HAZARD RESPONSE MODELING UNCERTAINTY (A QUANTITATIVE METHOD)

VOLUME I

USER'S GUIDE FOR SOFTWARE FOR EVALUATING HAZARDOUS GAS DISPERSION MODELS

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There are currently available many microcomputer-based hazard response models for calculating concentrations of hazardous chemicals in the atmosphere. The uncertainties associated with these models are not well-known and they have not been adequately evaluated and compared using statistical procedures where confidence limits are determined. The U.S. Air Force has a need for an objective method for evaluating these models, and this project provides a framework for performing these analyses and estimating the model uncertainties.

This volume of the final report provides a user's guide for the software that has been developed for the quantitative evaluation of the performance of hazardous gas dispersion models. The characteristics and uses of the software are described, the required components of input files are reviewed, and methods of presenting the output files are summarized.

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APPENDIX A

A. USER'S GUIDE FOR THE SIGPLOT PLOTTING PACKAGE

The SIGPLOT plotting package developed at Sigma Research Corporation is a versatile tool for producing different kinds of two-dimensional plots, such as scatter plots, graphs, box plots (sometimes called residual or whisker plots), or error bar plots. The user can specify many parameters including the number of frames per page, the aspect ratio of the frame, and the mapping of the coordinates. The graphics library routines used by SIGPLOT, together with the screen and printer drivers (described later) were originally developed by Dr. Arlindo daSilva of the University of Wisconsin at Milwaukee.

SIGPLOT requires two input files: 1) the template file that contains the control parameters which influence the appearance of the plots, and 2) the input data file that contains the data to be plotted. Tables A-1 and A-2 describe the formats of the template file and the input data file, respectively. Examples of the template file are shown in Figures A-1 and A-2 Examples of the input data file are shown in Figures A-3 and A-4.

SIGPLOT creates a Tektronix picture file that can be viewed directly on any kind of the PC graphics environments (e.g., Hercules, CGA, EGA, and VGA) using the screen driver, TEKPC. Hard copy output can also be generated from the Tektronix picture file with a printer driver. There are three printer drives, TEKEPS, TEKELQ, and PS, that are currently available. The first two drivers are used to drive an EPSON-compatible dot matrix printer, with TEKEPS for low resolution and TEKELQ for high resolution. The PS program is used to drive a PostScript printer, such as Apple LaserWriter, NEC LC-890, or TI MicroLaser PS35. It is recommended that the user have access to a PostScript printer to obtain the best results in the shortest time.

SIGPLOT requires about 200KB of memory. The other screen and printer drivers require less than 100KB of memory, except for TEKELQ, where 450KB of memory is required due to the high resolution and the use of the bitmap approach in the driver program. The SIGPLOT plotting package and the graphics library routines were written in FORTRAN. The screen and printer drivers were written in C.

TABLE A-1. THE FORMAT OF THE TEMPLATE FILE OF SIGPLOT. THE FOLLOWING KEY LETTERS ARE USED IN THE FORMAT COLUMN - FF: FREE FORMAT, C: CHARACTER, I: INTEGER, AND R: REAL.

The global control parameters are specified in the first section of the template file, lines 1 through 16.

LINE NO.	FORMAT	DESCRIPTION
1-3		Reserved for comments
4	FF/C	Name of the input data file, currently not used
5	FF/C	Name of the output Tektronix picture file, currently not used
6	FF/I	Flag for the frame aspect ratio, 1-5, 1: x:y = 1:1 2: x:y = 1:2 3: x:y = 2:1 4: x:y = 1:3 5: x:y = 3:1
7	FF/I	Number of frames per page, 1-4
8-9	A80	Title for the page (no title will be drawn if "0" appears as the first character of the line)
10	FF/C	Flag (PAXIS) for the axis along which the first column, representing the independent variable, of the data in the input data file (see Table A-2) will be plotted (x or y). PAXIS must = x if IPATTN (described below) = 4, and PAXIS must = y if IPATTN = 6
11	FF/I	Flag for mapping, 1-4, 1: linear in x, linear in y 2: linear in x, logarithmic in y 3: logarithmic in x, linear in y 4: logarithmic in x, logarithmic in y

TABLE A-1. THE FORMAT OF THE TEMPLATE FILE OF SIGPLOT. THE FOLLOWING KEY LETTERS ARE USED IN THE FORMAT COLUMN - FF: FREE FORMAT, C: CHARACTER, I: INTEGER, AND R: REAL. Continued.

LINE NO.	FORMAT	DESCRIPTION
12	FF/I	Flag (IPATTN) for plot pattern, 1-6, 1: scatter plot 2: line graph 3: scatter plot except line graph for the last variable 4: box plot 5: error bar plot 6: same as 5 but with extra labelling
13	FF/I	Flag for background, 0 or 2, 0: no background 2: gridded background
14	FF/C	Flag for system time, y or n, if y: system time will be printed out on the upper right corner of each page
15	5A1	Five point patterns for the scatter plot
16	FF/I	Flag (IEXTRA) for the plotting of extra lines, 1: x=0 will be plotted 2: y=0 will be plotted 3: x=0 and y=0 will be plotted 4: x=1 will be plotted 5: y=1 will be plotted 6: x=1 and y=1 will be plotted 7: diagonal line will be plotted 8: y=0.5 and y=2 (factor of two) will be plotted 9: x=-0.667, 0, and 0.667, and $y=4x^2/(4-x^2)$. (see text) will be plotted, else: no extra lines will be plotted. Note that IEXTRA = 9 is effective only if IPATTN = 6

TABLE A-1. THE FORMAT OF THE TEMPLATE FILE OF SIGPLOT. THE FOLLOWING KEY LETTERS ARE USED IN THE FORMAT COLUMN - FF: FREE FORMAT, C: CHARACTER, I: INTEGER, AND R: REAL. Continued.

The next section of the template file (lines 17 through 29) contains the parameters that are applicable to a frame. This section can be repeated if there are multiple frames to be plotted in a print job. However, the user can prepare just one such section if the same information is to be used repeatedly by all frames.

LINE NO.	FORMAT	DESCRIPTION
17-19		Reserved for comments
20	FF/R	Constants, a and b, for the linear transformation of the independent variable, where $x_{new} = a*x_{old} + b$, a=1 and b=0 means no transformation is needed
21	FF/R	Constants, a and b, for the linear transformation of the first dependent variable, where $y_{1,new} = a*y_{1,old} + b$, a=1 and b=0 means no transformation is needed
22	FF/R	Same as above, but for the second dependent variable
23	FF/R	Same as above, but for the third dependent variable
24	FF/R	Same as above, but for the fourth dependent variable

TABLE A-1. THE FORMAT OF THE TEMPLATE FILE OF SIGPLOT. THE FOLLOWING KEY LETTERS ARE USED IN THE FORMAT COLUMN - FF: FREE FORMAT, C: CHARACTER, I: INTEGER, AND R: REAL. Concluded.

LINE NO.	FORMAT	DESCRIPTION
25	FF/R	Same as above, but for the fifth dependent variable. Note that lines 22 through 25 cannot be omitted even if only one group of data were to be plotted
26	FF/R	xmin, xmax, and dx of the x-axis
27	FF/R	ymin, ymax, and dy of the y-axis
28	FF/C	Format specifier for the numerical labels of the x-axis. If "!" appears as the first character of the line, the appropriate format will be determined internally by the program; otherwise, the user should supply a simple FORTRAN I-, F-, or E-format specifier, enclosed in parentheses, e.g., (I5), (F6.3), and (E8.1) are accepted, but (3I5), (I5,f6.3), (1P,E8.1), and (G9.1) are not accepted
29	FF/C	Format specifier for the numerical labels of the y-axis

TABLE A-2. THE FORMAT OF THE INPUT DATA FILE OF SIGPLOT. THE FOLLOWING KEY LETTERS ARE USED IN THE FORMAT COLUMN - FF: FREE FORMAT, C: CHARACTER, I: INTEGER, AND R: REAL.

LINE NO.	FORMAT	DESCRIPTION
1	A40	Title for the frame (no title will be drawn if "0" appears as the first character of the line)
2	A40	Label for the x-axis (no label will be drawn if "0" appears as the first character of the line)
3	A40	Label for the y-axis (no label will be drawn if "0" appears as the first character of the line)
4	FF/I	Two integers specifying the number of points (NPTS) and the number of groups of data (MANY) to be plotted. MANY cannot be > 5 for IPATTN = 1, 2, 3, and 5, and MANY must be = 1 for IPATTN = 4 and 6. NPTS cannot be > 700 for IPATTN = 1, 2, and 3. NPTS cannot be > 50 for IPATTN = 4, 5, and 6 (see text).
Next NPTS lines:		
For IPATTN = 1, 2, and 3,		
	FF/R	There are 1+MANY real numbers in each line. The first number represents the independent variable, which can be plotted either along the x- or the y-axis depending the value of PAXIS (see Table A-1). The next MANY numbers represent the dependent variables. For example, if three curves (MANY=3), $f_1(x)$, $f_2(x)$, and $f_3(x)$ were to be plotted, then each line here should contain four real numbers, x_i, $f_{1,i}$ $f_{2,i}$, and $f_{3,i}$, where i=1, NPTS. If PAXIS = "x", the x will be plotted along the abscissa, and f_1, f_2, and f_3 will be plotted along the ordinate; vice versa PAXIS = "y".

TABLE A-2. THE FORMAT OF THE INPUT DATA FILE OF SIGPLOT. THE FOLLOWING KEY LETTERS ARE USED IN THE FORMAT COLUMN - FF: FREE FORMAT, C: CHARACTER, I: INTEGER, AND R: REAL. Continued.

LINE NO.	FORMAT	DESCRIPTION
For IPATTN = 4,		
	FF/R, I	There are six real numbers and one integer in each line. The first real number represents the independent variable. The next five real numbers represent the values of the dependent variable at the 2th, 16th, 50th, 84th, and 98th percentiles, respectively. Note that the value of the independent variable listed here frequently represents a range of the independent variable; for example, a wind speed of 7 m/s actually represents wind speeds in the range of 6 to 8 m/s. The integer represents the number of data points based on which the distribution of the dependent variable is derived. No box will be plotted if the number of data points is less than five since not enough information is available to define a distribution.
For IPATTN = 5,		
	FF/R	There are 1+3*MANY real numbers in each line. The first number represents the independent variable. The remaining numbers for the dependent variables are in MANY groups of three numbers. The three numbers, which must be in order, represent the distribution of a dependent variable. This distribution can be 1) $\mu-\sigma$, μ, and $\mu+\sigma$, where μ is the mean, and σ is the standard deviation, or 2) lower c.l., nominal value, and upper c.l., where c.l. is the confidence limit.

TABLE A-2. THE FORMAT OF THE INPUT DATA FILE OF SIGPLOT. THE FOLLOWING KEY LETTERS ARE USED IN THE FORMAT COLUMN - FF: FREE FORMAT, C: CHARACTER, I: INTEGER, AND R: REAL. Concluded

LINE NO.	FORMAT	DESCRIPTION
For IPATTN = 6,		
	FF/R,C	There are four real numbers and one character constant (no more than 17 characters long) in each line. The definition of the first four real numbers is identical to that when IPATTN = 5, except now MANY must = 1. The character constant, enclosed in apostrophes, is used to label each data point.

The above 4+NPTS lines provide enough information to plot a frame. Additional data, similar in structure, can be appended here if the plotting of more than one frames in a print job is desired.

```
!-------------------------------------------------------------------------
!      Main switches for plotting.
!--------0---------0---------0---------0-------------------------------
urrs.1    Name of input data file.
tek1.pic  Name of output tektronix file.
1         Aspect ratio (integer, 1 - 5).
1         Number of plots per page (integer, 1 - 4).
demo of ipattn=2
0
x         Which axis serves as independent variable (x or y).
1         Flag indicating log or linear mapping (1 - 4).
2         Pattern.
0         Background specification.
y         Print out system time on the upper right hand corner (y or n).
.+o$$     Patterns of scatter plots (5a1)
0   Extra line,1:x=0,2:y=0,3:x,y=0,4:x=1,5:y=1,6:x,y=1,7:diag,8:y=fac. 2.,9:fb-nmse, else:nothing.
!-------------------------------------------------------------------------
!      Parameters for plot 1.
!-------------------------------------------------------------------------
1. 0.     ascale, bscale for the independent variable axis.
1. 0.     ascale, bscale for curve 1.
1. 0.     ascale, bscale for curve 2.
1. 0.     ascale, bscale for curve 3.
1. 0.     ascale, bscale for curve 4.
1. 0.     ascale, bscale for curve 5.
-6.28319 6.28319 3.141595  xmin, xmax, and dx for the x axis.
-1.2 1.2 0.3 ymin, ymax, and dy for the y axis.
(f5.2)          format for x label
(f4.1)        format for y label
```

Figure A-1. An example of the template file of SIGPLOT. Refer to Figure A-6 for the results.

```
!-------------------------------------------------------------------------
!      Main switches for plotting.
!--------0---------0---------0---------0-------------------------------
urrs.1     Name of input data file.
tek1.pic   Name of output tektronix file.
1          Aspect ratio (integer, 1 - 5).
1          Number of plots per page (integer, 1 - 4).
demo of ipattn=5
0
x          Which axis serves as independent variable (x or y).
3          Flag indicating log or linear mapping (1 - 4).
5          Pattern.
0          Background specification. (0 or 2)
n          Print out system time on the upper right hand corner (y or n).
+o.#$      Patterns of scatter plots (5a1)
0    Extra line,1:x=0,2:y=0,3:x,y=0,4:x=1,5:y=1,6:x,y=1,7:diag,8:y=fac. 2.,9:fb-nmse, else:nothing.
!-------------------------------------------------------------------------
!      Parameters for plot 1.
!-------------------------------------------------------------------------
1. 0.      ascale, bscale for the independent variable axis.
1. 0.      ascale, bscale for curve 1.
1. 0.      ascale, bscale for curve 2.
1. 0.      ascale, bscale for curve 3.
1. 0.      ascale, bscale for curve 4.
1. 0.      ascale, bscale for curve 5.
200. 20000. 10. xmin, xmax, and dx for the x axis.
-1.5 1.5 0.5  ymin, ymax, and dy for the y axis.
(i5)
(f4.1)
```

Figure A-2. An example of the template file of SIGPLOT. Refer to Figure A-9 for the results.

```
0
x
y
        50 5
   -6.03186       0.248690       -0.368124       -0.844328       -0.998027       -0.770514
   -5.78053       0.481754       -0.125333       -0.684547       -0.982287       -0.904827
   -5.52920       0.684547        0.125333       -0.481753       -0.904827       -0.982287
   -5.27788       0.844328        0.368125       -0.248690       -0.770513       -0.998027
   -5.02655       0.951057        0.587786        0.397359E-06   -0.587785       -0.951056
   -4.77522       0.998027        0.770513        0.248690       -0.368125       -0.844328
   -4.52389       0.982287        0.904827        0.481754       -0.125333       -0.684547
   -4.27257       0.904827        0.982287        0.684547        0.125333       -0.481753
   -4.02124       0.770513        0.998027        0.844328        0.368125       -0.248690
   -3.76991       0.587785        0.951056        0.951057        0.587785        0.254308E-06
   -3.51858       0.368125        0.844328        0.998027        0.770513        0.248690
   -3.26726       0.125333        0.684547        0.982287        0.904827        0.481754
   -3.01593      -0.125333        0.481753        0.904827        0.982287        0.684547
   -2.76460      -0.368125        0.248690        0.770513        0.998027        0.844328
   -2.51327      -0.587785        0.397391E-07    0.587785        0.951056        0.951057
   -2.26195      -0.770513       -0.248690        0.368124        0.844328        0.998027
   -2.01062      -0.904827       -0.481754        0.125333        0.684547        0.982287
   -1.75929      -0.982287       -0.684547       -0.125334        0.481753        0.904827
   -1.50796      -0.998027       -0.844328       -0.368124        0.248690        0.770513
   -1.25664      -0.951057       -0.951057       -0.587785       -0.556284E-07    0.587785
   -1.00531      -0.844328       -0.998027       -0.770513       -0.248690        0.368124
  -0.753983      -0.684547       -0.982287       -0.904827       -0.481753        0.125333
  -0.502655      -0.481754       -0.904827       -0.982287       -0.684547       -0.125333
  -0.251328      -0.248690       -0.770513       -0.998027       -0.844328       -0.368125
   0.000000       0.000000       -0.587785       -0.951056       -0.951057       -0.587785
   0.251328       0.248690       -0.368124       -0.844328       -0.998027       -0.770513
   0.502655       0.481753       -0.125333       -0.684547       -0.982287       -0.904827
   0.753982       0.684547        0.125333       -0.481754       -0.904827       -0.982287
   1.00531        0.844328        0.368125       -0.248690       -0.770513       -0.998027
   1.25664        0.951056        0.587785       -0.381470E-06   -0.587786       -0.951057
   1.50796        0.998027        0.770513        0.248690       -0.368125       -0.844328
   1.75929        0.982287        0.904827        0.481754       -0.125333       -0.684547
   2.01062        0.904827        0.982287        0.684547        0.125333       -0.481754
   2.26195        0.770513        0.998027        0.844328        0.368125       -0.248690
   2.51327        0.587785        0.951056        0.951057        0.587785        0.190735E-06
   2.76460        0.368124        0.844328        0.998027        0.770513        0.248690
   3.01593        0.125334        0.684548        0.982287        0.904827        0.481753
   3.26726       -0.125333        0.481754        0.904827        0.982287        0.684547
   3.51858       -0.368124        0.248690        0.770514        0.998027        0.844328
   3.76991       -0.587785        0.341731E-06    0.587785        0.951057        0.951056
   4.02124       -0.770513       -0.248690        0.368125        0.844328        0.998027
   4.27257       -0.904827       -0.481754        0.125333        0.684547        0.982287
   4.52389       -0.982287       -0.684547       -0.125333        0.481754        0.904827
   4.77522       -0.998027       -0.844327       -0.368124        0.248691        0.770514
   5.02655       -0.951057       -0.951056       -0.587785        0.723200E-06    0.587786
   5.27787       -0.844328       -0.998027       -0.770513       -0.248689        0.368125
   5.52920       -0.684548       -0.982287       -0.904827       -0.481753        0.125334
   5.78053       -0.481754       -0.904827       -0.982287       -0.684547       -0.125333
   6.03186       -0.248690       -0.770513       -0.998027       -0.844328       -0.368124
   6.28319       -0.301992E-06   -0.587785       -0.951057       -0.951056       -0.587785
```

Figure A-3. An example of the input data file of SIGPLOT. Refer to Figure A-6 for the results.

```
all periods
n-s distance (m)
var(dws) / median 1-min var(ws) /2
6  3
     312.5 -0.029  0.002  0.034 -0.027  0.043  0.112  0.166  0.275  0.383
     625.0 -0.009  0.005  0.019  0.011  0.048  0.085  0.209  0.361  0.513
    1250.0 -0.035  0.012  0.059 -0.007  0.070  0.148  0.330  0.480  0.630
    2500.0 -0.155  0.015  0.185 -0.126  0.100  0.325  0.359  0.565  0.771
    5000.0 -0.033  0.170  0.373  0.013  0.323  0.633  0.440  0.751  1.062
   10000.0 -0.417  0.061  0.539 -0.137  0.369  0.876  0.406  0.873  1.339
```

Figure A-4. An example of the input data file of SIGPLOT. Refer to Figure A-9 for the results.

As one can see from Table A-1, SIGPLOT is capable of creating the following kinds of plots:

IPATTN = 1: scatter plot (e.g., Fig. A-5)

IPATTN = 2: line graph (e.g., Fig. A-6)

IPATTN = 3: scatter plot except line graph for the last variable (e.g., Fig. A-7)

IPATTN = 4: box plot (e.g., Fig. A-8)

IPATTN = 5: error bar plot (e.g., Fig. A-9)

IPATTN = 6: same as IPATTN = 5 but with extra labelling (e.g., Fig. A-10)

The usage of each option is described below.

For IPATTN = 1, groups of data are represented by different dot patterns that are defined in the template file (see Table A-1). At most, five groups of data (MANY = 5) can be plotted, with a maximum of 700 points for each group.

IPATTN = 2 is similar to IPATTN = 1 except that points are now connected. The following line patterns are used to represent different curves: solid, short-dashed, long-dashed, dot-dashed, and dotted. At most, five curves (MANY = 5) can be plotted, with a maximum of 700 points for each group. No user customization of the line patterns is allowed. It is important that the data points in the input file are sorted according to the independent variable.

IPATTN = 3, a combination of IPATTN = 1 and 2, is useful when the user wants to see how well a theoretical curve fits the observed data. Although the order of the data points does not matter for a scatter plot, in this case it is important that the data points in the input file are sorted according to the independent variable. At most, five groups of data (MANY = 5) can be plotted, with a maximum of 700 points for each group.

The IPATTN = 4 option is an alternative to the scatter plot when the number of data points is large. In preparing the input data file for SIGPLOT,

the user first defines certain ranges of the independent variable to be used for grouping the dependent variable. The distribution of the dependent variables within each group is then determined and represented by five significant points in the cumulative distribution function (cdf). These five values could be the 2th, 16th, 50th, 84th, and 98th percentiles of the cdf, or the mean and mean ± one and two standard deviations. SIGPLOT then uses a box pattern to represent the distribution of the dependent variable within each grouping or range of the independent variable. Only one set of data (i.e., MANY = 1, even though five points are needed to define a box) is accepted for this option, with a maximum of 50 boxes.

IPATTN = 5 is similar to IPATTN = 4 except that three values (vs. five) are needed to define an error bar (vs. a box). These three values can be the mean and mean ± one standard deviation of a dependent variable, or the nominal value of a dependent variable and its 95% confidence limits. At most, five groups (MANY = 5) of data can be plotted, with a maximum of 50 error bars for each group. The following error bar patterns are used: filled square, empty square, filled triangle, empty triangle, and cross.

IPATTN = 6 is similar to IPATTN = 5 except that the user can label each data point. Because of the additional information to be plotted, only one group of data (MANY = 1) is accepted, with a maximum of 50 error bars. This option is designed primarily to plot the FB (fractional bias), together with its confidence limits, against the NMSE (normalized mean square error), where

$$FB = \frac{(\bar{C}_o - \bar{C}_p)}{(0.5(\bar{C}_o + \bar{C}_p))} \qquad \text{(A-1)}$$

$$NMSE = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o C_p}} \qquad \text{(A-2)}$$

If IEXTRA = 9 (see Table A-1), SIGPLOT will plot the additional $x = -0.667$, 0, and 0.667 lines, representing the factor of two and zero FB lines, together with the $y = 4x^2/(4-x^2)$ line, representing the "minimum" NMSE (due only to the mean bias) as a function of FB.

The information concerning the usage of the driver programs, TEKPC, TEKELQ, TEKEPS, and PS, can be obtained by simply executing the programs without providing any arguments, and will not be repeated here.

Finally, an example is given below of the procedures followed to use the graphics package.

Step 1: The user prepares the template file (DEMO.INQ) and the input data file (DEMO.DAT) according to the formats described in Tables A-1 and A-2. The user can create his own template file by editing the sample template file. The input data file is usually generated by some other programs.

Step 2: After the execution of SIGPLOT, a Tektronix picture file (DEMO.PIC) is generated.

Step 3: The user can view the results on screen by typing:
TEKPC DEMO.PIC
if a Hercules graphics card is installed, or
TEKPC DEMO.PIC 16
if an EGA (with a resolution of 640x350 pixels) graphics card is installed.

Step 4: A high resolution hard copy output can be generated on an EPSON-compatible dot matrix printer by typing:
TEKELQ DEMO.PIC.

Step 5: Or if the user has access to a PostScript printer, a PostScript file (DEMO.PS) will be created by typing:
PS DEMO.PIC,
and this file can be printed out by typing:
PRINT DEMO.PS

DEMO OF IPATTN=1

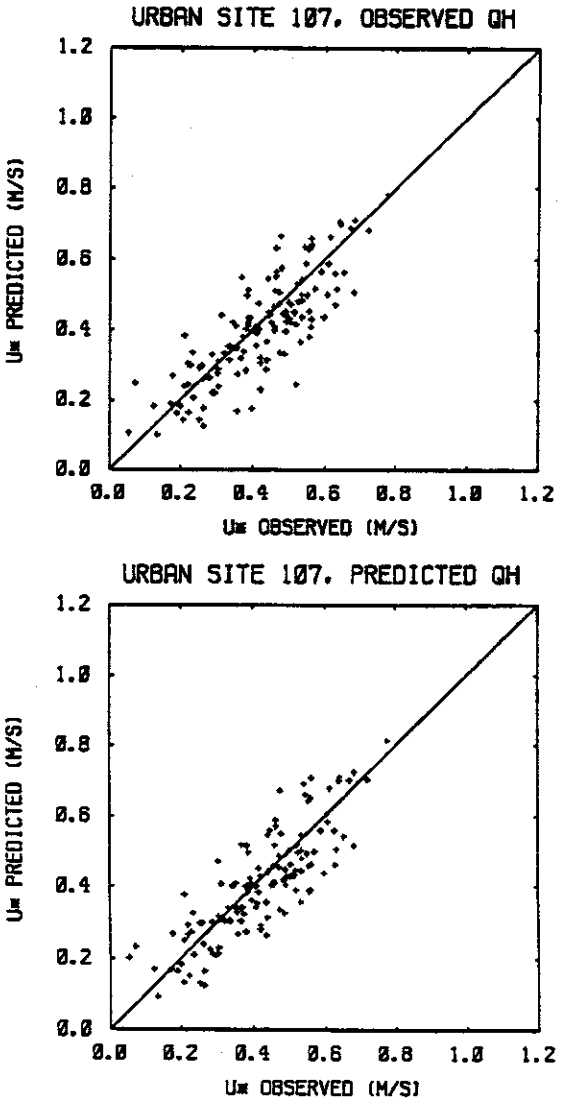

Figure A-5. A sample scatter plot (IPATTN = 1) generated by SIGPLOT.

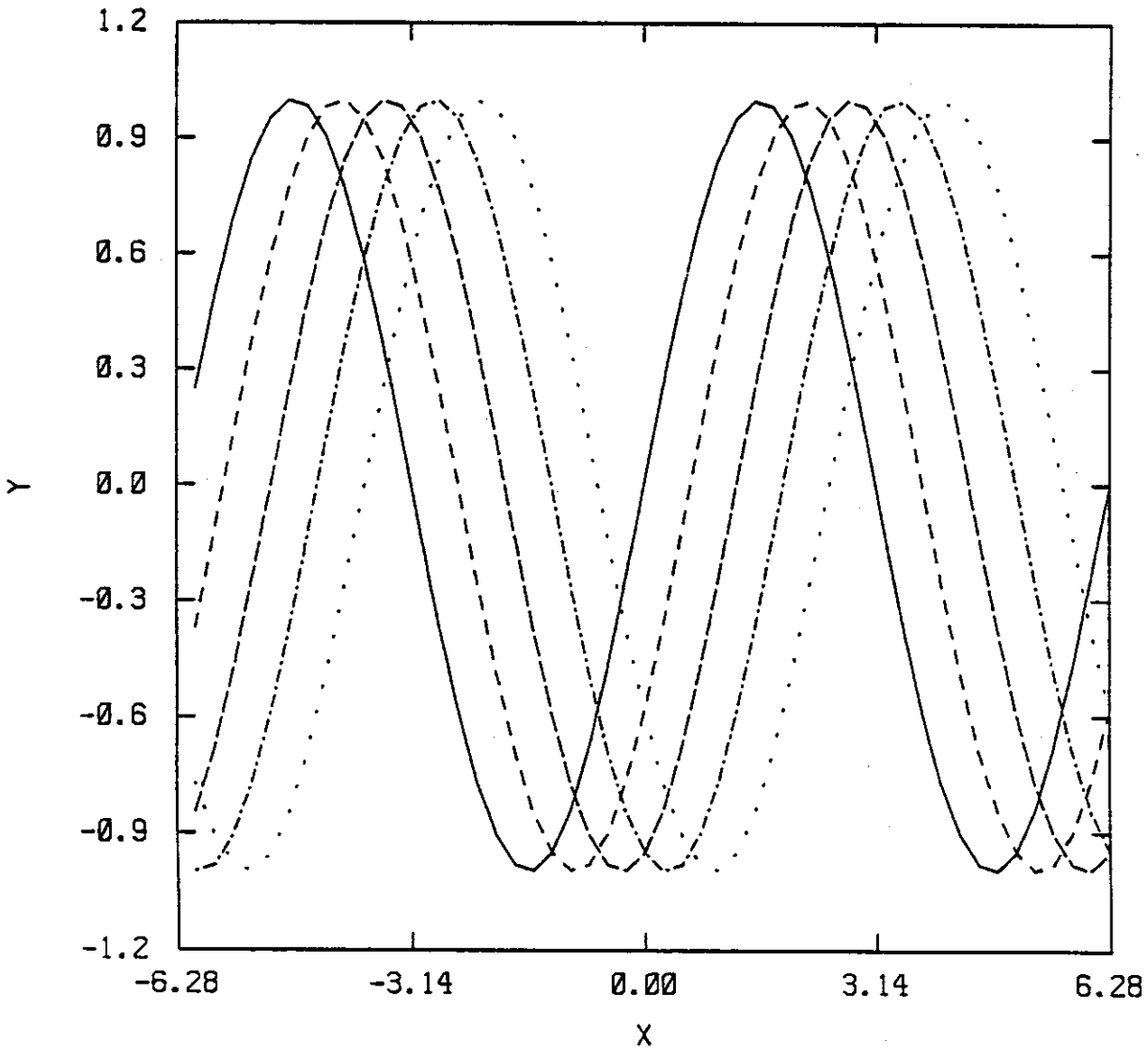

Figure A-6. A sample line graph (IPATTN = 2) generated by SIGPLOT. Refer to Figures A-1 and A-3 for the template and data files used for this figure.

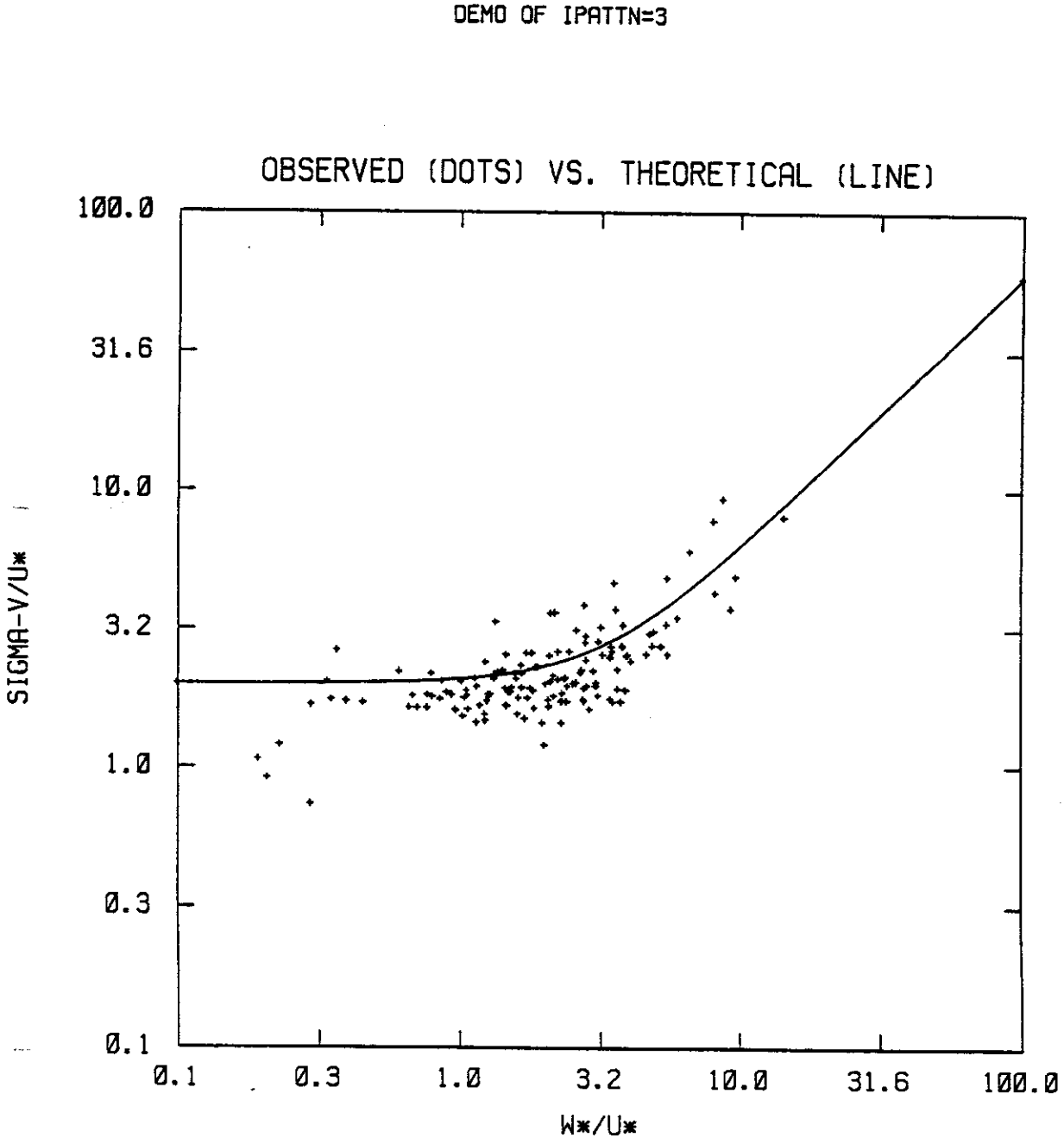

Figure A-7. A sample scatter plot and line graph (IPATTN = 3) generated by SIGPLOT.

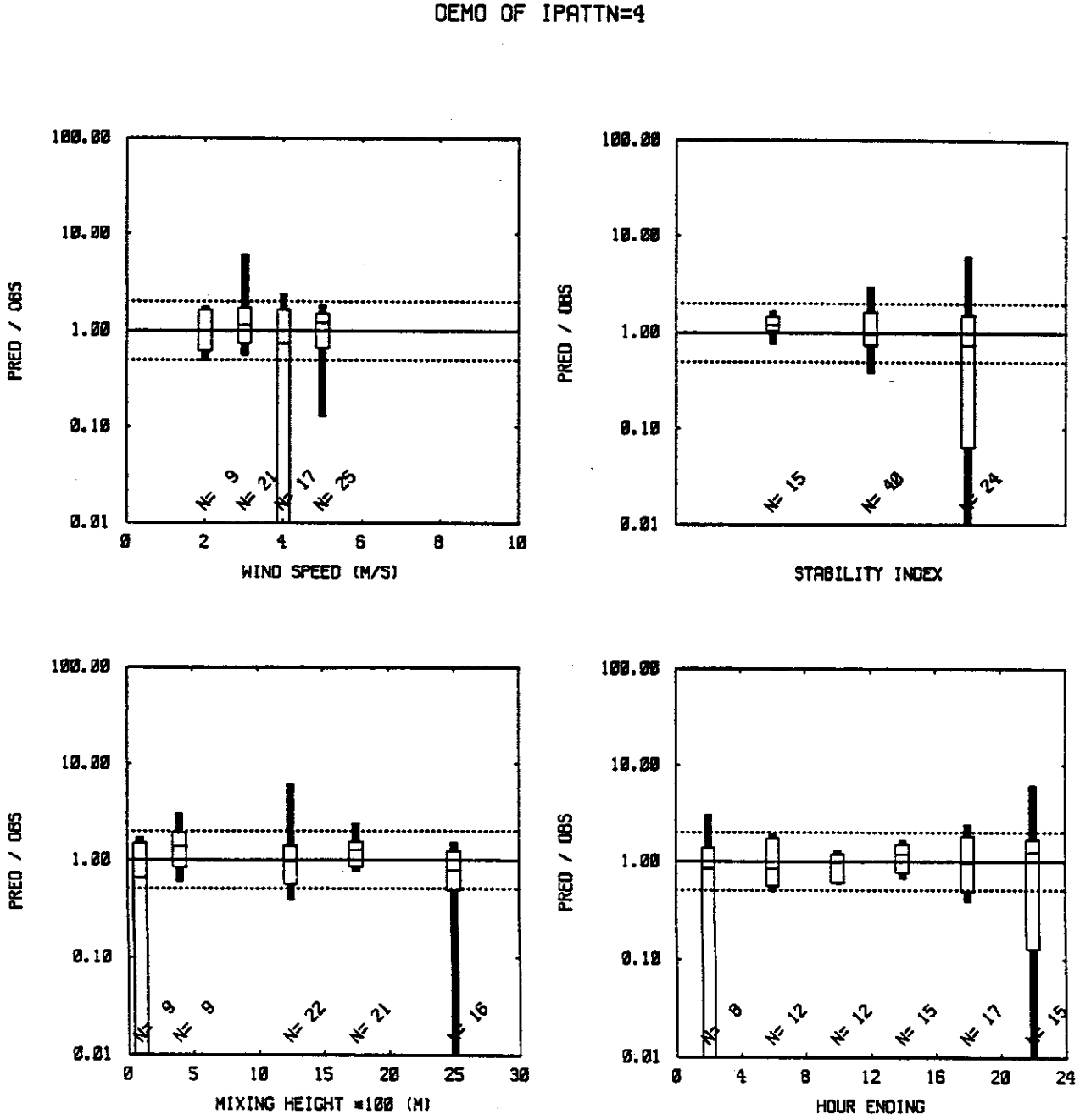

Figure A-8. A sample box plot (IPATTN = 4) generated by SIGPLOT.

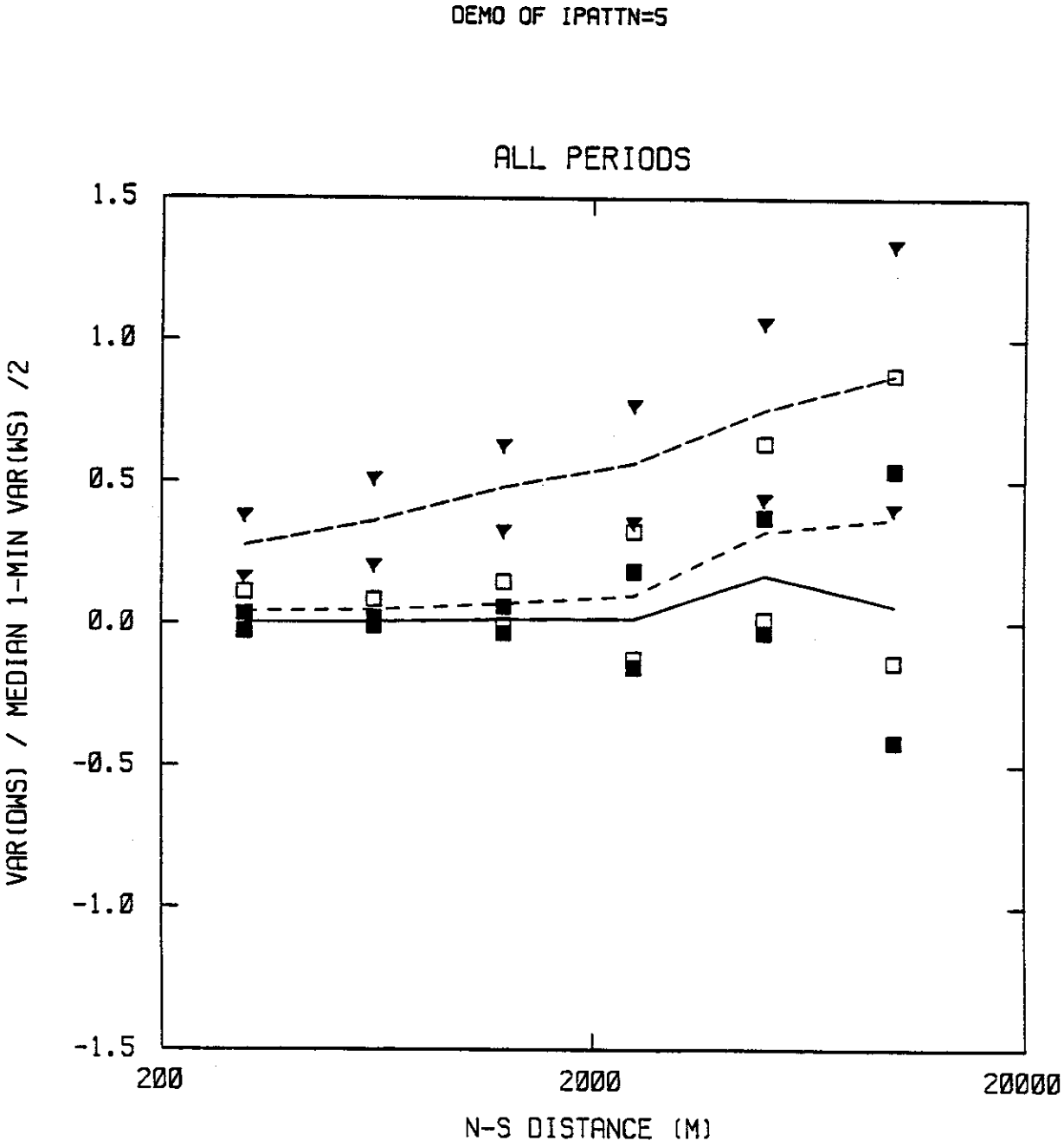

Figure A-9. A sample error bar plot (IPATTN = 5) generated by SIGPLOT. Refer to Figures A-2 and A-4 for the template and data files used for this figure.

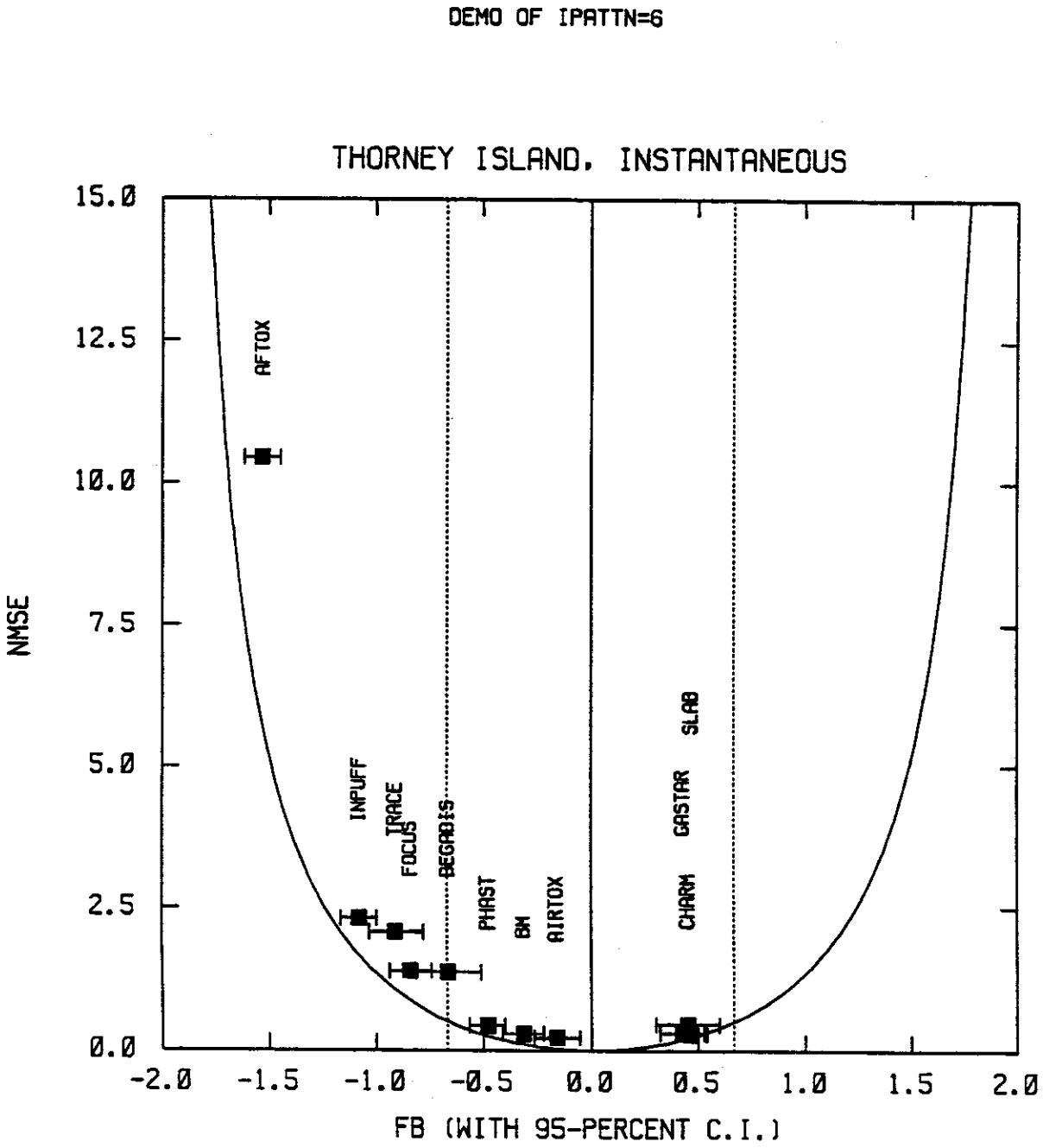

Figure A-10. A sample error bar plot with labelling (IPATTN = 6) generated by SIGPLOT.