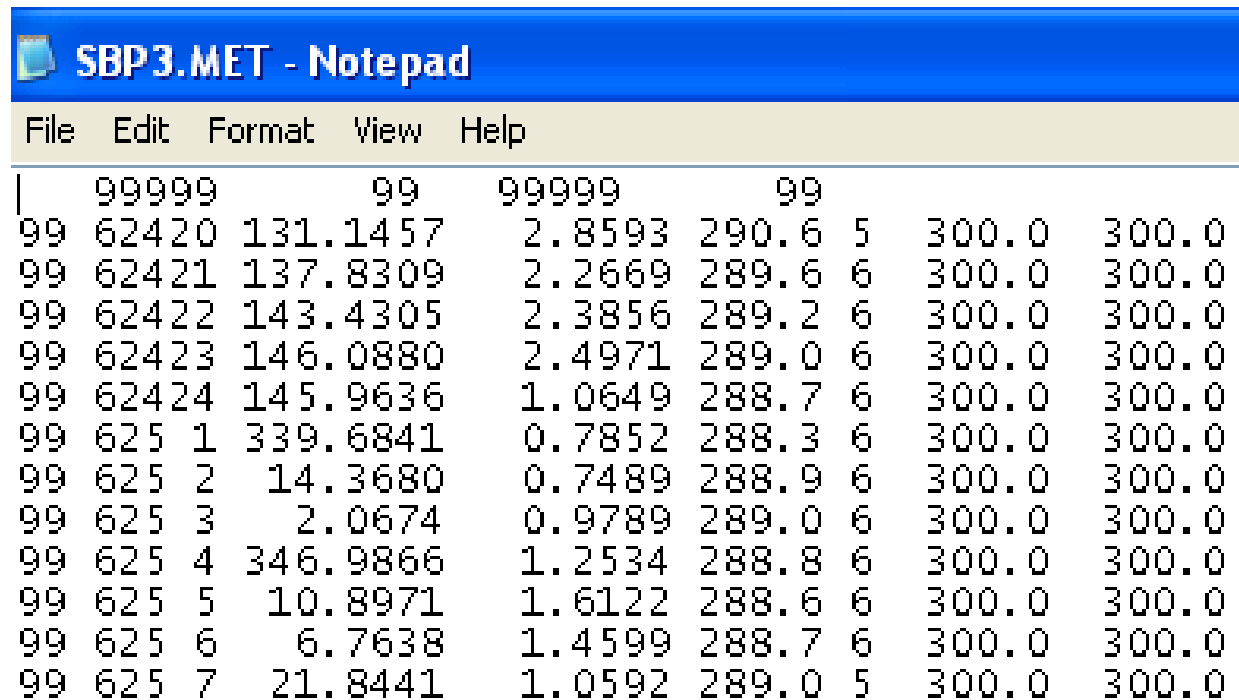
```
📄 sbisc.met - Notepad

File  Edit  Format  View  Help

    99999         99    99999        99
99 624 9    68.6439      0.7367 292.7 X   300.0    300.0
99 62410    36.0762      3.5957 292.6 X   300.0    300.0
99 62411    49.7803      4.1236 292.9 X   300.0    300.0
99 62412    55.6602      4.5357 293.0 X   300.0    300.0
99 62413    48.5289      4.6531 294.4 X   300.0    300.0
99 62414    58.2812      5.4138 295.4 X   300.0    300.0
```

8. One more step is required to prepare the met file for site application studies. The SBISC.MET file covers the whole monitoring study which consists of many periods when the sampling tubes or canisters are changed. In order to simulate each monitoring period, separate meteorological files must be created for each monitoring period. It is necessary to review the study, determine the start and stop times for each monitoring period, then use SBISC.MET to create individual met files for each of those periods. In each met file the first line must be the same as the first line in SBISC.MET. That is, it must include the 99999 99 99999 99. The year (99) must be the same as whatever the year designator is for each record. The 99999 only needs to match whatever code is used in the ISC control file in the ME pathway.

9. The finished met file for period 3 for Seal Beach study is shown below. The Xs have been replaced by the estimated stability class. This monitoring period 3 ran from 8PM on June 24 to 8AM on June 25. The stability classes reflect the high night time stability.

```
SBP3.MET - Notepad

File   Edit   Format   View   Help

|    99999          99    99999          99
99 62420 131.1457    2.8593 290.6 5    300.0    300.0
99 62421 137.8309    2.2669 289.6 6    300.0    300.0
99 62422 143.4305    2.3856 289.2 6    300.0    300.0
99 62423 146.0880    2.4971 289.0 6    300.0    300.0
99 62424 145.9636    1.0649 288.7 6    300.0    300.0
99 625 1 339.6841    0.7852 288.3 6    300.0    300.0
99 625 2  14.3680    0.7489 288.9 6    300.0    300.0
99 625 3   2.0674    0.9789 289.0 6    300.0    300.0
99 625 4 346.9866    1.2534 288.8 6    300.0    300.0
99 625 5  10.8971    1.6122 288.6 6    300.0    300.0
99 625 6   6.7638    1.4599 288.7 6    300.0    300.0
99 625 7  21.8441    1.0592 289.0 5    300.0    300.0
```

Section 06. Insert the flux, run an ISC control file several times.

1. In the DOS window, go to Section 06. List the directory and verify that PROB6A.IN, SBP1.MET are in the directory.
2. In the control file above (PROB6A.IN) the highlighted lines are those lines which most frequently will need to be changed for various simulations. One thing to keep in mind is that ISC will *write over existing files by the same name* without asking you. Therefore, if you plan a series of runs, you should change the output file names each time. In this case, there will be three output files: (1) the run output file which is specified when you run the ISC model (..\ISCST3 filename.in filename.out, in this case filename.out is the output file) (2) the ERRORS.OUT output file listed in line 8 above (3) the plotfile PROB6A.PLT, which will contain the output concentrations in a format more convenient for plotting or loading into Excel. Normally, I don't worry about overwriting the ERRORS.OUT file. I try to preserve the other output files however. Be intelligent about naming files. The control file names should conform to the old DOS rules for file names: max of 8 characters to the left of the decimal, max of 3 to the right, no spaces, use conventional characters such as letters and numbers. The input file above, PROB6A.IN was originally named SBBRP1.IN which stood for Seal Beach, Broadcast, Period 1.
3. **FLUX:** A key input is the flux. The ISC model cannot calculate flux. You, as the user, must input it on the SO SRCPARAM line. The flux value is input just after the name of this source unit (in the figure above, "acre1" is the name). The units for area sources are always grams per meter*meter*second. (g/m2s) The

```
CO STARTING
CO TITLEONE Seal Beach Broadcast Tarp June 24-26 1999
CO MODELOPT CONC    RURAL           NOSTD  NOBID  NOCALM
CO AVERTIME  period
CO POLLUTID OTHER
CO DCAYCOEF    .000000
CO RUNORNOT RUN
CO ERRORFIL ERRORS.OUT
CO FLAGPOLE 1.2
CO FINISHED


SO STARTING

** Source Location Cards:
**          SRCID SRCTYP      XS              YS              ZS

SO LOCATION    acre1 AREA          0.00          0.00          .0000

** Source Parameter Cards:
** POINT:    SRCID       QS          HS          TS          VS       DS
** VOLUME:   SRCID       QS          HS          SYINIT      SZINIT
** AREA:     SRCID       QS          HS          XINIT       YINIT

SO SRCPARAM    acre1    .10000000E-03      .0000      62.62      63.54

SO EMISUNIT    .100000E+07 (GRAMS/SEC)            (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED


RE STARTING
RE DISCCART 29.49 73.57
RE DISCCART 69.62 70.53
RE DISCCART 72.35 31.62
RE DISCCART 69.92 -6.99
RE DISCCART 31.92 -9.73
RE DISCCART -6.99 -6.99
RE DISCCART -10.03 31.92
RE DISCCART -7.9 70.53
RE FINISHED


ME STARTING
ME INPUTFIL SBP1.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT   10.000 METERS
ME SURFDATA 99999  1999              SURFNAME
ME UAIRDATA 99999  1999              UAIRNAME
ME WINDCATS   1.54    3.09    5.14    8.23   10.80
ME FINISHED


OU STARTING
OU PLOTFILE PERIOD ALL SBBRP1.PLT
OU FINISHED
```

line EMISUNIT permits you to convert these units in order to get concentration units that are desired. Common concentration units are ppb, ppm, and ug/m3. The file above shows the conversion in order to get ug/m3 in the concentration units. Search for EMISUNIT in the manual and read about this conversion factor line. What significant limitation on field names on the EMISUNIT line must be respected?

4. Go ahead and run the PROB6A.IN control file. The command to run from the DOS window when you are in the subdirectory of SECTION06 is ..\iscst3 file.in file.out (file.out=PROB6A.OUT, is listed in the appendix to this Tutorial)

5. Take a look at the "file.out" file from the run (I usually use the same name for the output file as the input file, except changing the extension from 'in' to 'out', so my command line would be ..\iscst3 prob6a.in prob6a.out) by running notepad within the DOS window (NOTEPAD FILE.OUT). Expand NOTEPAD to full screen and examine the output file.

6. There are several important things to pay attention to in the output file in order to help verify that the model is doing what you think it is doing and what you want it to do. The output file gives you a lot of information about how the ISCST3 program is interpreting your input.

    a. Note that the first part of the output file is simply a copy of the input file.

    b. Scroll down to the "Message Summary". You will see 8 messages. Are these serious errors? What do these messages mean? (Hint: Look up the message in the manual).

    c. Just past the Message Summary section is the "MODEL SETUP OPTIONS SUMMARY". This tells you how the program interpreted your input. Some of these interpretations relate to POINT sources and so are not relevant to us in this example which is an AREA source. The following line tells how many sources and receptors there are.

        i. This Run Includes: 1 Source(s);   1 Source Group(s); and   8 Receptor(s)

    d. In the next section "AREA SOURCE DATA" you can see important information about the sources. In the example, there is only one source. It is called ACRE1, the line gives convenient headers showing emission rate (flux), the southwest corner coordinates, the x and y dimensions of the field. This line is handy and shows in greater detail the meaning of the information that you put into the control file concerning the source.

    e. Next are the "DISCRETE CARTESIAN RECEPTORS" and the 8 monitor locations are listed. For each location, the first 2 numbers specify the location. The third number specifies the "elevation" (should be zero) and the fourth specifies the flagpole height (we wanted 1.2m and that's what we got – which is what the 8 warning messages told us).

    f. Skip down to "THE FIRST 5 HOURS OF METEOROLOGICAL DATA". This important section shows how the program interpreted the meteorological records. Again, as with the area source data above, there is a nice set of headers above the data providing detailed explanations for each of the fields. Below this meteorological data section are notes and one of the notes states : FLOW VECTOR IS DIRECTION TOWARD WHICH WIND IS BLOWING.

    g. Go to the next section, "THE PERIOD (5 HRS) AVERAGE CONCENTRATION   VALUES."

        i. Here you get the x and y coordinates along with the average modeled concentration for the five hour period in ug/m3.

       ii. This form of the modeled concentration output is hard to use for further calculations. That is why the control file also specified a PLT file (PROB6A.PLT).

7. Go back to the DOS window and use notepad to open up the PROB6A.PLT file.
   a. Note that there are 8 lines of text followed by the x,y locations and associated concentration estimates and other information.
   b. This file is much easier to read into Excel or into other programs, such as graphics programs.
   c. The concentrations in this file should match the concentrations found in the PROB6A.OUT file.
8. Exercise 6A. Modify PROB6A.IN file by changing the flux to .20000000E-03 and make whatever other changes you think are necessary to any relevant file names and run the modified file with the 2X flux. Compare the concentrations from the two runs (Hint: read the PLT files into Excel). Is the comparison what you expected? Why or why not.
9. Exercise 6X. You are reviewing a data package and the registrant has simulated a monitoring period. The file should run, but something is wrong with the output. Run the PROB-6X.IN file. Get the modeled concentrations from the PROB-6X.PLT file and compare the modeled concentrations to measured concentrations found the PROB-6X.MEA file. Develop a hypothesis about what is wrong.

Section 06 How to read in a *.plt file from ISCST3 into Excel.

1. You can specify an optional output file (a PLT file) using ISCST3. This file has the same concentration information that the regular ISCST3 output file has, but it is much easier to read into other programs using this file.
2. Below is a small PLT file from the Seal Beach Study.


```
* ISCST3 (02035): Seal Beach Broadcast Tarp June 24-26 1999
* MODELING OPTIONS USED:
*   CONC                        RURAL FLAT  FLGPOL             NOSTD   NOBID   NOCALM
*          PLOT FILE OF PERIOD VALUES FOR SOURCE GROUP: ALL
*          FOR A TOTAL OF     8 RECEPTORS.
*          FORMAT: (3(1X,F13.5),1X,F8.2,2X,A6,2X,A8,2X,I8.8,2X,A8)
*          X                Y           AVERAGE CONC   ZELEV     AVE      GRP         NUM HRS      NET ID

     29.49000        73.57000        153.21553     0.00   PERIOD   ALL       00000005       NA
     69.62000        70.53000        394.59613     0.00   PERIOD   ALL       00000005       NA
     72.35000        31.62000        374.55792     0.00   PERIOD   ALL       00000005       NA
     69.92000        -6.99000          0.36463     0.00   PERIOD   ALL       00000005       NA
     31.92000        -9.73000          0.00141     0.00   PERIOD   ALL       00000005       NA
     -6.99000        -6.99000          0.00000     0.00   PERIOD   ALL       00000005       NA
    -10.03000        31.92000          0.00000     0.00   PERIOD   ALL       00000005       NA
     -7.90000        70.53000          0.00000     0.00   PERIOD   ALL       00000005       NA
```

3. The important concentration data along with the x,y locations starts at LINE 9. In this file, it starts with 24.49000 and so on.

4. Open Excel, click on file, navigate to the Section06 subdirectory on your network drive for this class, type in *.plt into the "File name" field. You should see the file SBBRP1.PLT listed above this field in the large white area.

5. Double click on the file name SBBRP1.PLT. You will then get the "TEXT IMPORT WIZARD".
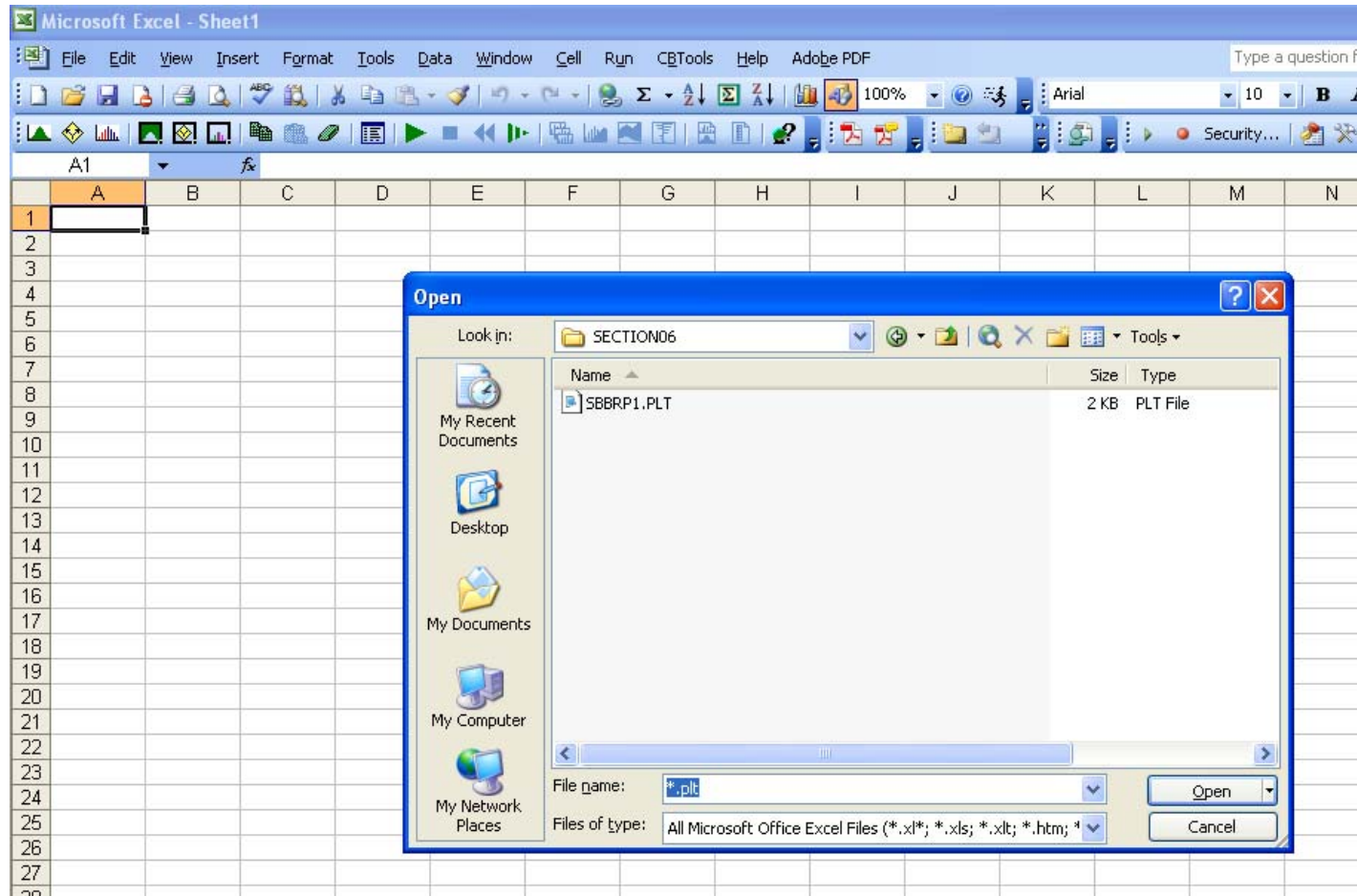
6. Click to check Delimited. Put a 9 into the field for "Start import at row" and click on "Next".
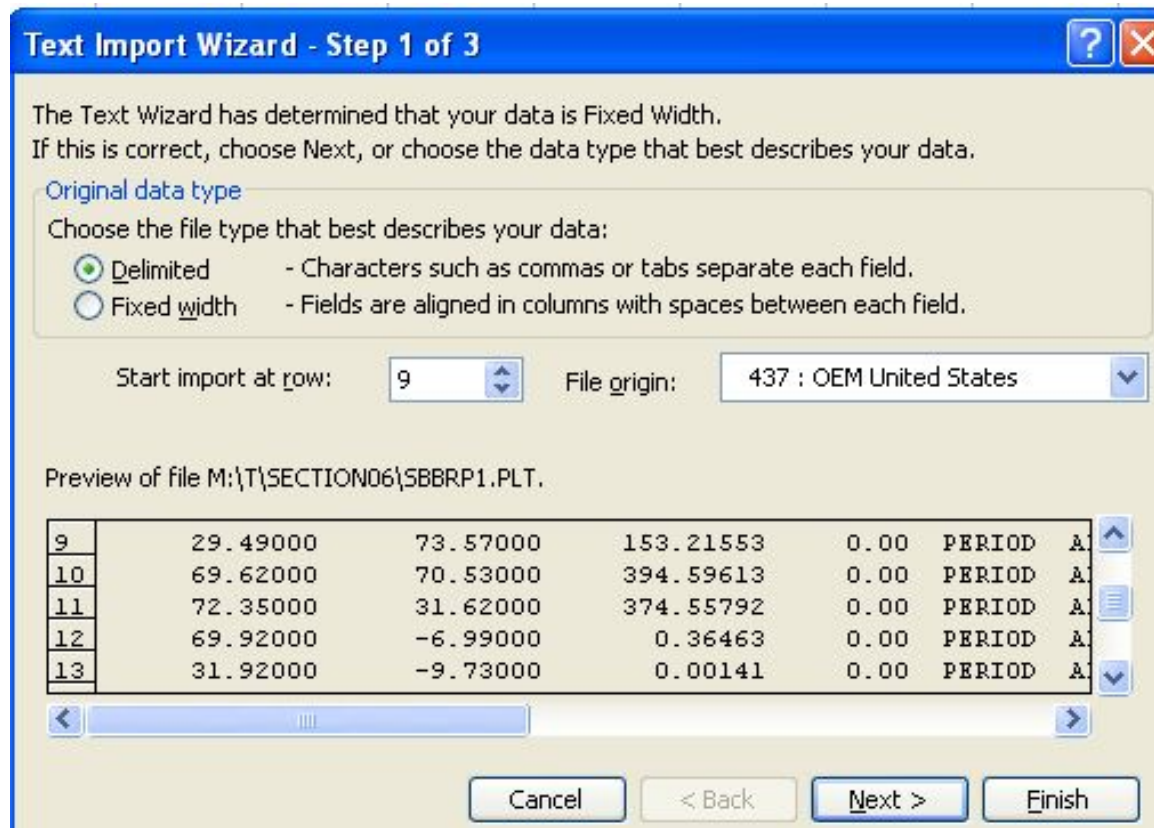
7. You will get STEP 2 of the Text Import Wizard. Click on Space (for delimiter) and Finish.

Text Import Wizard - Step 2 of 3

This screen lets you set the delimiters your data contains. You can see how your text is affected in the preview below.

Delimiters

☑ Tab   ☐ Semicolon   ☐ Comma   ☑ Treat consecutive delimiters as one

☑ Space ☐ Other: [   ]   Text qualifier: [" ▾]

Data preview

29.49000	73.57000	153.21553	0.00	PERIOD	ALL	00000005	NA
69.62000	70.53000	394.59613	0.00	PERIOD	ALL	00000005	NA
72.35000	31.62000	374.55792	0.00	PERIOD	ALL	00000005	NA
69.92000	-6.99000	0.36463	0.00	PERIOD	ALL	00000005	NA
31.92000	-9.73000	0.00141	0.00	PERIOD	ALL	00000005	NA

Cancel   < Back   Next >   Finish

8. You should now see the data entered into an Excel worksheet, something like below.

	A	B	C	D	E	F	G	H	I
1		29.49	73.57	153.2155	0	PERIOD	ALL	5	NA
2		69.62	70.53	394.5961	0	PERIOD	ALL	5	NA
3		72.35	31.62	374.5579	0	PERIOD	ALL	5	NA
4		69.92	-6.99	0.36463	0	PERIOD	ALL	5	NA
5		31.92	-9.73	0.00141	0	PERIOD	ALL	5	NA
6		-6.99	-6.99	0	0	PERIOD	ALL	5	NA
7		-10.03	31.92	0	0	PERIOD	ALL	5	NA
8		-7.9	70.53	0	0	PERIOD	ALL	5	NA
9									
10									

9. Notes: The delimiter refers to the signaling character that is inbetween the data fields. In this case, spaces were the delimiter. This WILL NOT WORK if there are NO spaces between adjacent data fields. For example, if the x and y values in the PLT file had no spaces inbetween, then using spaces as a delimiter wont work. You will have to use fixed format and insert lines between the fields. It is always wise to check down a ways in longer files and make sure that numbers got read the way you intended. Excel seems to sample the first 20-30 lines or so to figure out how to read them in, and if line 100 doesn't have the space, then it's going to be read in wrong.

10. The x,y data below will not be read correctly using spaces as delimiters because the x,y fields are contiguous. You must use fixed format and tell Excel where the fields are. Another common delimiter is the comma or tab.

```
File  Edit  Format  View  Help
*  ISCST3 (02035): Seal Beach Broadcast Tarp June 24-26
*  MODELING OPTIONS USED:
*    CONC                           RURAL FLAT   FLGPOL
*            PLOT FILE OF PERIOD VALUES FOR SOURCE GROUP:
*            FOR A TOTAL OF      8 RECEPTORS.
*            FORMAT: (3(1X,F13.5),1X,F8.2,2X,A6,2X,A8,2X,
*         X              Y          AVERAGE CONC    ZELEV      AVE
*
       _____    _____    _____    _____
       29.4900073.57000             153.21553     0.00   PERIOD
       69.6200070.53000             394.59613     0.00   PERIOD
       72.3500031.62000             374.55792     0.00   PERIOD
       69.92000-6.99000               0.36463     0.00   PERIOD
       31.92000-9.73000               0.00141     0.00   PERIOD
       -6.99000-6.99000               0.00000     0.00   PERIOD
      -10.0300031.92000               0.00000     0.00   PERIOD
       -7.9000070.53000               0.00000     0.00   PERIOD
```

Section 07. Running ISCST3 to estimate flux for a study.

1. In this section, an ISCST3 control file is run, the estimated concentrations put into Excel, the corresponding field measurements are put into Excel and a regression is run in Excel to derive an adjustment factor which is to estimate the field flux during this period.
2. The general information comes from Johnson and Wofford (1999), which was a methyl bromide monitoring study involving 6 approximately 1-acre fields. This study is included in the studies for this course (Mebr-study.pdf) or is available at (http://www.cdpr.ca.gov/docs/emon/methbrom/mb092499.pdf).
3. This exercise focuses on the case: broadcast, Seal Beach, period 3. To review, Johnson and Wofford (1999) contain the following information needed for simulation: the field size is shown in Table 1, monitoring periods in Table 2, air monitoring results in Table 3 (note: in PPM), field monitoring locations in Figure 3. The entire ISC-ready meteorological data for Seal Beach (except for stability class) can be found in Section05\sbcisc.met. Section 05 details how to estimate stability. So, you can review how to prepare the meteorology using these materials, or just use the file SBP3.MET which has already been prepared.
4.   (Note: the pathway in the following figures differs somewhat and in an obvious way from the pathway on the handout CD and on the network where these files are stored). First, run ISCST3 for period 3.

The graphic shows the directory listing for Section07 before running ISCST3 on this period. There are four files; the control file (SBBRP3.IN), the meteorological file (SBP3.MET) and two PDF documents. The ISCST3 program is then run using sbbrp3.out as the output file in the command line. Note that you must have a flux entered into the control file in order to run ISCST3. Since we

```
M:\T\SECTION07>dir
 Volume in drive M is Data2
 Volume Serial Number is F4D9-2235

 Directory of M:\T\SECTION07

04/26/2010  10:37 AM    <DIR>          .
04/26/2010  10:37 AM    <DIR>          ..
07/22/1999  04:16 PM             1,532 SBBRP3.IN
04/26/2010  10:06 AM             1,342 SBBRP3.PLT
07/28/1999  01:56 PM               634 SBP3.MET
04/12/2010  02:43 PM           201,093 Sec07 Simple linear regression with Excel
 Data Analsis Add In.pdf
04/26/2010  10:37 AM            25,339 Section 07-using ISCST3 to estimate flux.
pdf
               5 File(s)        229,940 bytes
               2 Dir(s)  166,599,008,256 bytes free

M:\T\SECTION07>_
```

don't know what the flux is (that's what we're trying to figure out), we have entered 100 ug/m2s. The relevant control file line is

```
SO SRCPARAM   acre1    .10000000E-03    .0000    62.62        63.54
```

The first number is 0.1E-3 g/m2s as the flux. Later we will adjust this assumed flux to estimate the actual flux based on the measured concentrations.

5. (Note: for some reason the operating system appears to change the subdirectory name from SECTION07 to SEA0E0~1 after you run ISCST3. It didn't actually change the name, but this is DOS attempt at dealing with a name that is longer than 8 characters. Just mentally substitute SECTION07 for this translated name). Three new files appear in the directory after running ISCST3: ERRORS.OUT, SBBRP3.OUT and SBBRP3.PLT.

```
cmd

M:\T\SECTION07>..\iscst3 sbbrp3.in sbbrp3.out
Now Processing SETUP Information

M:\T\SEA0E0~1>dir
 Volume in drive M is Data2
 Volume Serial Number is F4D9-2235

 Directory of M:\T\SEA0E0~1

04/26/2010  10:40 AM    <DIR>          .
04/26/2010  10:40 AM    <DIR>          ..
04/26/2010  10:40 AM             1,262 ERRORS.OUT
07/22/1999  04:16 PM             1,532 SBBRP3.IN
04/26/2010  10:40 AM            20,332 SBBRP3.OUT
04/26/2010  10:06 AM             1,342 SBBRP3.PLT
07/28/1999  01:56 PM               634 SBP3.MET
04/12/2010  02:43 PM           201,093 Sec07 Simple linear regression with Excel
 Data Analsis Add In.pdf
04/26/2010  10:37 AM            25,339 Section 07-using ISCST3 to estimate flux.
pdf
               7 File(s)        251,534 bytes
               2 Dir(s)  166,598,983,680 bytes free

M:\T\SEA0E0~1>
```

We will use SBBRP3.PLT. Review *SECTION06\How to read pltfile-intoExcel.pdf*. This explains how to get the estimated concentrations from the PLT file into Excel. After reading in the modeled concentrations, delete the unnecessary columns to the right of the modeled concentrations.

6. With the modeled concentrations input into Excel, then type in the concentrations from Johnson and Wofford (1999), the methyl bromide study for period 3 of the Seal Beach broadcast study. You must BE SURE that the typed in concentrations align properly with the modeled concentrations. That is, the worksheet shows the northeast measured concentrations next to the northeast modeled concentrations and so on for each of the 8 concentration pairs. The typed-in measured concentrations are in units of ppm and must be converted to ug/m3. Multiply the ppm values by 3880 to convert to ug/m3 (note: this conversion factor is temperature dependent). Your worksheet at this point should look something like below.

Microsoft Excel - SBBRP3.PLT

File   Edit   View   Insert   Format   Tools   Data   Window   Cell   Run   C

C13

	B	C	D	E	F	G
1	29.49	73.57	1071.34839	0.052	201.76	
2	69.62	70.53	386.97073	0.021	81.48	
3	72.35	31.62	193.96306	0.033	128.04	
4	69.92	-6.99	538.74335	0.037	143.56	
5	31.92	-9.73	277.39642	0.02	77.6	
6	-6.99	-6.99	0	nd	0	
7	-10.03	31.92	15.386	0.009	34.92	
8	-7.9	70.53	254.748	0.031	120.28	
9						
10	x coord	y coord	model conc	msrd ppm	msrd ug/m3	
11						
12						

7. Note, I have substituted 0 for the non detect in column F. The columns at this point are x and y coordinates (meters), modeled concentration (ug/m3), measured concentration (ppm), measured concentration (ug/m3).
8. Next conduct the regression of y (use the measured values in column F) against x (use the modeled values in column D).   Specific $H$1 for the location of the regression results. You can review how to perform simple linear regressions in Excel with the other document in this directory "Simple linear regression with Excel data analysis add-in.pdf". There are many cautions against using Excel for statistical analysis (see for example Pottel 2003 or McCullough and Wilson 2005 see "References" at end of this lesson). Specifically, in regard to regression, I have checked many regressions in Excel against other programs and always found that the results matched. However, Pottel (2003) presents a constructed example, in which Excel gives negative R2 values and negative sums of squares, which is a clearly impossible result. Sums of squares and R2 values should always be non-negative. Pottel's example takes advantage of the limits on numerical accuracy by using numbers like

$$10,000,000,009.000 \quad 1,000,000,000.000$$
$$10,000,000,010.000 \quad 1,000,000,000.001$$

It is unlikely that you will encounter numbers like this in performing regressions to analyze field results. For one thing, measured air concentrations are probably never reliable beyond 3 decimal places. Specifically, with regard to regression, McCullough and Wilson have a long history of looking at statistical problems with Excel and references can be obtained from their paper. McCullough and Wilson in the listed study concluded that Excel 2003 performance on linear regression was acceptable. However, they strongly discourage use of Excel for non-linear regression. If you contemplate conducting statistical analysis for areas other than simple linear regression, it would be prudent to look for a program besides Excel or familiarize yourself with the literature on Excel's statistical problems. And, as always, you should always check results to make sure that they seem reasonable (negative R2 values are not reasonable).

9. After doing the regression, your worksheet should look something like the one below.
The regression is significant at p=0.005641158 (extra decimal places so you can locate exactly which cell I'm referring to). The multiplicative coefficient was 0.160168 (extra decimals places so you can locate exactly what I'm referring to).

E	F	G	H	I	J	K	L	M	N	O	P	Q
0.052	201.76		SUMMARY OUTPUT									
0.021	81.48											
0.033	128.04		*Regression Statistics*									
0.037	143.56		Multiple R	0.864195								
0.02	77.6		R Square	0.746833								
	0		Adjusted R Square	0.704639								
0.009	34.92		Standard Error	34.68447								
0.031	120.28		Observations	8								
d ppm	msrd ug/m3		ANOVA									
				df	*SS*	*MS*	*F*	*Significance F*				
			Regression	1	21293.08	21293.08	17.6998	0.005641158				
			Residual	6	7218.073	1203.012						
			Total	7	28511.15							
				Coefficients	*Standard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*	
			Intercept	43.6265	17.89464	2.437964	0.050612	-0.1601161	87.41311	-0.16012	87.41311	
			X Variable 1	0.160168	0.038071	4.207113	0.005641	0.067012051	0.253323	0.067012	0.253323	

10. The simulation used 100 ug/m2s as the nominal flux. Since flux and concentration are proportional, we multiply the 100 ug/m2s by 0.16 (the multiplicative constant) and estimate the flux for this third measurement period as 16ug/m2s.

$$estimated\ flux = 100ug/m^2s * 0.16 = 16ug/m^2s$$

11. Check this result against the corresponding result in Table 7 of the methyl bromide study. The 1999 study shows the estimated flux was 16 ug/m2s, the R2 was 75% and the significance level as a percentage was 0.52, which differs slightly from the analysis above which shows 0.56%

Table 7. Summary of Regression Calculations Used t

Seal Beach

Broadcast	Flux Estimate (ug/m2s)	R2 (%)	p (%)
1	21	85	0.12
2	70	78	0.36
3	16	75	0.52
4	44	78	0.36
5	23	89	0.05

12. The other periods and other treatments in this study were analyzed similarly. This example, as with five periods in the Seal Beach broadcast treatment resulted in statistically significant regressions. When the regression is not significant, other procedures may be used. The workbook outlines some of these procedures.

References for Section 07 – using ISCST3 to estimate flux.doc

Johnson, Bruce and Pam Wofford. 1999. Memorandum to John Sanders on Monitoring results from a comparison test of bedded tarped application equipment dated September 24, 1999. http://www.cdpr.ca.gov/docs/emon/methbrom/mb092499.pdf

McCullough, B.D. and Berry Wilson. 2005. On the accuracy of statistical procedures in Microsoft Excel 2003. Computational Statistics and Data Analysis 49:1244-1252.

Pottel, Hans. 2003 (inferred). Statistical flaws in excel. http://www.mis.coventry.ac.uk/~nhunt/pottel.pdf

Section 07 Simple linear regression with Excel Data Analysis Add In.

1. This discussion starts with an excel spreadsheet that has 2 adjacent columns of numbers with the same number of values in each column.

2. Click on Tools. You should see a choice "Data Analysis" near the bottom. If you don't see "Data Analysis" as a choice, then you must install the Data Analysis Add Ins and until you do, you will be unable to execute the remainder of this lesson.
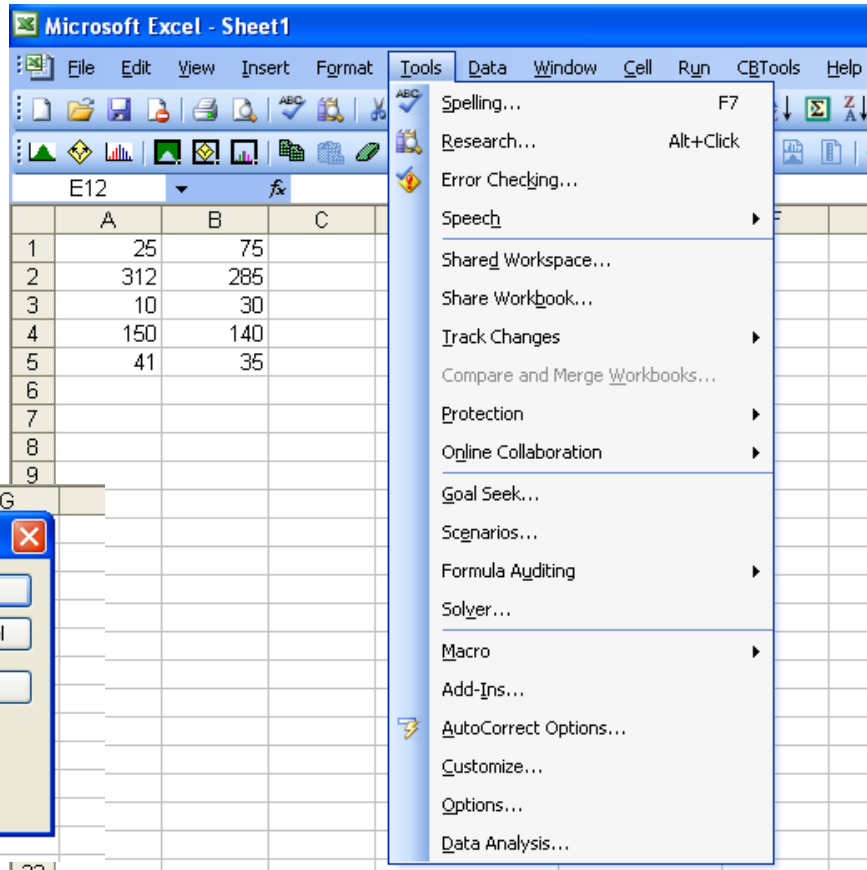
3. Click on Data Analysis. Scroll down to Regression and click on it to highlight it. Then click OK.
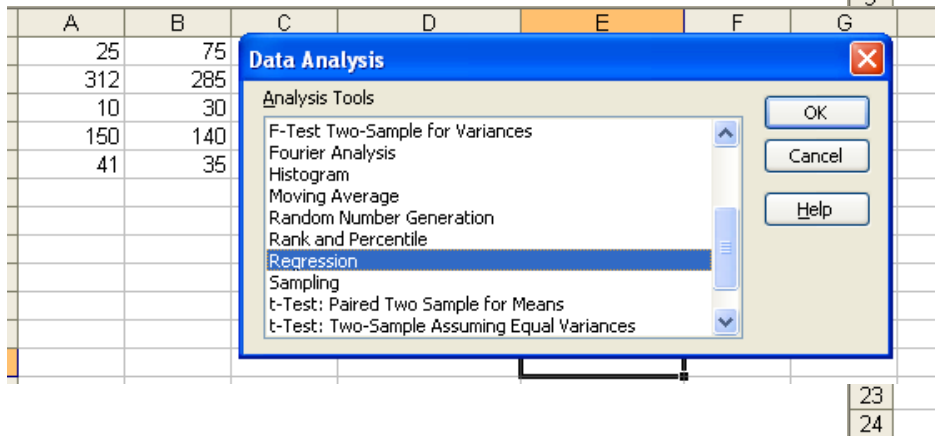
4. Click on the white entry field for "Input Y Range" so that the blinking cursor is in that field. Then using the mouse, highlight B1:B5 (this example has 5 data items and A1:A5 are the x values and B1:B5 are the y values for the equation y=mx+b). This procedure should put $B$1:$B$5 into this Input Y Range field.

5. Similarly, click in the Input X Range field, then highlight the five values in Column A. This should result in $A$1:$A$5 going into the Input X Range field.
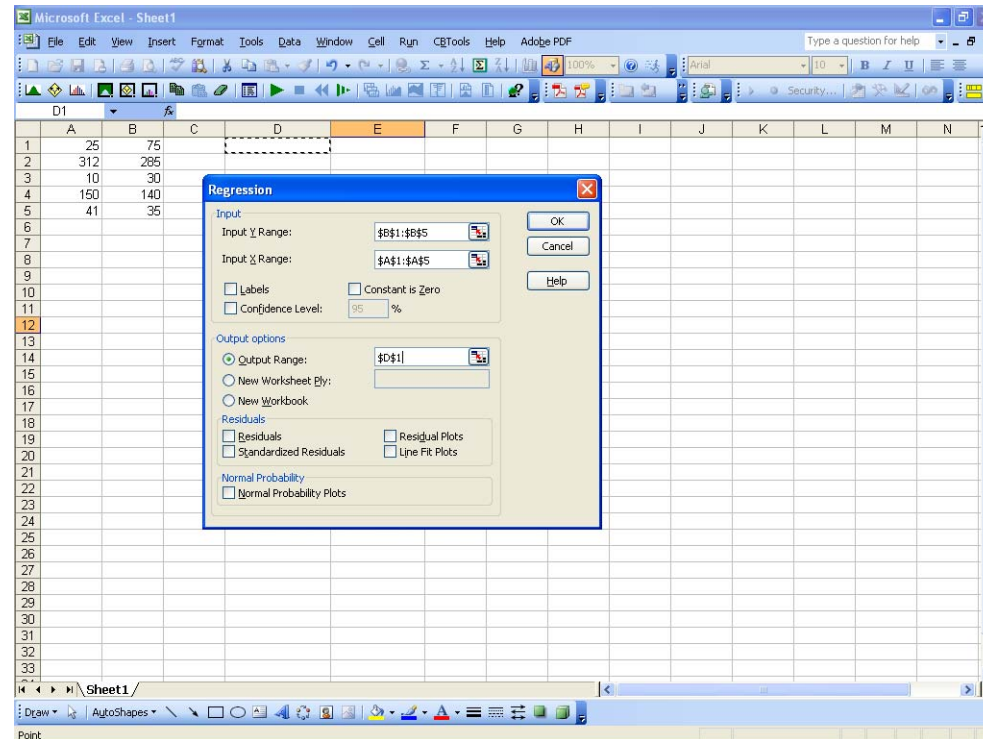
6. At this point, you can click OK and Excel will, by default, create the regression output on a new worksheet. If you want the regression output on this same page as the data, you must do a little extra. Click on the button "Output Range" in order to put the green check there. PAY ATTENTION: Excel will cutely place the blinking cursor back into the Input Y Range and if you click on a cell in the worksheet, you will wipe out the $A$1:$A$5 and will have to reenter it. So, after clicking on "Output Range" button, then click into the empty field for Output Range, THEN click on the cell D1, say.
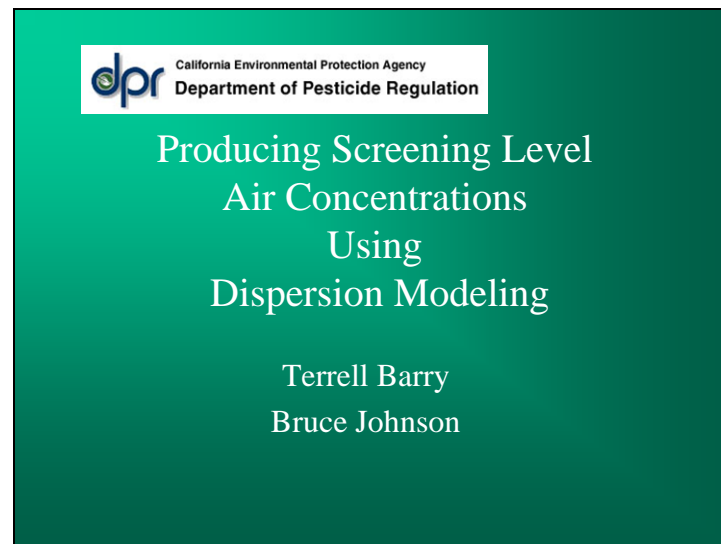
7. You can now click on OK and you will get regression results which start at the cell D1 and generally go down and across to the right.

	A	B	C	D	E	F	G	H	I	J	K	L
1	25	75		SUMMARY OUTPUT								
2	312	285										
3	10	30		Regression Statistics								
4	150	140		Multiple R	0.982869074							
5	41	35		R Square	0.966031617							
6				Adjusted R Square	0.954708822							
7				Standard Error	22.50485719							
8				Observations	5							
9												
10				ANOVA								
11					df	SS	MS	F	ignificance F			
12				Regression	1	43210.59	43210.59	85.31742	0.002685			
13				Residual	3	1519.406	506.4686					
14				Total	4	44730						
15												
16					Coefficients	tandard Err	t Stat	P-value	Lower 95%	Upper 95%	ower 95.0%	pper 95.0%
17				Intercept	24.8351802	13.87087	1.790456	0.171311	-19.3081	68.97847	-19.3081	68.97847
18				X Variable 1	0.819375649	0.088708	9.236743	0.002685	0.537066	1.101685	0.537066	1.101685
19												
20												
21												
22												

8. The slope in this example was 0.82 and it was statistically significant at the <5% level The regression was significant at p=0.002685 and the 95% confidence interval for the slope did NOT include 0. The corresponding values for the intercept suggested that the intercept was not significant (p>.05, in fact p=0.171311).

Section 08 Producing Screening Level Air Concentrations using Dispersion Modeling

Slide 1

Slide 2

dpr

Overview

- ISCST3 uses a steady-state Gaussian plume dispersion equation to estimate downwind air concentrations
- For fixed meteorological conditions, the Gaussian plume algorithm produces downwind air concentrations that are directly proportional to the emission rate (flux) of a pollutant.
- DPR assumes that flux is directly proportional to the application rate
- The resulting proportional linkage between application rate and concentration simplifies calculations under fixed meteorological conditions.

2

Slide 3

dpr

Methods

- The ISCST3 model can be used in three distinct ways:

  - (1) the screening mode
  - (2) the PERFUMmodel
  - (3) the FEMS model

3

Slide 4

Slide 5

Slide 6

Temperature, wind speed, and other meteorological conditions (e.g., stability class).

Slide 7

dpr

Generic Components

- The generic ISCST3 simulation results consist
- of downwind air concentration estimates
  generated using :
  - fixed meteorological conditions
  - a nominal flux of 100 ug/m2s.

- Sets of generic concentration estimates are
  produced for different acreages and
  meteorological condition combinations.

7

Slide 8

Slide 9

Slide 10

Slide 11

Flux Estimates from Field Studies

- The relationship between the flux profile averaging times and the time of day should be preserved in the process of adjusting the generic centerline concentrations
  - a day flux is used only with the day conditions centerline
  - a night flux is used only with the night conditions centerline
- In cases of averaging intervals that span sunrise or sunset, both day and night air concentration estimates are calculated

Slide 12

Slide 13

Slide 14

Slide 15

Estimated Iodomethane Air Concentrations

- Three averaging times were requested by WHS for the DPR iodomethane exposure appraisal
  – (24, 8, and 1 hr)
- flux estimates for the three averaging times were obtained from each study flux profile
- The highest flux values were obtained using the study flux profiles and a rolling average method where necessary

15

Slide 16

Table 2. Flux estimates for iodomethane studies used to estimate off-site air concentrations. With the exception of LaSelva Beach, the 8 hr and 1 hr scenarios both exhibited the highest flux and highest air concentrations during the day. Both day and night air concentrations were provided for the LaSelva Beach study (See Appendix A). The remainder of the studies focused on the day scenario.

Study Location	Application Method	Study Application Rate[a]	Study Effective Broadcast Application Rate	24 hr flux (ug/m²sec) (hrs)[b]	8 hr flux (day) (ug/m²sec) (hrs)	1 hr flux (day) (ug/m²sec) (hrs)
Watsonville, California	Broadcast/ Tarp	252	252	120.9 (22.0)[b]	234.2 (8.1)	N/A[c]
Manteca, California	Broadcast/ Tarp	242	242	160.2 (19.0)	313.7 (8.0)	481.0 (3.3)
Oxnard, California	Bed/Tarp	244	171	186.4 (18.9)	265.6 (8.2)	535.0 (2.6)
Guadalupe, California	Bed/Tarp	179	143	117.7 (21.0)	153.1 (7.0)	171.4 (3.0)
LaSelva Beach, California	Drip/Tarp	235	162	87.6 (19.0)	187.5 (7.0)	198.0 (3.0)
Camarillo, California	Drip/Tarp	175	119	81.4 (22.0)	153.4 (8.0)	242.1 (4.0)
Guadalupe, California	Drip/Tarp	174	139	131.1 (23.0)	296.1 (7.0)	429.8 (3.0)

a. This application rate is the "treated acre" rate. For broadcast application methods the Study Application Rate and the Study Effective Broadcast Application Rate will be the same. For bed type applications an adjustment must be made to the Study Application Rate to account for the portions of the field that are untreated. See the text for details of the calculation.
b. The number in parentheses is the sampling interval duration in hrs.
c. It was not possible to estimate a 1 hr flux for this study.

16

Slide 17

Slide 18

Supplementary Material

Answer to Problem 6A

X	Y	6A (UG/M3)	6B (UG/M3)
29.49	73.57	47.4521	94.90419
69.62	70.53	67.14664	134.2933
72.35	31.62	109.5967	219.1934
69.92	-6.99	126.6627	253.3255
31.92	-9.73	198.6105	397.221
-6.99	-6.99	28.80057	57.60115
-10.03	31.92	52.53577	105.0716
-7.9	70.53	0.59658	1.19316

Answer to Problem 6A.

SUMMARY OUTPUT

Regression Statistics

Multiple R	1
R Square	1
Adjusted R	1
Standard E	7.26E-06
Observatio	8

ANOVA

	df	SS	MS	F	ignificance F
Regression	1	112070.9	112070.9	2.13E+15	7.02E-45
Residual	6	3.16E-10	5.27E-11		
Total	7	112070.9			

	Coefficient	andard Err	t Stat	P-value	Lower 95%	Upper 95%	ower 95.0%	pper 95.0%
Intercept	2.27E-06	4.28E-06	0.5306	0.614751	-8.2E-06	1.27E-05	-8.2E-06	1.27E-05
X Variable	2	4.34E-08	46110187	7.02E-45	2	2	2	2
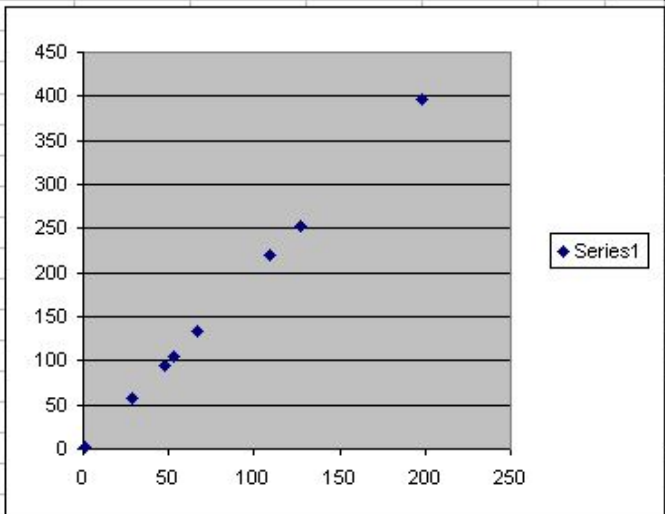
The relationship between the two sets of concentrations is that doubling the flux has doubled the concentrations. The regression results show that this is nearly perfect relationship. This is because the gaussian equation basically maintains a proportional relationship between concentration and flux (C=QK, where K is a large complicated expression which is fixed by the geometry and meteorology for that hour.)

Answer to Problem 6X

measured	values		prob6x	location			Measured values found in PROB6X.MEA		
location	ug/m3			x	y		msrd	modeled	the modeled values from PROB6X.PLT file
n	49			29.49	73.57		49.00	197.5383	
ne	61.4			69.62	70.53		61.40	28.79613	
e	99			72.35	31.62		99.00	52.99294	
se	130.4			69.92	-6.99		130.40	0.58752	
s	210			31.92	-9.73		210.00	49.68333	
sw	20.8			-6.99	-6.99		20.80	67.17444	
w	55			-10.03	31.92		55.00	106.9111	
nw	nd			-7.9	70.53		0.00	121.2408	

When you plot the measured vs modeled
values, they seem to be inversely related.
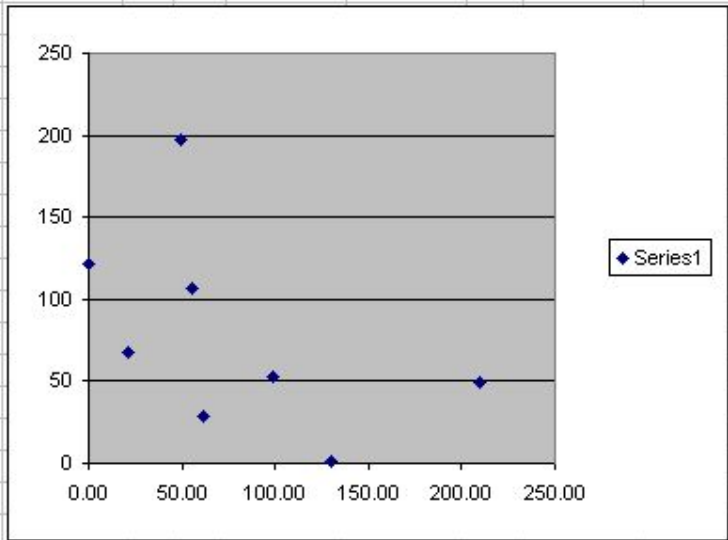
Scatter plot: measured (y-axis, 0–250) vs modeled (x-axis, 0.00–250.00), Series1.

Answer to Problem 6X:

wind directions from prob6x.met file with hour

strongest and most persistent direction is to the northwest, but NW measured value is 0 and highest msrd value is 210 to the south — 2nd highest 130 to SE — hypothesis: wind directions are off by 180°!

Example 07, Seal Beach Period 3, Broadcast, regression of measured vs. modeled to estimate flux.

x coord	y coord	model conc	msrd ppb	msrd ug/m3					
29.49	73.57	1071.34839	0.052	201.76	SUMMARY OUTPUT				
69.62	70.53	386.97073	0.021	81.48					
72.35	31.62	193.96306	0.033	128.04	Regression Statistics				
69.92	-6.99	538.74335	0.037	143.56	Multiple R	0.864195			
31.92	-9.73	277.39642	0.02	77.6	R Square	0.746833			
-6.99	-6.99	0	nd	0	Adjusted R Square	0.704639			
-10.03	31.92	15.386	0.009	34.92	Standard Error	34.68447			
-7.9	70.53	254.748	0.031	120.28	Observations	8			

ANOVA

	df	SS	MS	F	Significance F
Regression	1	21293.08	21293.08	17.6998	0.005641158
Residual	6	7218.073	1203.012		
Total	7	28511.15			

	Coefficients	Standard Err	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	43.6265	17.89464	2.437964	0.050612	-0.1601161	87.41311	-0.16012	87.41311
X Variable 1	0.160168	0.038071	4.207113	0.005641	0.067012051	0.253323	0.067012	0.253323

Pre-class reading material: atmospheric stability concepts

Please take 15 minutes to look at the following two articles:

1. Wikipedia article on Air Pollution Dispersion Terminology and the related link on rising air parcels and stability.

http://en.wikipedia.org/wiki/Air_pollution_dispersion_terminology

In particular
- study the vertical and horizontal pollution concentration profiles in the figure (normal distribution)
- read the paragraph on the Gaussian model (the link mainly discusses elevated point sources, whereas we will focus more on ground-level area sources)
- read the paragraph on Air Pollution Emission Sources and understand the difference between area, point, line and volume sources
- read the section "Characterization of Atmospheric Turbulence" and "The Pasquill atmospheric stability classes"
- read about inversion layers and mixing height

2. Look at the three diagrams of rising air parcels versus the environmental and adiabatic lapse rates and try to understand why some conditions are called stable and some conditions are called unstable at the following URL:

http://www.ux1.eiu.edu/~jpstimac/1400/stability.html

Coarse grid template file (specifying gridded set of receptors)

```
CO STARTING
CO TITLEONE Seal Beach Broadcast Tarp June 24-26 1999
CO MODELOPT CONC    RURAL          NOSTD  NOBID  NOCALM
CO AVERTIME  period
CO POLLUTID OTHER
CO DCAYCOEF    .000000
CO RUNORNOT RUN
CO ERRORFIL ERRORS.OUT
CO FLAGPOLE 1.2
CO FINISHED


SO STARTING

** Source Location Cards:
**           SRCID SRCTYP        XS              YS              ZS

SO LOCATION    acre1 AREA        0.00          0.00          .0000

** Source Parameter Cards:
** POINT:   SRCID        QS              HS        TS        VS        DS
** VOLUME:  SRCID        QS              HS        SYINIT    SZINIT
** AREA:    SRCID        QS              HS        XINIT     YINIT

SO SRCPARAM  acre1    .03120000E-03    .0000    62.62      63.54

SO EMISUNIT    .100000E+07 (GRAMS/SEC)        (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED
```

```
RE STARTING
RE GRIDCART COARSE STA
RE GRIDCART COARSE XYINC -78.275 15 15.655 -79.425 15 15.885
RE GRIDCART COARSE END
RE FINISHED


ME STARTING
ME INPUTFIL SBREQ.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT   10.000 METERS
ME SURFDATA  99999  1999            SURFNAME
ME UAIRDATA  99999  1999            UAIRNAME
ME WINDCATS    1.54    3.09    5.14    8.23   10.80
ME FINISHED


OU STARTING
OU PLOTFILE PERIOD ALL SBBRREQC.PLT
OU FINISHED
```

24 hour met file used for coarse grid simulation

```
    99999       99    99999       99
99 624  9   68.6439    0.7367 292.7 2   300.0   300.0
99 62410   36.0762    3.5957 292.6 2   300.0   300.0
99 62411   49.7803    4.1236 292.9 2   300.0   300.0
99 62412   55.6602    4.5357 293.0 2   300.0   300.0
99 62413   48.5289    4.6531 294.4 2   300.0   300.0
99 62414   58.2812    5.4138 295.4 3   300.0   300.0
99 62415   60.9318    5.1967 296.2 3   300.0   300.0
99 62416   64.1872    6.1775 294.8 4   300.0   300.0
99 62417   63.9935    4.5952 294.5 3   300.0   300.0
99 62418  118.1665    3.5326 296.0 3   300.0   300.0
99 62419  132.4641    3.7558 293.4 4   300.0   300.0
99 62420  131.1457    2.8593 290.6 5   300.0   300.0
99 62421  137.8309    2.2669 289.6 6   300.0   300.0
99 62422  143.4305    2.3856 289.2 6   300.0   300.0
99 62423  146.0880    2.4971 289.0 6   300.0   300.0
99 62424  145.9636    1.0649 288.7 6   300.0   300.0
99 625  1  339.6841    0.7852 288.3 6   300.0   300.0
99 625  2   14.3680    0.7489 288.9 6   300.0   300.0
99 625  3    2.0674    0.9789 289.0 6   300.0   300.0
99 625  4  346.9866    1.2534 288.8 6   300.0   300.0
99 625  5   10.8971    1.6122 288.6 6   300.0   300.0
99 625  6    6.7638    1.4599 288.7 6   300.0   300.0
99 625  7   21.8441    1.0592 289.0 5   300.0   300.0
```

Course grid receptor plot

Grid Layout for Receptors
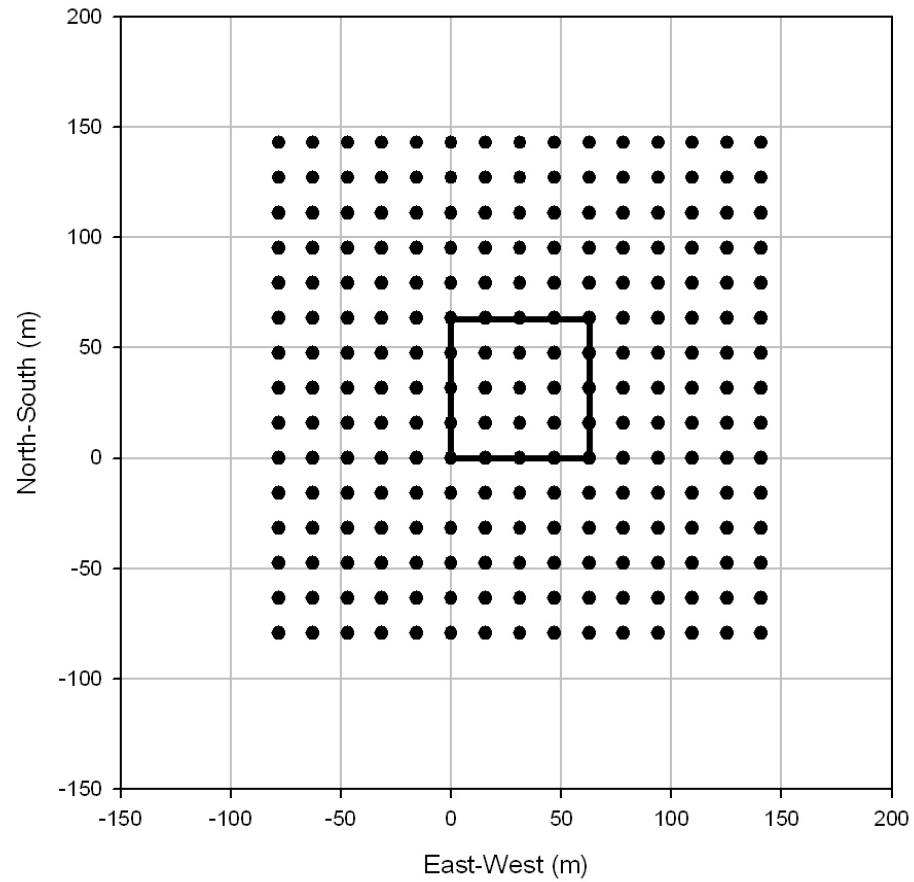
Coarse grid isopleths made from output file SBBREQC.PLT.

Seal Beach Broadcast - Reqd BZ Coarse
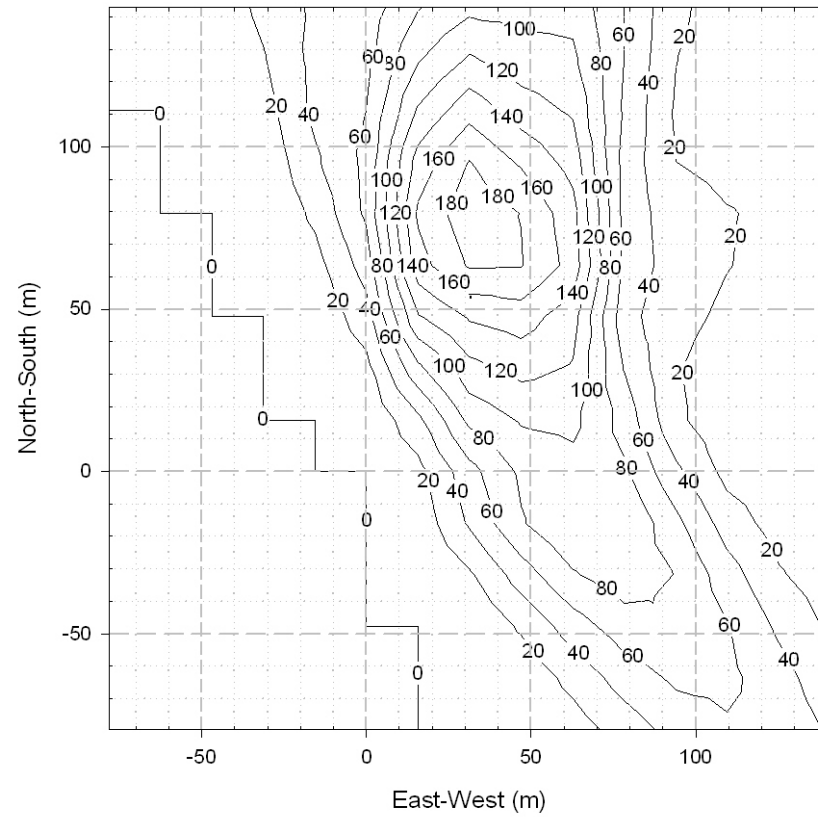
References for ISCST3 Class April 13, 2010

Barry, Terrell. 2008. SCREENING LEVEL AIR CONCENTRATION ESTIMATES FOR WORKER HEALTH AND SAFETY EXPOSURE APPRAISALS. Memorandum to Randy Segawa dated August 21, 2008.
http://www.cdpr.ca.gov/docs/emon/pubs/ehapreps/analysis_memos/
2071_segawa.pdf

Barry, Terrell. 2008. SCREENING LEVEL AIR CONCENTRATION ESTIMATES FOR WORKER HEALTH AND SAFETY EXPOSURE APPRAISALS. Memorandum to Randy Segawa dated August 21, 2008.
http://www.cdpr.ca.gov/docs/emon/pubs/ehapreps/analysis_memos/
2071_segawa.pdf

Budney, Laurence J. 1977. Guidelines for air quality maintenance planning and analysis — Volume 10 (Revised): Procedures for evaluating air quality impact of new stationary
sources. Report No. EPA-450/4-77-001. U.S. Environmental Protection Agency, Office of Air and Waste Management, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711.

Johnson, Bruce, Terrell Barry and Pamela Wofford. 1999. Workbook for gaussian modeling analysis of air concentration measurements. EH99-03. State of California, Environmental Protection Agency, Department of Pesticide Regulation, Environmental Monitoring and Pest Management Branch, Environmental Hazards Assessment Program Sacramento, California 95814-3510
http://www.cdpr.ca.gov/docs/emon/pubs/ehapreps/eh9903.pdf

Johnson, Bruce and Pam Wofford. 1999. Memorandum to John Sanders on Monitoring results from a comparison test of bedded tarped application equipment dated September 24, 1999. http://www.cdpr.ca.gov/docs/emon/methbrom/mb092499.pdf

Johnson, Bruce. 2010. Documentation for WEATHER6A.EXE. Environmental Monitoring, March 26, 2010.

USEPA. Code of Federal Regulations. 2003. APPENDIX W TO PART 51— GUIDELINE ON AIR QUALITY MODELS Pt. 51, App. W 40 CFR Ch. I (7–1–03 edition) http://www.epa.gov/scram001/guidance/guide/appw_03.pdf calms processing, from section

9.3.4 "Treatment of Near-calms and calms" page 481 states as follows: "If the total number of valid hours is less than 18 for 24-hour averages, less than 6 for 8-hour averages or less than 3 for 3-hour averages, the total concentration should be divided by 18 for the 24-hour average, 6 for the 8-hour average and 3 for the 3-hour average. For annual averages, the sum of all valid hourly concentrations is divided by the number of noncalm hours during the year."

U.S.E.P.A. 1995. User's guide for the industrial source complex (ISC3) disperson models. Volume 1 - User Instructions. EPA-454/B-95-003a. U.S. Environmental Protection Agency. Office of Air Quality Planning and Standards Emissions, Monitoring and Analysis Division Research Triangle Park, North Carolina 27711. September 1995.

U.S.E.P.A. 1995. User's guide for the industrial source complex (ISC3) disperson models. Volume 2 - Description of model algorithms. EPA-454/B-95-003b. U.S. Environmental Protection Agency. Office of Air Quality Planning and Standards Emissions, Monitoring and Analysis Division Research Triangle Park, North Carolina 27711. September 1995

Woodrow, James E., James N. Seiber, and Lynton W. Baker. 1997. Correlation techniques for estimating pesticide volatilization flux and downwind concentrations. Environ. Sci. Technol 31:523:529.

Appendix 1. Listing of the PROB6A.OUT file from problem 6.

```
CO STARTING
CO TITLEONE ISC Class Problem 6A
CO MODELOPT CONC    RURAL          NOSTD  NOBID  NOCALM
CO AVERTIME  period
CO POLLUTID OTHER
CO DCAYCOEF    .000000
CO RUNORNOT RUN
CO ERRORFIL ERRORS.OUT
CO FLAGPOLE 1.2
CO FINISHED


SO STARTING

** Source Location Cards:
**          SRCID SRCTYP         XS              YS              ZS

SO LOCATION   acre1 AREA         0.00      0.00          .0000

** Source Parameter Cards:
** POINT:   SRCID        QS           HS         TS          VS          DS
** VOLUME:  SRCID        QS           HS       SYINIT       SZINIT
** AREA:    SRCID        QS           HS        XINIT        YINIT

SO SRCPARAM  acre1   .10000000E-03      .0000    62.62       63.54

SO EMISUNIT    .100000E+07 (GRAMS/SEC)          (MICROGRAMS/CUBIC-METER)
SO SRCGROUP ALL
SO FINISHED


RE STARTING
RE DISCCART 29.49 73.57
RE DISCCART 69.62 70.53
RE DISCCART 72.35 31.62
RE DISCCART 69.92 -6.99
RE DISCCART 31.92 -9.73
RE DISCCART -6.99 -6.99
RE DISCCART -10.03 31.92
```

```
RE DISCCART -7.9 70.53
RE FINISHED


ME STARTING
ME INPUTFIL PROB6A.MET (4I2,2F9.0,F6.1,I2,2F7.1)
ME ANEMHGHT   10.000 METERS
ME SURFDATA  99999  1999            SURFNAME
ME UAIRDATA  99999  1999            UAIRNAME
ME WINDCATS    1.54    3.09    5.14    8.23   10.80
ME FINISHED


OU STARTING
OU PLOTFILE PERIOD ALL PROB6A.PLT
OU FINISHED


 *** Message Summary For ISC3 Model Setup ***

 --------- Summary of Total Messages --------

A Total of            0 Fatal Error Message(s)
A Total of            8 Warning Message(s)
A Total of            0 Informational Message(s)


   ******** FATAL ERROR MESSAGES ********
            ***  NONE  ***


   ********   WARNING MESSAGES   ********
RE W228    33 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    34 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    35 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    36 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    37 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    38 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    39 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    40 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART

**********************************
```

```
*** SETUP Finishes Successfully ***
**********************************
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                    ***
04/08/10
                                   ***                                                         ***
14:15:12
**MODELOPTs:
PAGE   1
CONC                    RURAL FLAT  FLGPOL              NOSTD  NOBID  NOCALM


                                     ***    MODEL SETUP OPTIONS SUMMARY     ***
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
- - -


**Intermediate Terrain Processing is Selected

**Model Is Setup For Calculation of Average CONCentration Values.

  -- SCAVENGING/DEPOSITION LOGIC --
**Model Uses NO DRY DEPLETION.  DDPLETE =  F
**Model Uses NO WET DEPLETION.  WDPLETE =  F
**NO WET SCAVENGING Data Provided.
**NO GAS DRY DEPOSITION Data Provided.
**Model Does NOT Use GRIDDED TERRAIN Data for Depletion Calculations

**Model Uses RURAL Dispersion.

**Model Uses User-Specified Options:
          1. Final Plume Rise.
          2. Not Use Stack-tip Downwash.
          3. Not Use Buoyancy-induced Dispersion.
          4. Not Use Calms Processing Routine.
          5. Not Use Missing Data Processing Routine.
          6. Default Wind Profile Exponents.
          7. Default Vertical Potential Temperature Gradients.

**Model Assumes Receptors on FLAT Terrain.

**Model Accepts FLAGPOLE Receptor Heights.

**Model Calculates PERIOD Averages Only

**This Run Includes:    1 Source(s);     1 Source Group(s); and     8 Receptor(s)
```

```
**The Model Assumes A Pollutant Type of:  OTHER

**Model Set To Continue RUNning After the Setup Testing.

**Output Options Selected:
        Model Outputs Tables of PERIOD Averages by Receptor
        Model Outputs External File(s) of High Values for Plotting (PLOTFILE Keyword)

**Misc. Inputs: Anem. Hgt. (m) =    10.00 ;   Decay Coef. =    0.000     ;   Rot. Angle =     0.0
                Emission Units = (GRAMS/SEC)                      ; Emission Rate Unit Factor =   0.10000E+07
                Output Units   = (MICROGRAMS/CUBIC-METER)

**Approximate Storage Requirements of Model =    1.2 MB of RAM.

**Input Runstream File:        PROB6A.IN
**Output Print File:           PROB6A.OUT
**Detailed Error/Message File:  ERRORS.OUT
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                      ***        04/08/10
                                   ***                                                          ***        14:15:12
**MODELOPTs:                                                                                               PAGE   2
CONC                      RURAL FLAT  FLGPOL              NOSTD  NOBID  NOCALM
```

```
                                            *** AREA SOURCE DATA ***

                 NUMBER EMISSION RATE  COORD (SW CORNER)  BASE     RELEASE  X-DIM    Y-DIM    ORIENT.  INIT.   EMISSION RATE
        SOURCE   PART.  (USER UNITS       X        Y      ELEV.    HEIGHT   OF AREA  OF AREA  OF AREA  SZ      SCALAR VARY
          ID     CATS.   /METER**2)    (METERS) (METERS) (METERS) (METERS) (METERS) (METERS) (DEG.)   (METERS)    BY
     - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

       ACRE1       0   0.10000E-03      0.0      0.0      0.0      0.00     62.62    63.54    0.00     0.00
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                                       ***
04/08/10
                                        ***                                                                       ***
14:15:12
**MODELOPTs:
PAGE   3
CONC                      RURAL FLAT  FLGPOL              NOSTD  NOBID  NOCALM


                                   *** SOURCE IDs DEFINING SOURCE GROUPS ***

GROUP ID                                              SOURCE IDs


 ALL        ACRE1    ,
```

```
 *** ISCST3 - VERSION 02035 ***     *** ISC Class Problem 6A                                                    ***
04/08/10
                                   ***                                                                          ***
14:15:12
**MODELOPTs:
PAGE   4
CONC                        RURAL FLAT  FLGPOL                    NOSTD  NOBID  NOCALM


                                     *** DISCRETE CARTESIAN RECEPTORS ***
                                        (X-COORD, Y-COORD, ZELEV, ZFLAG)
                                                  (METERS)

      (     29.5,      73.6,      0.0,      1.2);          (     69.6,      70.5,      0.0,      1.2);
      (     72.3,      31.6,      0.0,      1.2);          (     69.9,      -7.0,      0.0,      1.2);
      (     31.9,      -9.7,      0.0,      1.2);          (     -7.0,      -7.0,      0.0,      1.2);
      (    -10.0,      31.9,      0.0,      1.2);          (     -7.9,      70.5,      0.0,      1.2);
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                          ***
04/08/10
                                    ***                                                              ***
14:15:12
**MODELOPTs:
PAGE   5
CONC                       RURAL FLAT  FLGPOL                NOSTD  NOBID  NOCALM
```

```
                        *** METEOROLOGICAL DAYS SELECTED FOR PROCESSING ***
                                      (1=YES; 0=NO)


      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 1 1   1 1 1 1 1 1

         NOTE:  METEOROLOGICAL DATA ACTUALLY PROCESSED WILL ALSO DEPEND ON WHAT IS INCLUDED IN THE DATA FILE.



                        *** UPPER BOUND OF FIRST THROUGH FIFTH WIND SPEED CATEGORIES ***
                                              (METERS/SEC)

                          1.54,   3.09,   5.14,   8.23,  10.80,


                                    *** WIND PROFILE EXPONENTS ***



            STABILITY                          WIND SPEED CATEGORY
            CATEGORY          1            2            3            4            5            6
               A          .70000E-01   .70000E-01   .70000E-01   .70000E-01   .70000E-01   .70000E-01
               B          .70000E-01   .70000E-01   .70000E-01   .70000E-01   .70000E-01   .70000E-01
               C          .10000E+00   .10000E+00   .10000E+00   .10000E+00   .10000E+00   .10000E+00
               D          .15000E+00   .15000E+00   .15000E+00   .15000E+00   .15000E+00   .15000E+00
               E          .35000E+00   .35000E+00   .35000E+00   .35000E+00   .35000E+00   .35000E+00
               F          .55000E+00   .55000E+00   .55000E+00   .55000E+00   .55000E+00   .55000E+00
```

```
                *** VERTICAL POTENTIAL TEMPERATURE GRADIENTS ***
                          (DEGREES KELVIN PER METER)


STABILITY                         WIND SPEED CATEGORY
CATEGORY          1              2              3              4              5              6
    A         .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00
    B         .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00
    C         .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00
    D         .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00     .00000E+00
    E         .20000E-01     .20000E-01     .20000E-01     .20000E-01     .20000E-01     .20000E-01
    F         .35000E-01     .35000E-01     .35000E-01     .35000E-01     .35000E-01     .35000E-01
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                      ***
04/08/10
                                      ***                                                        ***
14:15:12
**MODELOPTs:
PAGE   6
CONC                     RURAL FLAT  FLGPOL              NOSTD  NOBID  NOCALM


                *** THE FIRST   5 HOURS OF METEOROLOGICAL DATA ***

       FILE:   PROB6A.MET
       FORMAT: (4I2,2F9.0,F6.1,I2,2F7.1)
       SURFACE STATION NO.:  99999               UPPER AIR STATION NO.:  99999
                    NAME: SURFNAME                             NAME: UAIRNAME
                    YEAR:  1999                                YEAR:  1999

              FLOW   SPEED  TEMP  STAB  MIXING HEIGHT (M)  USTAR  M-O LENGTH   Z-0  IPCODE PRATE
YR MN DY HR VECTOR   (M/S)  (K)  CLASS   RURAL   URBAN     (M/S)    (M)        (M)        (mm/HR)
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
- - - - - -

99 06 24 09  168.6   1.74  292.7   2    300.0   300.0   0.0000      0.0  0.0000   0   0.00
99 06 24 10   36.1   3.60  292.6   2    300.0   300.0   0.0000      0.0  0.0000   0   0.00
99 06 24 11  149.8   4.12  292.9   2    300.0   300.0   0.0000      0.0  0.0000   0   0.00
99 06 24 12  255.7   4.54  293.0   2    300.0   300.0   0.0000      0.0  0.0000   0   0.00
99 06 24 13  101.5   4.65  294.4   2    300.0   300.0   0.0000      0.0  0.0000   0   0.00


*** NOTES:  STABILITY CLASS 1=A, 2=B, 3=C, 4=D, 5=E AND 6=F.
            FLOW VECTOR IS DIRECTION TOWARD WHICH WIND IS BLOWING.
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                              ***
04/08/10
                                    ***                                                                   ***
14:15:12
**MODELOPTs:
PAGE   7
CONC                    RURAL FLAT  FLGPOL              NOSTD  NOBID  NOCALM

                        *** THE PERIOD (    5 HRS) AVERAGE CONCENTRATION   VALUES FOR SOURCE GROUP: ALL     ***
                           INCLUDING SOURCE(S):       ACRE1   ,

                                *** DISCRETE CARTESIAN RECEPTOR POINTS ***

                              ** CONC OF OTHER    IN (MICROGRAMS/CUBIC-METER)           **

       X-COORD (M)   Y-COORD (M)      CONC                   X-COORD (M)   Y-COORD (M)      CONC
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
- - - - -
            29.49        73.57      47.45210                     69.62        70.53      67.14664
            72.35        31.62     109.59670                     69.92        -6.99     126.66274
            31.92        -9.73     198.61050                     -6.99        -6.99      28.80057
           -10.03        31.92      52.53577                     -7.90        70.53       0.59658
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                        ***
04/08/10
                                   ***                                                             ***
14:15:12
**MODELOPTs:
PAGE   8
CONC                    RURAL FLAT  FLGPOL            NOSTD  NOBID  NOCALM

                              *** THE SUMMARY OF MAXIMUM PERIOD (     5 HRS) RESULTS ***


                              ** CONC OF OTHER    IN (MICROGRAMS/CUBIC-METER)              **

                                                                                     NETWORK
GROUP ID                     AVERAGE CONC         RECEPTOR  (XR, YR, ZELEV, ZFLAG)   OF TYPE  GRID-ID
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

ALL      1ST HIGHEST VALUE IS     198.61050 AT (      31.92,      -9.73,      0.00,      1.20) DC   NA
         2ND HIGHEST VALUE IS     126.66274 AT (      69.92,      -6.99,      0.00,      1.20) DC   NA
         3RD HIGHEST VALUE IS     109.59670 AT (      72.35,      31.62,      0.00,      1.20) DC   NA
         4TH HIGHEST VALUE IS      67.14664 AT (      69.62,      70.53,      0.00,      1.20) DC   NA
         5TH HIGHEST VALUE IS      52.53577 AT (     -10.03,      31.92,      0.00,      1.20) DC   NA
         6TH HIGHEST VALUE IS      47.45210 AT (      29.49,      73.57,      0.00,      1.20) DC   NA
         7TH HIGHEST VALUE IS      28.80057 AT (      -6.99,      -6.99,      0.00,      1.20) DC   NA
         8TH HIGHEST VALUE IS       0.59658 AT (      -7.90,      70.53,      0.00,      1.20) DC   NA
         9TH HIGHEST VALUE IS       0.00000 AT (       0.00,       0.00,      0.00,      0.00)
        10TH HIGHEST VALUE IS       0.00000 AT (       0.00,       0.00,      0.00,      0.00)


 *** RECEPTOR TYPES:  GC = GRIDCART
                      GP = GRIDPOLR
                      DC = DISCCART
                      DP = DISCPOLR
                      BD = BOUNDARY
```

```
 *** ISCST3 - VERSION 02035 ***    *** ISC Class Problem 6A                                      ***
04/08/10
                                    ***                                                          ***
14:15:12
**MODELOPTs:
PAGE    9
CONC                      RURAL FLAT  FLGPOL              NOSTD  NOBID  NOCALM


*** Message Summary : ISCST3 Model Execution ***

 --------- Summary of Total Messages --------

A Total of            0 Fatal Error Message(s)
A Total of            8 Warning Message(s)
A Total of            0 Informational Message(s)


   ******** FATAL ERROR MESSAGES ********
            ***  NONE  ***


   ********   WARNING MESSAGES   ********
RE W228    33 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    34 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    35 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    36 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    37 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    38 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    39 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART
RE W228    40 DISCAR:Default(s) Used for Missing Parameters on Keyword  DISCCART


   **********************************
   *** ISCST3 Finishes Successfully ***
   **********************************
```