



ASSESS

User's Guide

A large, stylized graphic of the word "ASSESS" in a bold, blocky font. The letters are white with a thick black outline, set against a background of a grey and white halftone dot pattern. The graphic is positioned horizontally across the lower half of the page.

NOTICE

Version 1.0 of this software is a prototype. Additional modifications are planned for the future. The information in this document does not represent the views or policy of the Environmental Protection Agency.

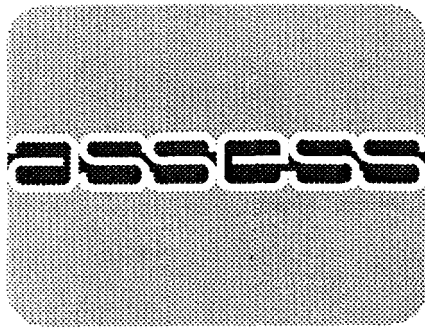
DISCLAIMER

ASSESS software and documentation are provided "as is" without guarantee or warranty of any kind, expressed or implied. The Environmental Monitoring Systems Laboratory, U. S. Environmental Protection Agency and Computer Sciences Corporation will not be liable for any damages, losses, or claims consequent to use of this software or documentation.



Contents

	Contents	iii
	List of Figures	v
<hr/>		
1. Introduction	1.1 OVERVIEW	1-1
	1.2 EQUIPMENT REQUIREMENTS	1-3
	1.3 USER PROFILE	1-3
	1.4 INSTALLING THE SYSTEM	1-3
	1.4.1 ASSESS Data Files	1-3
	1.4.2 Hard Disk Installation	1-4
	1.4.3 Using ASSESS on Floppy Diskette	1-4
	1.4.4 Using ASSESS from DOS	1-4
	1.5 GRAPHICS	1-4
	1.5.1 On-Screen Graphics	1-4
	1.5.2 Metacoda-Based Graphics	1-4
	1.6 ERROR AND RECOVERY PROCEDURES	1-5
<hr/>		
2. System Operation	2.1 DATA	2-1
	2.1.1 ASSESS Data Files	2-1
	2.2 INTERACTIVE SCREENS	2-2
	2.2.1 Screen Format	2-2
	2.2.2 Types of Screen input Fields	2-3
	2.2.3 The Menu Tree	2-4
	2.2.4 ASSESS Screens and Menus	2-4
<hr/>		
3. Using ASSESS in an Assessment Study: Example	3.1 OVERVIEW	3-1
	3.2 THE EXAMPLE SET	3-2
	3.3 DATA INPUT THROUGH THE KEYBOARD: AN EXAMPLE . .	3-13
	3.4 ALTERNATIVE DESIGN: AN EXAMPLE	3-15
<hr/>		
	Appendix A - DATA FILES	A-1
	Appendix B - REFERENCES	B-1
	Appendix C - NOMENCLATURE	C-1



List of Figures

Number		Page
2-1	Example Interactive Screen	2-2
2-2	The Menu Hierarchy	2-5
3-1	ASSESS Main Screen	3-3
3-2	Sampling Considerations Screen	3-4
3-3	Historic Assessment Screen	3-5
3-4	Quality Assessment Data Screen	3-6
3-5	Scatter Plot of the QA Data	3-7
3-6	Transforms Screen	3-8
3-7	The Scatter Plot of the Log Transformed Data	3-8
3-8	The Results Screen	3-10
3-9	The Intermediate Results Screen	3-11
3-10	The Error Bar Graph	3-11
3-11	The Results Screen	3-14
3-12	Alternative Design Results Screen	3-15
3-13	Alternative Design Error Bar Graph	3-16
3-14	Variance Estimates for the Alternative Design	3-17



Section 1

Introduction

1.1 OVERVIEW

ASSESS is an interactive program designed to assist the user in statistically determining the quality of data from field samples. The program permits quality assessment data and historical information (historical information is for notational purposes only) such as data quality objectives, sampling considerations, and historical assessments to be saved. Measurement-error variances are computed. Scatter plots of the variance (represented as $\sqrt{2}$ times the standard deviation) versus the average concentration may be produced for Routine Samples (RS) with either Field Duplicates (FD) or Preparation Splits (PS). Transforms may be applied to the entire data set. Error bar graphs of variance estimates from quality assessment (QA) samples may be produced. Hardcopies of all plots may be obtained by depressing the <P> key. The plots may also be stored in a file of device independent plotting commands (metacode). An HPGL plotter instruction file may be produced using the program HPPLLOT with the metacode file as input. The historical information, measurement-error variances, and data set may be written in a report format to either an output file or sent to a printer. The printer must be either an Epson- or IBM-compatible dot matrix printer, HP Laserjet, or HP Deskjet.

ASSESS may be used to provide a foundation for answering two basic questions:

How many, and what type, of samples are required to assess the quality of data in a field sampling effort? How can the information from the QA samples be used to identify and control sources of error and uncertainties in the measurement process?

Once the analytical results are received, bias and precision values will be computed. Note that ASSESS will only compute the precision.

An alternative QA design that does not employ field evaluation samples (FES) and external laboratory evaluation samples (ELES) is also discussed and error variances are computed.

ASSESS uses two temporary files called scratch files to store and process data read from an ASSESS data file. These scratch files are assigned the names XXXXXXXX.XXX and ZZZZZZZZ.ZZZ.

The concentrations (units) of the samples may be specified for notational purposes, but unit conversions cannot be made by ASSESS.

It is recommended that the EPA publication "A Rationale for the Assessment of Errors in the Sampling of Soils"(1), from which the program ASSESS has been derived, be used in conjunction with this user manual.

Please forward any questions, comments, or bug reports to the following address:

Jeff van Ee (Assess)
USEPA EMSL-LV, EAD
P.O. Box 93478
Las Vegas, NV 89193-3478

1.2 EQUIPMENT REQUIREMENTS

ASSESS was designed to run under DOS (Disk Operating System) on an IBM PC, XT, AT, PS2, or compatible. Graphics capability is not required, but is highly recommended as graphics output is produced. Graphics support is provided for the Hercules graphics card, laptops with monochrome displays having graphic capabilities, the Color Graphics Adapter (CGA), and the Enhanced Graphics Adapter (EGA). Support for Video Graphics Array (VGA) is not available, however, VGA does emulate EGA and therefore graphics support is provided for VGA indirectly. At least 512 kilobytes (Kb) of random access memory (RAM) is required, but 640 Kb is recommended. An arithmetic co-processor chip is recommended due to the computational intensive nature of the program, but is not required for use. ASSESS may be run from floppy diskette or from a fixed disk. The system storage requirement is approximately 420 kilobytes. For a hardcopy of results, a graphics printer (IBM graphics compatible) is required. Support is provided for plotters which accept HPGL plotting commands.

1.3 USER PROFILE

To use ASSESS, one should have some familiarity with personal computers and DOS (Disk Operating System). One should also understand basic DOS commands such as DIR (directory), CD (change directory), and how to insert and use diskettes. For more information on these topics, consult a DOS user's manual. The manual titled "A Rationale for the Assessment of Errors in the Sampling of Soils"(1) must be followed. For a list of references, refer to Appendix B, References.

1.4 INSTALLING THE SYSTEM

1.4.7 ASSESS Data Files

ASSESS in its executable form is entirely in the public domain. In the future, it may be downloaded from the U.S. EPA Bulletin Board System.

ASSESS.exe is the only file required to run ASSESS. If a metacode file is to be converted to a file with an HPGL format, then Hpplot.exe and Hershy.bar are required. Hershy.bar is a character font file and is required to execute Hpplot.exe.

The executable file, example data set, and optional files are as follows:

ASSESS	422778 bytes (required)
---------------	--------------------------------

Optional:

Standard	.fil	2576 bytes (example data set)
Alt1	.fil	1471 bytes (example data set)
Alt2	.fil	1636 bytes (example data set)
Saved1	.fil	4744 bytes (used for comparison)
Saved2	.fil	3771 bytes (used for comparison)
Barchart	.met	1440 bytes (wad for comparison)
Scatter	.met	2880 bytes (used for comparison)
Results	.fil	4744 bytes (used for comparison)
Smdata	.fil	1714 bytes (example data set)
Example	.fil	4744 bytes (example data set)
Hpplot	.exe	98417 bytes (conversion program)
Hershy	.bar	176000 bytes (required with Hpplot.exe)

The files denoted as "Used for Comparison" will be created by ASSESS as you run through the program. Therefore, these files may reside somewhere

outside the directory where ASSESS resides and thus will not be overwritten.

The source code is written in FORTRAN 77 for the Microsoft (Microsoft Corporation, Redmond, WA) FORTRAN compiler (version 4.01). With the exception of slightly modified proprietary Graflib Version 1.0 (Sutrasoft, Sugarland, TX) subroutines used for generating screen graphics, the source code is also in the public domain.

1.4.2 Hard Disk Installation

To install the system on a fixed disk, a subdirectory should first be created (for example, ASSESS). Copy ASSESS. exe and any other optional files into the subdirectory. For more information on creating subdirectories and copying files from a diskette into a subdirectory, refer to your DOS user's manual.

1.4.3 Using ASSESS on Floppy Diskette

ASSESS. exe is too large to fit on a 360 kilobyte diskette. This means that if only a 360 kilobyte disk drive (and no fixed disk) is available, then ASSESS cannot be used. Either a 3.5 disk drive or a 1.2 megabyte (or larger) 5.25" disk drive is needed to run both ASSESS and the optional program Hpplot.exe (with Hershy.bar)

1.4.4 Using ASSESS from DOS

To run ASSESS or Hpplot from DOS, type ASSESS or Hpplot at the DOS prompt. For example, to start program ASSESS type:

ASSESS <enter>

ASSESS uses most of the available memory. If an error message occurs after typing ASSESS, try to free other existing memory-resident programs, and type ASSESS to restart the program.

1.5 GRAPHICS

1.5.1 On-Screen Graphics

ASSESS plots graphics directly on the screen. This approach is used to provide a quick look at data or program results. Such graphics displays may be printed on a dot-matrix printer. When a graphics screen is displayed, the program will wait for a key to be pressed. Pressing <Q> will cause an interactive screen and menu to be displayed. Pressing <P> will produce a hard copy of the screen on a graphics printer. It is important to make sure that a graphics printer is connected to your computer if you choose this option, or the program will "lock-up". Also make sure that the printer is turned on and "on-line". If the program "locks up", the computer will probably have to be re-started.

1.5.2 Metacode-Based Graphics

The graphics displays may also be written to a "metacode" file when the "Save Plot" menu option is selected. A metacode file is a file of device-independent plotting instructions. This file can be converted to a HPGL (Hewlett Packard Graphics Language) formatted file using the program Hpplot (refer to section 1.4.1 ASSESS Data Files concerning Hpplot.exe). The advantage of using a metacode file is that higher-quality graphic output can be obtained on a pen plotter or other graphics device. The HPGL format is directly supported by WordPerfect.

Example: To import a metacode file generated by ASSESS into WordPerfect 5.0, perform the following steps*

- 1.) Generate a metacode file called 'Metacode.met' using ASSESS. Either of the two graphs generated by ASSESS may be saved to a metacode file. Note that the name "Metacode.met" is a generic name and it may be referred to by any other name. The 'met' extension is used as a means of distinguishing these files and the regular ASCII text files.
- 2.) Run the program HPPLLOT. Enter 'Metacode.met' as the input file and 'Metacode.pit' as the output file. HPPLLOT will convert 'Metacode.met' to an HPGL formatted file called 'Metacode.plt', which is supported by WordPerfect*.
- 3.) If you have a VGA adapter, the HPGL formatted file may require one more conversion using the WordPerfect conversion program Graphcnv.exe. To convert, call GRAPHCNV, and then enter "Metacode.pit" as the input file and "Metacode.wpg" as the output file. GRAPHCNV will generate "Metacode.wpg" which can be successfully imported into WordPerfect on PC's using a VGA adapter.

1.6 ERROR AND RECOVERY PROCEDURES

Normal Error Processing

ASSESS performs error checking on such items as file existence, file Input/Output and bounds checking on numeric parameters. When errors of these types are encountered in programs, error messages are displayed on the message line at the bottom of the screen. These messages are displayed in a black-on-white format (reverse video) and are accompanied with a buzz sound. To return to the interactive screen after such a message is displayed, press any key.

Problems

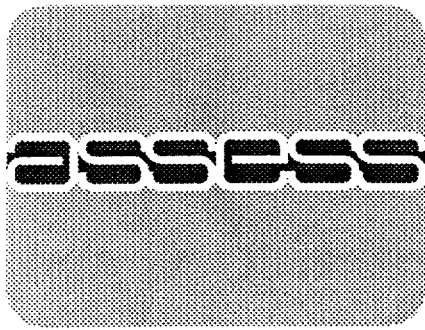
Although ASSESS has been tested and debugged it is still possible that there are situations which will cause ASSESS to "crash" or "fail" (terminate prematurely), or to "lock-up" (pause indefinitely with no response). If ASSESS "locks-up", the computer must be re-started. The problem may be due to a bug, or due to a printer or disk-drive problem (see below).

ASSESS may crash when a binary operation in the Transform menu is chosen which would produce a very large or very small number. An example would be the operation $1.0/X$, or 10 to the power of X, when X is a very small or very large ($1.E-1\ 000$, $1.E1\ 000$). This type of program error cannot be trapped or handled by ASSESS. In such cases the result cannot be produced due to hardware limitations in the precision of the numeric coprocessor (or floating-point emulation software). Since there is no remedy for this situation, the only solution is to avoid such operations.

There are several error conditions which the program was specifically not designed to check for. These involve checking to see if disk or printer peripherals are connected and ready for data transfer. The user should ensure that printers are attached and on-line, or that disk drives have the correct density media and are ready for read/write operations, when Read, Save, or Write options are selected. The following actions are guaranteed to create a "lock-up" situation.

**WordPerfect is a registered trademark of WordPerfect Corporation.*

- Trying to print a text or graphics screen when the printer is not connected or on-line. If a printer is connected, make sure it is turned "on" and is ready to accept output from the computer (on-line). If a printer is not connected to your system, it may be necessary to "re-boot" the computer.
- Accessing a file on a floppy diskette drive when the disk drive door is open, or no diskette is present. In some cases, DOS may respond with a message: Device not ready (Abort, Retry, Ignore). Insert a diskette and press <R> (for Retry). If this does not work, you must re-start the computer.



Section 2

System Operation

2.1 DATA

2.1.1 ASSESS Data Files

ASSESS employs a particular format for its data files. An ASSESS data file is an ASCII text file and is different from the Metacode files used by the HPLOT program. The ASSESS data files may be created with any text editor. For instance, WordPerfect* files may be converted to ASCII text files before being supplied to the program. Make sure your data files are compatible with the input format, or the program will not be able to read them, ASSESS will also operate without an input data file, in which case the screen layout for data input will be self explanatory. Three example data files included with the distribution diskette will be used as examples in this manual. Copy these files into the subdirectory where the Program ASSESS resides. They are called "standard. fil", "(altl .fil", and "smdata.fil". Below is an explanation of the "standard. fil" data file. The format of the other two files is the same and will be discussed later. It is helpful to obtain a print-out of these files using the DOS print command before proceeding to the next section.

Line 1 to 42

These lines of data represent the historical information. The data file includes information about the site, methods, desired accuracy, precision, etc. Note that these input lines are inconsequential to the data processing phase of ASSESS and are merely supplied to keep track of sampling considerations and historical assessments.

Line 43 to End of File - The Data Entries

This is where the data are stored. Each row represents a batch sample consisting of a pair of QA samples. For the regular design, these QA samples are stored under the following columns: Routine Sample (RS), Field Duplicate (F D), Preparation Split (PS), Field Evaluation Sample Pairs (FES1 and FES2), and External Laboratory Evaluation Sample pairs (ELES1 and ELES2).

For the "Alternative QA design, only FES1 and ELES1 values used for detection of bias are included; and two new columns are provided for Batch Field Duplicates (BFD) and their locations.

**WordPerfect is a registered trademark of WordPerfect Corporation.*

The data may be in "free format" which means that in a given line in the file, values must be separated by at least one space or a single comma. For readability, columns of numbers should line up; although this style is not required. Variable values must be numeric with no embedded blanks. Whenever a value could not be obtained for a variable, a special value of -9999.0 will be assigned to it. This value, referred to as missing, will not be included in the calculations. The file "standard.fil" contains the historical data and 23 batch samples. Examine the contents of this file using the DOS "Type" command or your editor.

Note: Refer to Appendix A for further discussions of the different data file formats.

2.2 INTERACTIVE SCREENS

2.2.1 Screen Format

This section will show the basic components of screens used in ASSESS. A menu tree of the entire program is presented to observe the flow of the program's interaction.

ASSESS initially displays an introduction screen. Upon pressing any key, the first interactive screen is displayed. ASSESS is composed of several screens for selection of program options and display of results. Figure 2-1 displays the first interactive screen. Below is a description of common components.

Figure 2-1
Example Interactive Screen

1 DATA QUALITY OBJECTIVES (1.0)

Data File:

Site : **4**

Method :

Analyte :

Analytical Method:

Desired Accuracy +/- %

Desired Precision +/- %

Desired Confidence Ranges (95%)

Bias +/- %

Precision +/- %

2

Data Alternative Revise Sampling Considerations Evaluate Data Quit **3**

Specify the input data file

❶ The Screen Frame

This is the rectangular box which encloses each screen. Program inputs and results are displayed in this area. Typically, the screen frame is divided into smaller, single-line rectangles. Each of these smaller rectangles contains a functionally related group of one or more input parameters or program results.

❷ The Message Line

This is the rectangle at the bottom of the screen frame. This area is used to display program error messages, yes/no prompts, prompts for additional information, or instructions for using a program option.

❸ The Menu Line

This is the line of text just below the screen frame. It contains a set of menu option names and a highlighted box (cursor bar). The cursor bar can be moved along the menu line by using the <left> and <right> arrow keys. As the cursor bar is moved over a menu option name, a short description of the menu option is displayed on the line just below the menu line. This line is called the menu description line. You may explore the possible choices in a program by moving the cursor bar and reading the descriptive messages which accompany each menu option. To select a menu option, move the cursor bar over the desired menu option name, and press <enter>. An alternative (and faster) way to select a menu option is to press the key which corresponds to the first letter in the menu option name. The result is the same as using the cursor control keys and pressing <enter>. For example, you would choose the "Revise" option by pressing <R> from the main menu.

❹ Parameter Groups

Typically, a functionally related group of program input parameters (fields) are enclosed together on the screen by a single-line rectangle. These groups of parameters are accessed through the menu. When a menu option is selected, a cursor bar appears at the screen field, and a message describing what action to take appears on the message line. When such a group contains several fields, the cursor control keys are used to move to subsequent fields. Exiting from the last field in the group will return the cursor bar to the menu line.

2.2.2. *Types of Screen input Fields*

Several types of input files are provided to allow flexibility in program parameter specification. Below is a list of these types and an example of each field type in the first screen of ASSESS (Figure 2-1).

Alphanumeric Fields — These fields may contain character strings of alphabetic or numeric characters. Any alphanumeric characters may be entered. The "Data" menu option in the screen of Figure 2-1 requires an alphanumeric value to be entered. To specify a data file name, select the data option on the menu; and type the name of the input data file.

Numeric Fields — Only numeric data may be entered into numeric fields. Some numeric fields will only accept integer (non-decimal) numbers. The program will respond to any erroneous keystrokes (such as alphabetic keys) with a low-pitched error tone. An example of numeric fields in the screen of Figure 2-1 are the desired accuracy and desired precision fields. Only integers may be entered for these two fields.

Toggle Fields — A toggle field is a special type of field which contains a list of 2 or more preset choices. Only one of these choices is displayed in the field. The <space> key is used to change the displayed choice, and the <enter> key is used to make the selection. Two examples of toggle fields in the screen of Figure 2-1 are the "Data" field and the "Alternative" field. Once the data option is selected, the toggle field will contain a "Yes" and "No" in response to the prompt "Do you want to specify a data file <use space bar>:" The toggle field will be highlighted; and each time the <space> key is pressed, "Yes" or "No" will appear. Press the <enter> key to make a selection. If "Yes" is selected, the toggle fields "Input (with labels)" and "Standard (with no labels)" may then be selected. Alternative option allows for two toggle fields, "Yes" and "No", in response to the prompts regarding the sample locations.

Yes/No prompts, prompts for additional information — These prompts are for information which will not be displayed permanently on the screen. They will appear temporarily on the message line. A Yes/No prompt will typically have the form: "Question...<Y/N>?". To respond Yes, press the <Y> key; to respond in the negative, press any other key. A typical Yes/No prompt is the "Do you really want to quit <Y/N>?" prompt which is displayed after the "Quit" (terminate program) option is selected. Another example is when you attempt to write over an existing file.

2.2.3 The Menu Tree

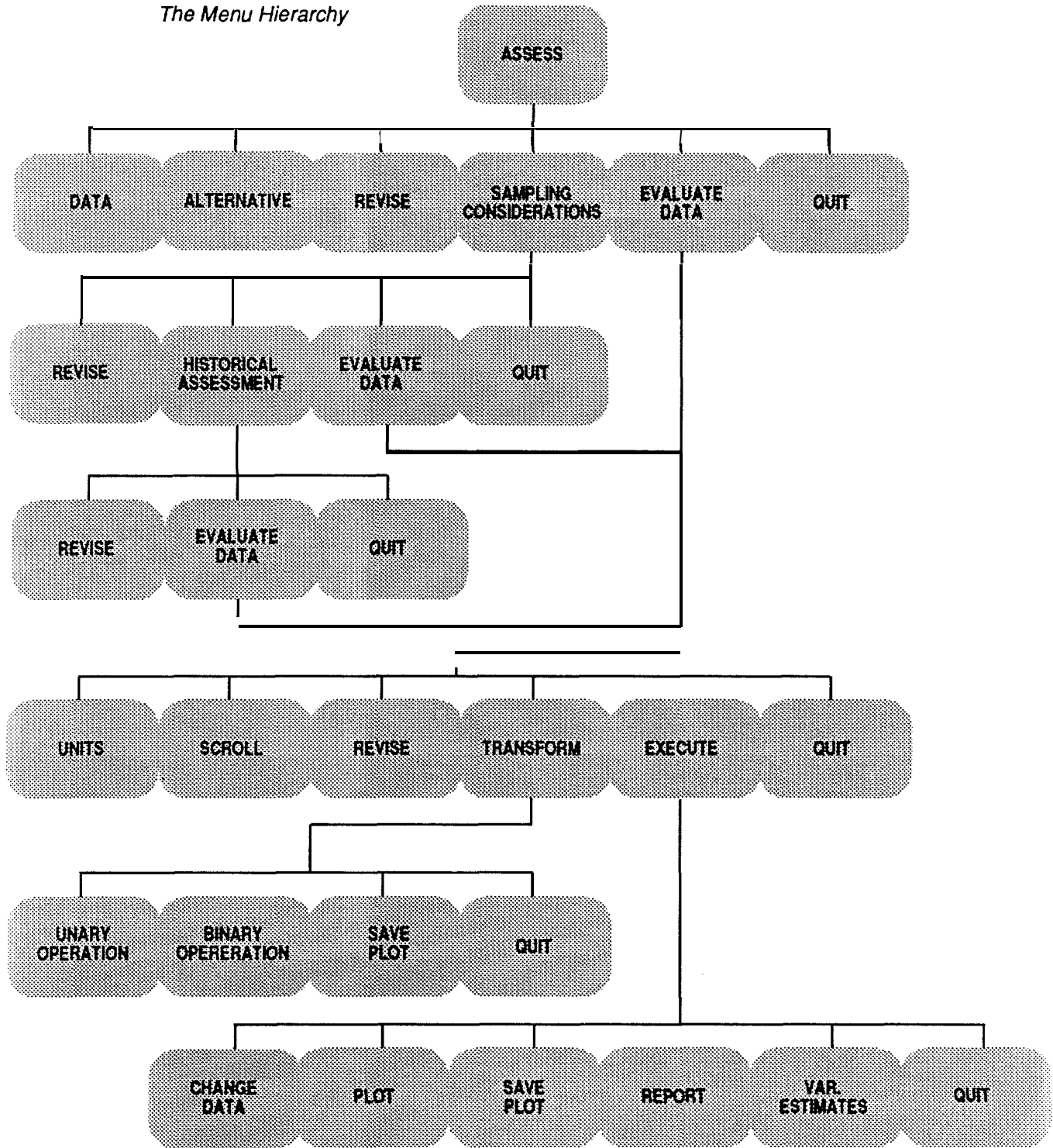
ASSESS typically requires input from data files and through interactive screens. These program inputs are arranged in a hierarchy of functionally related groups. Each group or individual program parameter value is accessed through a menu of choices. Some choices will lead to other menus, while some will lead to prompts for groups of one or more inputs. Such an arrangement can be represented in a menu hierarchy as illustrated in Figure 2-2.

The "menu tree" representation of program options provides a "road map" for ASSESS which summarizes the functional capabilities of a program. You may explore the hierarchy of options by traversing the menu tree and reading the descriptive messages which appear at the bottom of each screen.

2.2.4 ASSESS Screens and Menus

ASSESS initially displays an introduction screen. Upon pressing any key, the first interactive screen is displayed. The information entered or displayed on the succeeding three screens, namely the "Data Quality Objectives" screen, the "Sampling Considerations" screen and the "Historical Assessment" screen, are used presently for information purposes. No calculations are performed using the information from these three screens. The information is written to a user-specified file, along with the results of other calculations.

Figure 2-2
The Menu Hierarchy





Section 3

Using ASSESS in an Assessment Study: Example

3.1 OVERVIEW

This section will demonstrate how to use the ASSESS software to conduct an assessment study. We start with an example data set obtained from an actual Superfund site which was contaminated by lead deposition from a smelter; however, the arrangement of the data into batches and data from field evaluation samples are fictional and are included for illustrative purposes. Through this example data set, we will explore the ASSESS utilities and analyze its results. Two other data sets for the alternative QA design will also be shown. The data set "standard.fil" has been included with the software, so that you may repeat the exercise as a tutorial or to test the software. For a detailed explanation of the data, refer to the "Rationale document"(I).

The pilot study was conducted over a representative area to determine spatial variability and extent of the lead contamination in order to develop an efficient sampling network for obtaining representative measurements of contamination over a large area. The quality assessment program was implemented to assess variability from the collection, handling, and analysis of the samples.

3.2 THE EXAMPLE DATA SET

The "standard.fil" data set is an ASCII file in the ASSESS format. It contains data grouped into 23 batches. The file structure is described in Section 2. The first few lines of data without the historical information are as follows:

```
1  -9999.000  -9999.000  -9999.000  448.000  505.000  -9999.000  -9999.000
2  -9999.000  -9999.000  -9999.000  475.000  488.000  -9999.000  -9999.000
3  -9999.000  -9999.000  -9999.000  423.000  424.000  -9999.000  -9999.000
4    389.000  -9999.000    430.000 -9999.000 -9999.000  -9999.000  -9999.000
```

Each row represents a batch. The first through the third rows indicate that only Field Evaluation Sample pairs (FES1 and FES2) exist, and all other samples are unknown (i.e., missing). The fourth batch indicates that only a routine sample (RS) and a preparation split sample (PS) exist.

Notice that the ASSESS data files for the regular design consist of the following columns in the given order: RS, FD, PS, FES1, FES2, ELES1, ELES2.

Assuming that you have already copied the software and data into a directory called ASSESS on your hard disk and have used the command "CD\ASSESS" to access the directory, you can run ASSESS by typing the command:

ASSESS <enter>.

When the program begins execution, it first displays a screen with introductory information. When you press a key to proceed, you will see the program main screen and menu as displayed in Figure 2-1.

The bottom line on the screen provides the list of available options. The first three options move you to an area on the screen (or to a new screen) where you can input or select program parameters.

We begin by running through the program using the menu options.

Throughout this tutorial you will see the phrase "select an option" used often. You "select" an option by positioning the cursor on the option or field, and pressing the <enter> key.

In the data analysis section of this document the following points are noted:

1. The line "**Insufficient samples exist for this variance**" for any error variance estimates means that enough samples do not exist to assess the variance.
2. if the value of any variance estimate is less than zero, a value of zero will be assigned to that variance.

Data

The "Data" option is used to decide whether a data file is present or data is to be entered on the screen. Select the data option and answer Yes to the prompt "Do you want to specify a data file? (use <space> bar):"? This is done by pressing the <enter> key on the toggle field "Yes". You are then asked about the format of the input file. Hit the space bar to toggle through the options, and select the "standard (with no labels)" field in response to the "What is the input file format? (use <space> bar):" prompt. As before, select

a particular field by pressing the <enter> key. You are then prompted for a data file name. Notice the cursor jumps to the "Datafile:" field on the screen. Type the name of the input data file, which in this case is "Standard.fil", and press the <enter> key. A short tuned noise will be generated, and the message "ERROR - data file not found (press any key)" will be displayed if an incorrect or a non-existent file is entered. In such a case, select the Data option and proceed with correct entries. The following screen will be displayed (Figure 3-1).

Figure 3-1
ASSESS Main Screen

```

DATA QUALITY OBJECTIVES (1.0)

Data File: standard.fil

Site      : Palmerton, Penn. (Phase I)
Method    : core
Analyte   : Pb
Analytical method:

Desired Accuracy +/- 20 %
Desired Precision +/- 20 %

Desired Confidence Ranges (95%)

Bias      +/- 0 %
Precision +/- 0 %

Data Alternative Revise Sampling Considerations Evaluate Data Quit
Pick the alternative QA design without FES and ELES

```

Alternative

This option allows the user to select the alternative QA design without the FES and ELES values. Since the first example does not employ the alternative design, DO NOT select this option. Use your cursor keys to move to the "Revise" option.

Revise

This option is used to revise the screen parameters. Note that the parameters on the second part of the screen displaying the site, method, etc. are only for historical notations and have no bearing on the result of the analysis. Note also that the displayed information is the result of the input given in the file "standard.fil". You may proceed to the next option by not selecting the "Revise" option, thus accepting the listed parameters. However, for illustration purposes, select the "Revise" option, move the cursor key to the "Analyte:" field, and type in "lead" over "Pb" and press the <enter> key. Pressing the <enter> key till the end of the screen parameters or the <left arrow> key at anytime, will take you back to the "Revise" option on the menu fields.

Sampling Considerations

This option displays the "Sampling Considerations" menu. It is designed only for historical notations, and is merely a summary of the contents of parts

of the data file. DO NOT this option yet. We will discuss this after examining the remaining options on the screen.

Evaluate Data

This option displays the "Evaluate Data" menu. Through this menu, ASSESS does all of its computing work. It computes and displays measurement error variances. It also performs data transformations, produces reports and plots data. This option may be selected immediately after the specification of data input type and will bypass the sampling consideration and historical assessment screens. Experienced users will select this option first if quick data evaluation is required, thus bypassing the historical screens.

Quit

This option is used to exit the program. Using the analogy of the menu tree, the "Quit" option also allows you to "move up" one level in the tree. The "Quit" option will also appear in other successive screens. When this option is used from the main menu of the program, a Yes/No prompt is issued: "Do you really want to quit <Y/N>?". The <Q> key is typically used to select this option. The Yes/No prompt is a means of ensuring that a series of <Q> keystrokes will not cause inadvertent termination of the program.

You may now select the "Sampling Considerations" option from the menu bar. The following screen will be displayed:

Figure 3-2
Sampling Considerations

SAMPLING CONSIDERATIONS (1.0)			
Number of Samples :	300	Batch Data	
Number of Batches :	20	Number	Sampling Crew
Costs	1	single	Analytical Lab
Sample Collection:	.00		single
Analysis :	.00		
Revise Historical Assessment Evaluate Data Quit			
Revise the sampling considerations			

We will now discuss the options accessed through this screen.

Revise

This option is exactly similar to the discussion of the "Revise" option above. Let us change the analysis cost to \$500.00. Select the "Revise" option, use

the <down arrow> key to move to the "Analysis" field, and type 500.00. Notice that if you hit an <enter> key after entering the number 500.00, you will be placed into the next part of the screen regarding the batch data. To get back to the "Revise" option, move your cursor bar to the extreme left or right sides of the screen frame using the arrow keys.

Historical Assessment

This option displays the "Historical Assessment" menu. This menu shows a screen with the bias and measurement data of the input data file. DO NOT select this option yet. We will discuss it after examining the remaining options on the screen.

Evaluate Data

This option is exactly similar to the option discussed for the main screen.

Quit

This option will return the user to the main menu of the main screen. We may now select the "Historical Assessment" option. After pressing the <enter> key on the "Historical Assessment" option, the following screen will be displayed.

Figure 3-3
Historical Assessment Screen

HISTORICAL ASSESSMENT (1.0)			
Precision	IVARI	Measurement Bias	(%)
Sampling	: .10	Sampling (no contamination)	: .00
Source: this is some thing new		(contamination)	: .00
Handling/Preparation	: .07	Source:	
Source:		Handling/Prep (no contamination):	.00
Subsampling	: .05	(contamination):	.00
Source: this is old		Source:	
Laboratory analytical	: .20	Subsampling (no contamination)	: .00
Source:		(contamination)	: .00
Data analysis	: .05	Source:	
Source:		Analytical (no contamination)	: .00
Between batch	: .00	(contamination)	: .00
Source:		Source:	
Total measurement variance:	.00	Data Handling	: .00
Source:		Source:	
Revise Evaluate Data Quit			
Revise the precision and measurement bias assessments			

We will now discuss the options accessed through this screen.

Revise

Through this option, you may alter any of the screen fields as discussed in the previous explanation of Revise. Select the "Revise" option, and change the "Total Measurement Variance:" field to 0.09.

Evaluate Data

This option is essentially the same as previously discussed.

Quit

This option will return you to the previous menu which is the "Sampling Considerations" screen.

We will now select the "Evaluate Data" menu option to display the "Quality Assessment Data" screen.

Figure 3-4
Quality Assessment Data

Row	Batch	RS	FD	PS
1	1			
2	2			
3	3			
4	4	389.000		430.000
5	5	244.000	410.000	
6	6	33.400		32.100
7	7	960.000	780.000	
8	8	221.000		244.000
9	9	100.000	200.000	
10	10	00.000		72.000

Concentrations (Units): Transform: None

Units Scroll Revise Transform Execute Save Data Quit

The screen above shows the contents of your input data file. It only shows data for 10 batches within the RS, FD, and PS columns. The "Scroll" option described below will let you explore the additional batches and the remaining columns not seen on the screen.

We will now discuss the options accessed through this screen.

Units

This option will allow you to enter the concentration unit. Select this option and type "mg/kg". When you hit the <enter> key after typing in the concentration unit, you will be back on the units option.

Scroll

This option will allow you to scroll through the input screen. The data file "standard.fil" contains 23 batches, but only 10 are shown on the screen. Select the "Scroll" option. In the message frame, you will notice the message "Use <arrow> key to scroll or <Q> to Quit." As you push the <right arrow> key, you will notice that additional columns of input will appear on the screen. Note that missing values are represented by blanks on the screen, thus improving readability. The <down arrow> key will let you scroll and observe additional batches, if any. After scrolling through the screen, press the letter <Q> to get back to the "Scroll" option.

Revise

This option is the same as previously discussed. You may alter any of the input values by a sequence of arrow keys (to get to the correct position) and typing over the old values. Note that the "Save Data" option must be selected to save any new changes before proceeding to transformations of the data, or execution of the program. For the time being, do not alter any of the data. Proceed to the following option.

Transform

The Transform option is used as a tool to determine if the data needs to be transformed and to carry out various data transformations.

The "Transform" option plots a scattergram of the data. When the 'Transform' option is selected, you will have a choice as to the type of data to be plotted. Select this option, and you will be prompted by "Specify plot of which concentration to use? (use <space> bar):. Toggle through the possible fields which are "RS&FD" and "RS&PS". Remember to use the space bar to toggle throughout the possible options. Select the "RS&FD" field and press the <enter> key. Note the message on the message line, and press any key to view the scattergram. The following is the plot of the original data (untransformed).

Figure 3-5
Scatter plot of the QA data

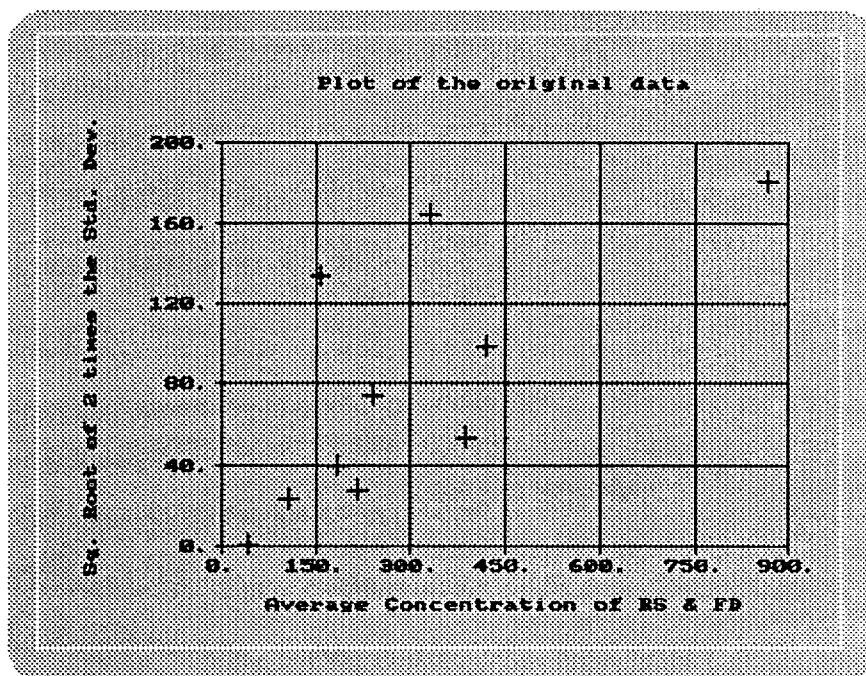


Figure 3-5 illustrates the need for a transform of the original data. The plot shows that the standard deviation of the data (multiplied by $\sqrt{2}$) from routine samples and field duplicates increases with the average concentration of these samples. A logarithmic transform of the data will stabilize the variance of the data over measured concentration range. After this transformation has occurred, the variances may be computed for the purpose of assessing variability throughout the measurement process.

Press the letter <Q> to quit the graph, and observe the following "Transforms" screen.

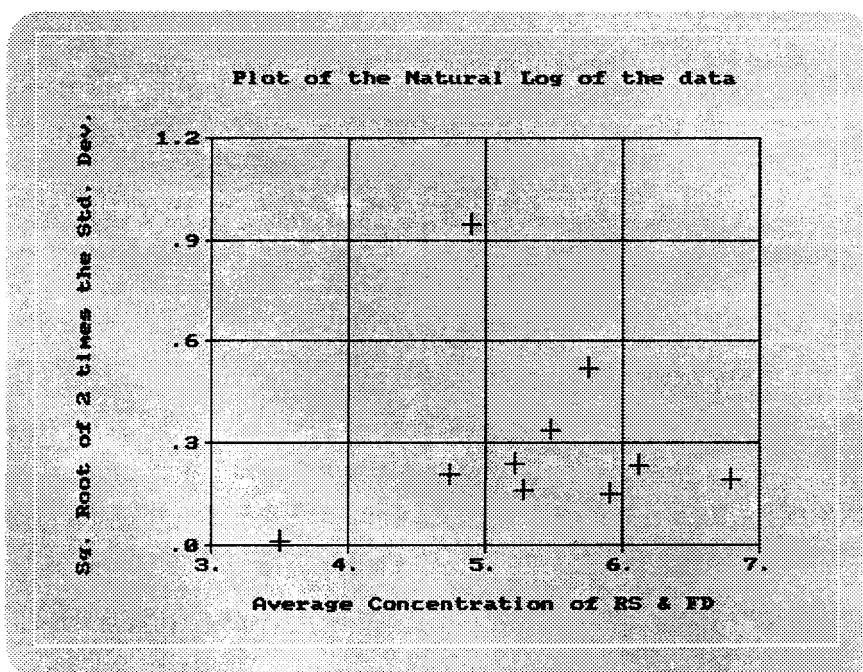
Figure 3-6
Transforms Screen

TRANSFORMS (1.0)	
Meta File:	
Operation:	Operator
<p>Description</p> <p>The transform is applied to the entire data set. Five unary operations are provided:</p> <p>Sqrt : square root of x Log : Log of x to the base 10 Ln : Log of x to the base e Truncate : Truncation of the decimals of x Exp : e to the power of x Retain : Retain the original data</p>	
<p>Unary Operation Binary Operation Save Plot Quit</p> <p>Select a unary operation</p>	

Unary Operation

This option allows the user to toggle through five unary operations, as well as a "Retain" option, which allows the original data to be retained thereby eliminating any confusion as to the type of data being transformed. These six options are also listed on the screen. Select the "Unary operation", and use the space bar to toggle through the possible selections. Select the "Ln" operator to take the log base e of the original data. After selecting this option you will remain in this screen. In order to view the newly created plot, select the "Quit" option. Notice the message at the bottom of the screen when the cursor bar is moved to the "Quit" option. This option will return you to the "Quality Assessment Data" screen. Notice the data displayed on the screen. The values are log base e of the original data. Select the "Transform" option and the "RS&FD" toggle field. Press <enter> to view the following graph:

Figure 3-7
The Scatter Plot of the Log Transformed Data



The data now fall along a straight horizontal line. The variance of the data is now said to be “stabilized.”

Press the letter <Q>, and select the “Quit” option to return to the “Quality Assessment Data” screen. Notice that the screen shows the log-transformed data of the input data.

In order to explore the remaining options of the “Transforms” menu, select the “Transform” option. Select the “RS & PS” toggle field and view the graph. Press the letter <Q> to quit the graph and enter the “Transform” screen. The “Unary Operation” option was discussed above. It may be used to retain the original data, so that additional transforms may be applied to the untransformed data.

Binary Operation

This option allows data transformation using the given binary operators on the screen. This option has the same features as the “Unary Operation” option, and allows you to perform multiplication, division, addition, subtraction, exponentiation, and retain the original data.

Save Plot

This option saves the generated plot through the “Transform” option. The plot that will be saved is the plot just observed prior to reaching this screen layout. Conceptually, it saves the plot that is no longer visible by the user, though it still exists. In order to save the plot just viewed, select this option and enter “Scatter.met” for the “Meta File:” prompt.

Quit

This option will return to the “Quality Assessment Data” screen. Select this option to return to the “Quality Assessment Data” screen.

Execute

This option will display the results obtained by applying the equations in table 5 of the “Rationale Document”(1). The primary purpose here is to estimate measurement-error variance components. The measured lead concentrations in soil (in mg/kg) are given for 10 Preparation Spilt (PS) pairs and for 10 Field Duplicate (FD) pairs. The amount of data used has been kept small for readability and to illustrate the use of the computer program to calculate variances. Select the “Execute” option. The following screen will be displayed:

Figure 3-8
The Results Screen

RESULTS (1.0)		
Report File:		
Meta File:		
Number of RS :	28	Transform:
FD :	18	
PS :	18	
YES :	1	
ELES:	0	
Concentrations: mg/kg		
Total Measurement Error Variance: .077		
Sample-Collection Variance:Insufficient samples exist for this variance		
Between-batch Variance:004		
Subsampling Variance:Insufficient samples exist for this variance		
Handling Variance:Insufficient samples exist for this variance		
Analytical Variance:Insufficient samples exist for this variance		
Change Data Plot Save Plot Report Var. Estimates Quit Return to Evaluate Data menu		

Figure 3-8 shows a summary of the results. Note that when enough samples do not exist to assess any of the variances, "Insufficient samples exist for this variance" will be displayed. For example, sample-collection variance can not be calculated, because the error estimate calculated from external laboratory evaluation samples (ELES) does not exist. Refer to Table 5 of the "Rationale Document" (1) for the formulas. Also note that the analytical variance could not be computed, since the estimate from external laboratory evaluation samples (ELES pairs) can not be obtained. This screen also displays a summary of the number of QA samples present. Note that the number of ELES values is equal to zero.

The options on this screen will now be discussed.

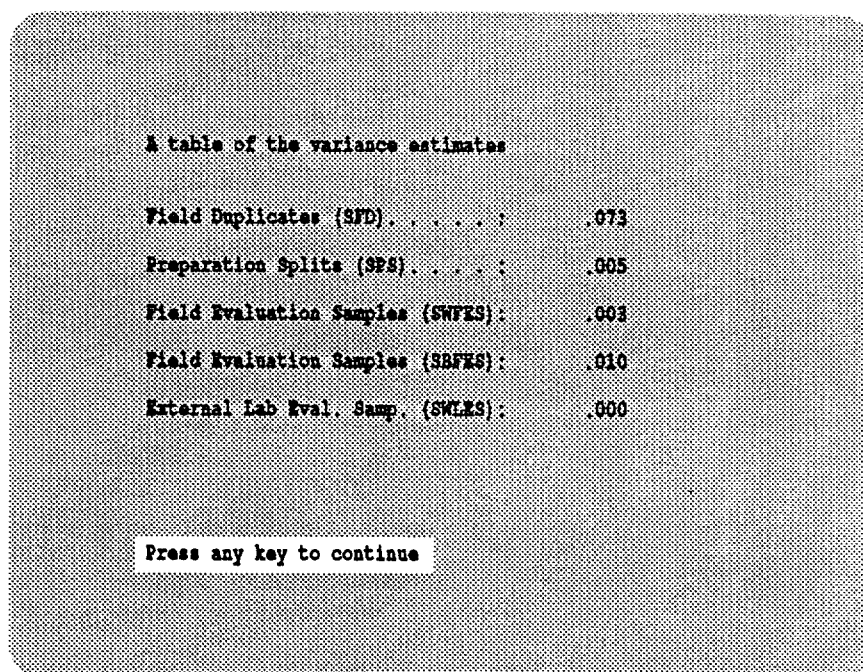
Change Data

This option will return the user to the "Evaluate Data" menu to make additional changes. The user will examine the result on the screen and decide if changes are necessary. This option will not do anything computationally, but is only a means for accessing the data screen. You may select this option, if there is a need for additional changes. This option will take you back to the "Quality Assessment Data" screen. After making changes, the "Execute" option will bring you back to the "Results" screen. This option will be selected after explaining the following options.

Var. Estimates

This option will display a screen showing the values of various variance estimates. Select the "Var. Estimates" option. The following screen will be displayed.

Figure 3-9
The Intermediate Results
Screen

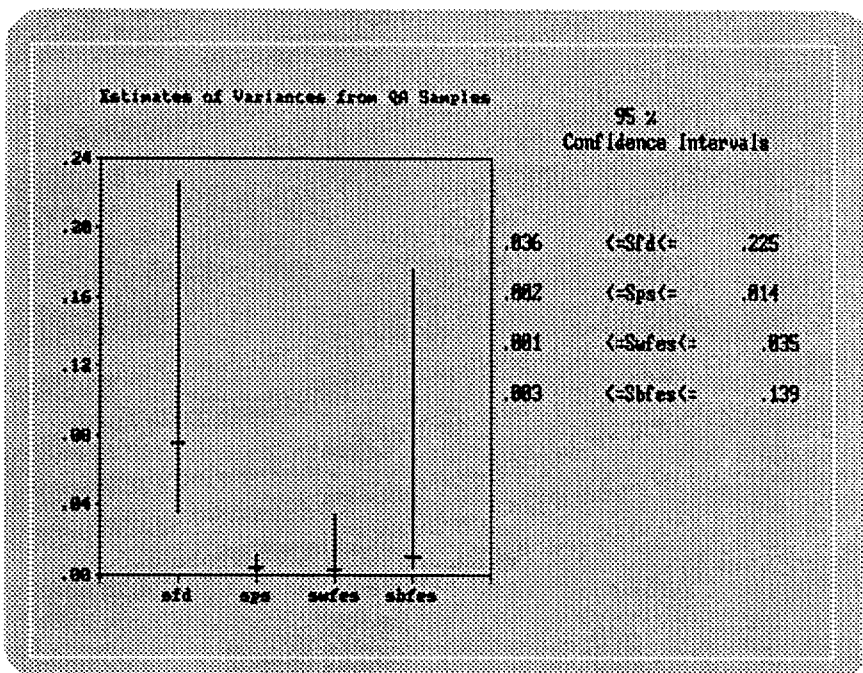


The table shows the variance estimates given in Table 5 of the "Rationale Document"(I). Press any key to return to the "Results" screen.

Plot

This option is used to display a plot of the error bar graph. (Note the message on the message line.) Select the "Plot" option, and press any key to view the following plot.

Figure 3-10
The Error Bar Graph



The plot illustrates the range in which the estimates of the various variance components may be expected to occur within a 95% confidence interval. It is clear from the length of the line for "sbfes" (Field Evaluation Samples estimate) that greater use of field evaluation samples would have improved the assessment of between-batch variability, as well as total measurement error variance. Table 3 of the "Rationale Document"(1) is used to determine the 95% confidence intervals for variances based on the degrees of freedom. Press the letter <Q> to return to the "Results" screen.

Save Plot

This option saves the error bar chart of the plot just viewed. Select this option, and type in "barchart.met" in response to the "Mets File:" prompt. After the metacode file has been written, press any key to return to the menu bar. A Metacode file is a device-independent file used by the program HP PLOT to produce a hardcopy of the plot on an HP plotter. Notice that you may also press the letter <P> to produce a hardcopy of the plot (Make sure that the printer is on-line). For more information on how to port this file into WordPerfect, refer to section 1.5.2, and consult your WordPerfect manuals.

Report

This option generates a report of the data and its results in three formats. The output may go to a file with input format, a file with report format, and to the printer. Select this option and select the "file (report format)" toggle field. Type in "results.fil" after the "Report File:" prompt.

Quit

This option will return the user to the main menu.

In order to return to the "Evaluate Data" menu, select the "Change Data" option. You are now located at the "Quality Assessment Data" screen.

Save Data

This option allows the user to save the contents of the screen in a data file with the input format. Select this option, and type in "Saved1.fil" in response to the "File:" prompt.

Quit

This option will return the user to the main menu. This is a good time to take a break. Select the "Quit" option of the "Quality Assessment Data" screen. The resulting screen is the main screen of ASSESS. Select the "Quit" option to end this session of ASSESS. We will return to ASSESS to demonstrate input from keyboard.

Now the basic concept of ASSESS has been studied, two shorter examples dealing with input data from the keyboard and using alternative QA design will be offered.

As discussed earlier, the second and third screens in ASSESS are used in reviewing or revising the historical data. These two screens may be skipped without any effects on the computational aspect of ASSESS. In this example, we will allow the user to access the "Evaluate Data" menu, input pair data, carry out computations and sketch plots, and finally save input data at anytime during the calculation phase. Obtain a hardcopy of the file "smdata.fil". The data in this file will be used as input to the program. At the DOS prompt in the appropriate subdirectory, type the command:

ASSESS <enter>

After observing the introductory screen, the screen of Figure 3-1 will be displayed. In the previous section, the sequence of actions needed to display various results were explained in a long-hand notation, where every keystroke was thoroughly explained.

To simplify our explanations, an abbreviated notation for the sequence of events will be used. A general formula exists for each option: Initiate the option, then take one or more actions, each of which may result in a screen field taking a particular value.

In order to get to the "Evaluate Data" menu, without a data file, use the following set of actions:

Option	Action	Field	Value
Data	Enter	Data File	No
Evaluate Data	Enter	Number of Rows	13
Revise	Enter		

Enter the values from the file "smdata.fil" using the <arrow keys> to move the cursor bar. Notice that the first 42 lines are historical information and will be ignored. You may pass over a field, thus assigning a missing value to that particular field ("-9999.0" in the data file represents a missing value).

Notice that by pressing the <enter> key, you will be positioned at the "Revise" option on the menu bar. Select it again to return to the input screen. Once all of the data is entered, take the following actions.

Option	Action	Field	Value
Save Data	Enter	Data file	Saved2.fil
Execute	Enter		

The screen of Figure 3-11 will be displayed. Notice that through the "Save Data" option, you may save your data at anytime. The format of this file is "Input (with labels)". This point is important if you would want to use this file again to add or delete information. Therefore, on the first screen, you would select the "Input (with labels)" toggle field of the Data Option, if there is a need to use this file as input to ASSESS. This example is used to verify your results. Analysis of data is similar to the analysis discussed in the previous section.

Quit	Enter		
Quit	Enter	Quit Prompt	Y

Figure 3-11
The Results Screen

RESULTS (1.0)	
Report File:	
Meta File :	
Number of RS :	7
PD :	3
PS :	4
FES :	3
ELES:	3
Transform: None	
Concentrations:	
Total Measurement Error Variance: 9.627	
Sample-Collection Variance. . . . : .000	
Between-batch Variance. : 6.833	
Subsampling Variance. : 22.364	
Handling Variance. : .000	
Analytical Variance. : 4.823	
Change Data Plot Save Plot Report Var. Estimates Quit	
Return to Evaluate Data menu	

3.4 ALTERNATIVE DESIGN: AN EXAMPLE

The alternative QA design was developed to assess measurement error variances in absence of FES and ELES pairs. Formulas in Table 6 in the "Rationale Document"(I) are used to calculate the results. The required data for the alternative design are RS, FD, PS, BFD (Batch Field Duplicates), the location of BFD values, and FES1, and ELES1 values. The FES1 and ELES1 values are not used in the computations and are only used to represent bias. Note: ASSESS presently does not calculate bias in the data.

In the following example the data file "Alt1.fil" is used to illustrate the case where batch field duplicates are all obtained from one sampling location. The format of the file "Alt1.fil" is the same as for the data file "standard.fil". Take the following sequence of actions to display the variance estimates, produce error bar graphs and scattergrams.

Option	Action	Field	Value
Data	Enter	Data File	Yes, Standard (with no labels), Alt1.fil
Alternative	Enter	Sample Location	Yes, No

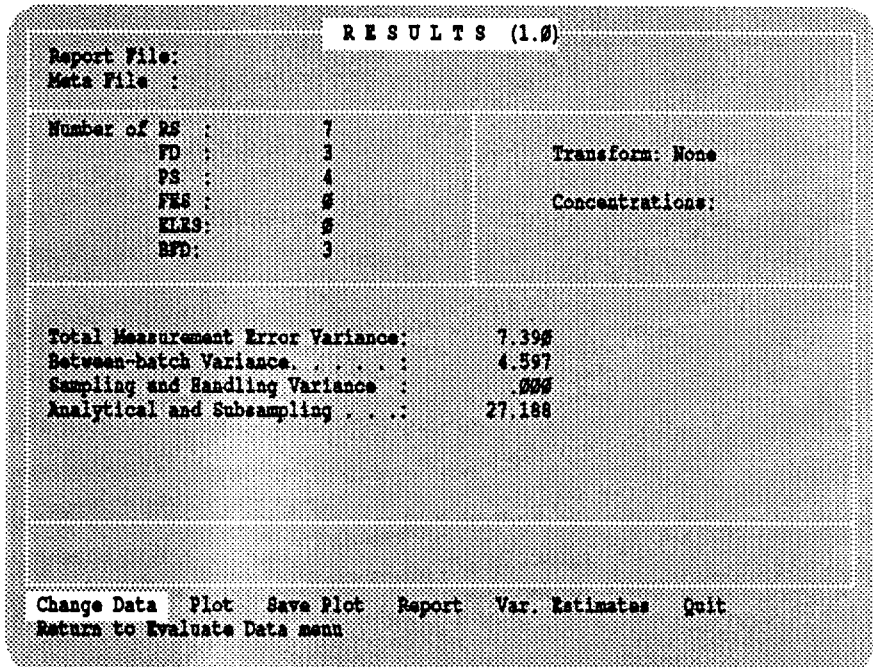
If you answer either "Yes" to both questions or "No" to both, you will be notified by an error message asking you to start over. Cursor bar returns to "Data" option.

Evaluate Data Enter

Execute Enter

The following screen will be displayed.

Figure 3-12
Alternative Design Results
Screen



Note that the variance component associated with handling cannot be separated from that associated with sample collection, and that the variance component associated with subsampling cannot be separated from that associated with analysis. This loss of information is a consequence of not using FES and ELES values in the study. The sampling and handling variance is equal to zero. This variance is the result of subtracting the error estimate for the preparation splits s_{ps}^2 from the error estimate for the field duplicates.

$$\sigma_h^2 + \sigma_s^2 = \sigma_{fd}^2 - \sigma_{ps}^2$$

For this example

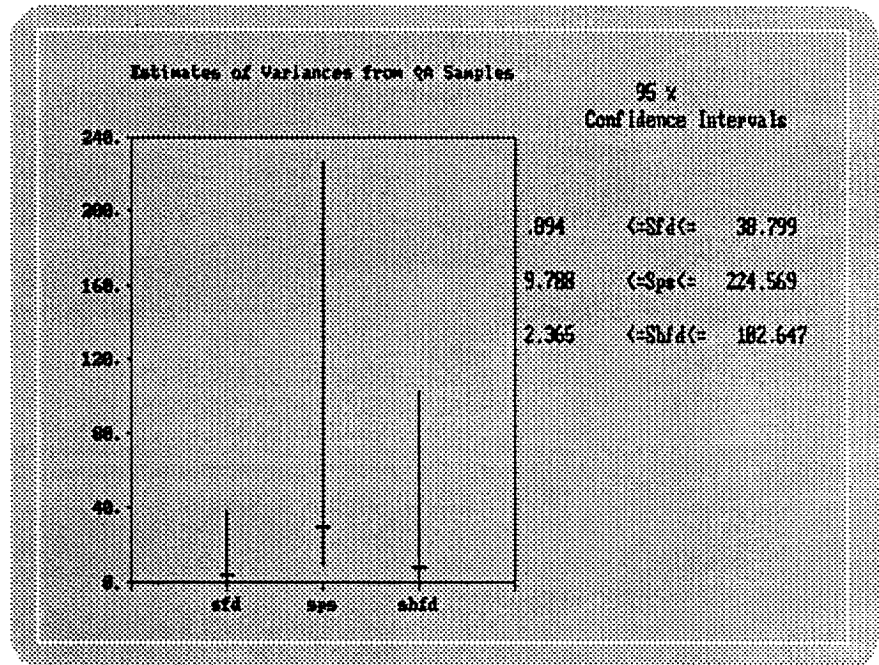
$$\sigma_h^2 + \sigma_s^2 = 2.793 - 27.188 = -24.395$$

ASSESS will report a value of zero, when the measured variance is a negative number. Follow the sequence of keystrokes:

Option	Action
Plot	Enter

The resulting graph is displayed in Figure 3-13.

Figure 3-13
Alternative Design Error
Bar Graph

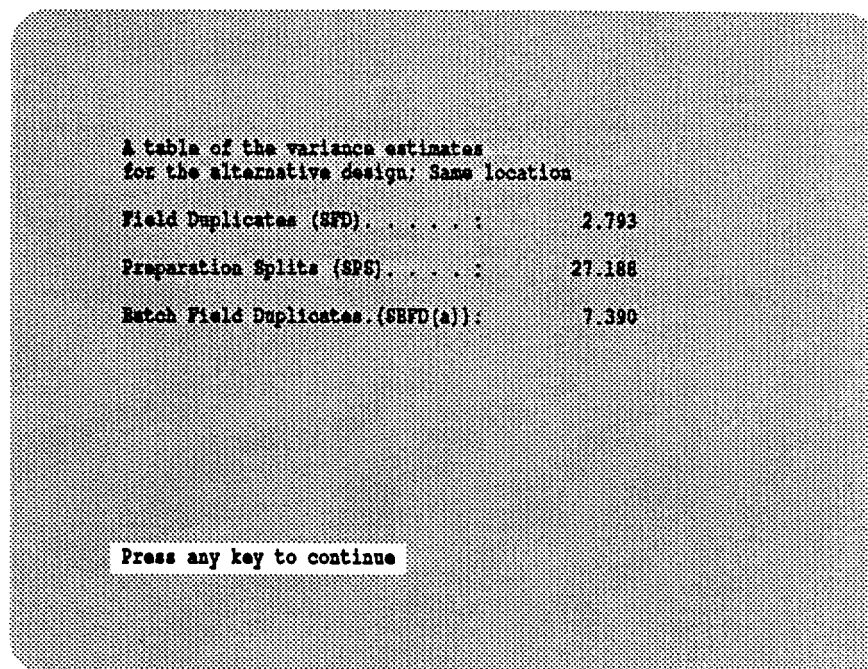


Notice the large confidence interval for the preparation split samples. Perhaps more preparation split samples could be taken to reduce this large interval.

Option	Action
<Q>	Enter
Var. Estimates	Enter
Press any key	Enter

The resulting table is displayed in Figure 3-14.

Figure 3-14
Variance estimates for the
Alternative Design



The displayed data in this figure is a summary of the computed error estimates for the alternative design. Note that the estimate for the batch field duplicates is the one computed for condition (a). This condition is appropriate when the batch field duplicates are all taken from one sampling location.

You may end this session by the following given keystrokes or proceed with the data transformation as previously discussed.

Option	Action	Field	Value
Press any key	Enter		
<Q>	Enter		
<Q>	Enter	Prompt	Yes

The file "Alt2.fil" is also included in the distribution diskette. This file contains data necessary to carry out the alternative design where Field Duplicate Samples are taken from different locations. Table (6) of the "Rationale Document"(I) is used for the calculations. Note that for this design the error estimate for batch field duplicate (s_{BFD}^2) is calculated using the equation denotated for part (b).



Appendix A

Data Files

The data files are simple ASCII text files which may be created with any text editor, and can be printed using the DOS print command. ASSESS can produce two types of output files; both of which contain the historical information (for notational purposes only) displayed on the screens, the summary of results, and the quality assessment data. One of these output files can be read in as a data file by ASSESS (see "Example.fil", next page), whereas the other output file uses a report- like format (see Report of Results which follows) and is not readable by ASSESS. A third file (see "Standard.fil" which follows), produced only by the user, is readable by ASSESS but lacks the descriptive labels included in the other two output files. The third file type is provided so that the user may edit an input file without having to enter all the data via ASSESS; (this method is faster in cases where the number of quality assessment data is large).

Two example data files are provided. As noted above "Example.fil" is an example of a file generated by ASSESS that can be used as an input file. When selecting the Data option in the Data Quality Objectives menu, a question appears asking which format to use. If the toggle "Input (with labels)" is chosen, then the file "Example.fil" may be selected. If the toggle "Standard (no labels)" is chosen, then the file "Standard.fil" may be selected.

An explanation of the formats used in "Example. fil", the reporting of results (report sent to the printer) and in "Standard.fil" follow.

Certain lines of historical information will have no information after the descriptive label. This is specific to the example at hand and not representative of data files in general.

"Example.fil" is a data file, created by ASSESS, that contains the computed variances as well as any historical information (for notational purposes) displayed on the screens. Quality assessment data is also included. This file is also an input data file; so if results and data changes are to be saved for later use, this file type should be created.

This file is generated by selecting the Report option of the Results screen menu and then selecting the option "File (input format)". The quality assessment data is listed at the end of the file. It includes "-9999" values which represent missing values (see the description in *Data File Example - "Standard.fil"* concerning the format for the quality assessment data, line 43). These "-9999" values permit ASSESS to read the data and convert the "-9999's" to empty fields.

Screen labels precede the entries, making the file self explanatory.

Figure A-1
Example.fil data file

DATA QUALITY OBJECTIVES				subsampling (no contamination) : .0000			
Site : Palmerton, Penn. (Phase I)				subsampling (contamination) : .0000			
Method : core				source:			
Analyte : Pb				analytical (no contamination) : .0000			
Analytical Method:				analytical (contamination) : .0000			
Desired Accuracy : +/- 20%				source:			
Desired Precision: +/- 20%				data handling : .0000			
Desired Confidence Ranges (95%)				source			
Bias : +/- 0%				SUMMARY OF RESULTS			
Precision: +/- 0%				number of RS : 20			
SAMPLING CONSIDERATIONS				number of FD : 10			
Number of Samples: 300				number of PS : 10			
Batches : 20				number of FES : 3			
Costs for				number of ELES : 0			
Sample Collection: .00				Total Measurement Error Variance: 5438.338000			
Analysis : .00				Sample-Collection Variance : Insufficient number of samples			
Batch Data				Between-batch Variance : 748.083400			
Number	Sampling Crew	Analytical Lab		Subsampling Variance : Insufficient number of samples			
1	single	single		Handling Variance : Insufficient number of samples			
END OF BATCH DATA				QUALITY EVALUATION DATA Transform: None			
HISTORICAL PRECISION ASSESSMENTS [VAR]				Concentrations: mg/kg			
Batch	RS	FD	PS	FES1	FES2	ELES1	ELES2
1	-9999.000	-9999.000	-9999.000	448.000	505.000	-9999.000	-9999.000
2	-9999.000	-9999.000	-9999.000	475.000	488.000	-9999.000	-9999.000
3	-9999.000	-9999.000	-9999.000	423.000	424.000	-9999.000	-9999.000
4	389.000	-9999.000	430.000	-9999.000	-9999.000	-9999.000	-9999.000
5	246.000	410.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
6	33.400	-9999.000	32.100	-9999.000	-9999.000	-9999.000	-9999.000
7	960.000	780.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
8	221.000	-9999.000	244.000	-9999.000	-9999.000	-9999.000	-9999.000
9	180.000	208.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
10	60.000	-9999.000	72.000	-9999.000	-9999.000	-9999.000	-9999.000
11	87.000	221.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
12	275.000	-9999.000	233.000	-9999.000	-9999.000	-9999.000	-9999.000
13	349.000	400.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
14	474.000	-9999.000	446.000	-9999.000	-9999.000	-9999.000	-9999.000
15	478.000	382.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
16	33.500	-9999.000	32.700	-9999.000	-9999.000	-9999.000	-9999.000
17	33.000	33.300	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
18	1360.000	-9999.000	1340.000	-9999.000	-9999.000	-9999.000	-9999.000
19	104.000	128.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
20	313.000	-9999.000	294.000	-9999.000	-9999.000	-9999.000	-9999.000
21	201.000	161.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
22	67.000	-9999.000	67.000	-9999.000	-9999.000	-9999.000	-9999.000
23	275.000	199.000	-9999.000	-9999.000	-9999.000	-9999.000	-9999.000
HISTORICAL MEASUREMENT BIAS ASSESSMENTS [%]				-2-			
sample collection (no contamination) : .0000							
sample collection (contamination) : .0000							
source:							
handling/preparation (no contamination): .0000							
handling/preparation (contamination) : .0000							
source:							

Data File Example - Report of Results

The report data file is created by ASSESS and contains the computed variances as well as any historical information displayed on the screens. Quality assessment data are also included. This file is the same as the "Example.fil" discussed in the preceding section with one exception: the quality assessment data has blanks where the "-9999" values were located. As a result this file cannot be used as an input data file.

This file is generated by selecting the Report option of the Results screen menu and then selecting the option "File (report format)". The file may be sent to the printer by selecting the "Printer" option.

Only the quality assessment data are shown below as the rest of the file is the same as "Example.fil" shown on the previous page. Note that the "-9999" values have been replaced with blanks.

Figure A-2
Report data file without the
historical information

QUALITY EVALUATION DATA				Transform: None			
Concentrations: mg/kg							
Batch	RS	FD	FS	FES1	FES2	ELIS1	ELIS2
1				448.000	505.000		
2				475.000	488.000		
3				423.000	424.000		
4	389.000		430.000				
5	246.000	410.000					
6	33.400		32.100				
7	960.000	780.000					
8	221.000		244.000				
9	180.000	208.000					
10	60.000		72.000				
11	87.000	221.000					
12	275.000		233.000				
13	349.000	400.000					
14	474.000		446.000				
15	478.000	382.000					
16	33.500		32.700				
17	33.000	33.300					
18	1360.000		1340.000				
19	104.000	128.000					
20	313.000		294.000				
21	201.000	161.000					
22	67.000		67.000				
23	275.000	199.000					

Data File Example - "Standard.fil"

"Standard.fil" is an input data file created by the user and stripped of any descriptive (screen) labels. ASSESS can read but cannot generate such a file. All entries must start in column 1. The number (e.g., '1.') that appears on each line is used as a line number reference and does not appear in the actual file. For descriptions of each line, referenced by the line number, follow the example.

Figure A-3
Explanation of standard.fil
data file

```
1.)Palmerton, Penn. (Phase I)
2.)coored
3.)Pb
4.)
5.)20
6.)20
7.)0
8.)0
9.)300
10.)20
11.) .00
12.) .00
13.)1      single      single
14.)END OF BATCH DATA
15.) .1000
16.)
17.) .0700
18.)
19.) .0500
20.)
21.) .2000
22.)
23.) .0500
24.)
25.) .0000
26.)
27.) .0600
28.)
29.) .0000
30.) .0000
31.)
32.) .0000
33.) .0000
34.)
35.) .0000
36.) .0000
37.)
38.) .0000
39.) .0000
40.)
41.) .0000
42.)
43.) 1 -9999.000 -9999.000 -9999.000 448.000 505.000 -9999.000 -9999.000
44.) 2 -9999.000 -9999.000 -9999.000 475.000 488.000 -9999.000 -9999.000
```

-1-

Descriptions: The descriptions are broken down into screens and include the screen label, type of field (A: Alphanumeric, 1: Integer, F: Floating point), and length of field.

Figure A-4

Explanation of Standard.fil
data file, continued

```
33.) Handling/Prep (contamination), F, 6.4
34.) Source, A, 26
35.) Subsampling (no contamination), F, 6.4
36.) Subsampling (contamination), F, 6.4
37.) Source, A, 26
38.) Analytical (no contamination), F, 6.4
39.) Analytical (contamination), F, 6.4
40.) Source, A, 26
41.) Data Handling, F, 6.4
42.) Source, A, 26
```

Quality Evaluation Data

43.) This is the first row of quality evaluation data. There are eight columns. The first column represents the batch number and is an integer. The remaining seven columns represent the routine subsample (RS), the field duplicate subsample (FD), the preparation split subsample (PS), the first field evaluation sample (FES1), the second evaluation sample (FES2), the first external laboratory evaluation sample (ELES1), and the second external laboratory evaluation sample (ELES2), respectively. All seven samples are floating point.

!!IMPORTANT!!

The -9999 represents an empty field. On line 43 of the above example only columns five and six have values other than -9999. This means that FES1 and FES2 have values of 448 and 505, respectively; and that RS, FD, PS, ELES1 and ELES2 have no values for that row of data. The -9999 must be entered in the column of the sample that has no value for that row. If it is not entered then Assess will either read the data incorrectly or will display an error message.

44.) Second row of quality evaluation data. A maximum of 1000 rows of such data may be entered.

-3-

Descriptions:

Data Quality Objectives screen

```
1.) Site, A, 64
2.) Method, A, 14
3.) Analyte, A, 14
4.) Analytical Method, A, 14
5.) Desired Accuracy, I, 4
6.) Desired Precision, I, 4
7.) Bias, I, 4
8.) Precision, I, 4
```

Sampling Considerations screen

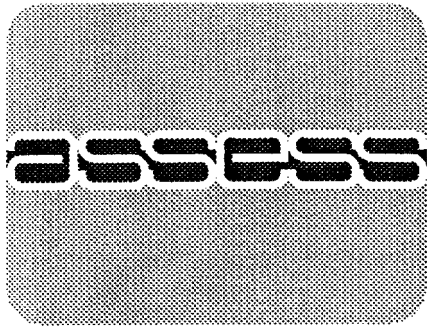
```
9.) Number of Samples, I, 10
10.) Number of Batches, I, 10
11.) Sample Collection, F, 10.2
12.) Analysis, F, 10.2

The following line is historical information about each batch of data. A
maximum of 10 such lines is permitted. If more than 10 are present then
the program will report an error in reading the data.
13.) Number, A, 7, Occupies columns 1-7.
13.) Sampling Crew, A, 15, Occupies columns 9-23.
13.) Analytical Lab, A, 15, Occupies columns 25-39.
14.) END OF BATCH DATA must appear. This tells Assess that the last line
of batch data descriptions (eg. line 13) has been written. An "E" or "e"
in the first column of this line is sufficient.
```

Historical Assessment screen

```
15.) Sampling, F, 6.4
16.) Source, A, 26
17.) Handling/Preparation, F, 6.4
18.) Source, A, 26
19.) Subsampling, F, 6.4
20.) Source, A, 26
21.) Laboratory analytical, F, 6.4
22.) Source, A, 26
23.) Data analysis, F, 6.4
24.) Source, A, 26
25.) Between batch, F, 6.4
26.) Source, A, 26
27.) Total measurement variance, F, 6.4
28.) Source, A, 26
29.) Sampling(no contamination), F, 6.4
30.) Sampling(contamination), F, 6.4
31.) Source, A, 26
32.) Handling/Prep (no contamination), F, 6.4
```

-2-



Appendix B

Reference

-
- (1) U. S, EPA. 1990. A Rationale for the Assessment of Errors in the Sampling of Soils. Environmental Monitoring Systems Laboratory, Las Vegas, Nevada. EPA/600/4-90/013.



Appendix C

Nomenclature

RS	Routine sample
FD	Field duplicate
PS	Preparation split
FES1	Field evaluation sample 1
FES2	Field evaluation sample 2
ELES1	External laboratory evaluation sample 1
ELES2	External laboratory evaluation sample 2
BFD	Batch field duplicate
Location	Location of a batch field duplicate sample
s_{FD}^2	Field duplicates error estimate
s_{PS}^2	Preparation splits error estimate
s_{WFES}^2	Field evaluation samples error estimate within batches
s_{BFES}^2	Field evaluation samples error estimate between batches
s_{WLES}^2	External laboratory evaluation samples error estimate
s_{BFD}^2	Batch field duplicates error estimate
σ_m^2	Total measurement error variance
σ_s^2	Sampling error variance
σ_b^2	Between-batch variance
σ_{ss}^2	Subsampling variance
σ_h^2	Handling variance
σ_a^2	Analytical variance
$\sigma_s^2 + \sigma_h^2$	Sampling and handling variance
$\sigma_a^2 + \sigma_{ss}^2$	Analytical and subsampling variance
n	Number of sample pairs
m	Number of batch field duplicate samples
L	Number of sample locations for the alternative design

