Agilent G1701DA MSD Productivity Software EnviroQuant Mode

EnviroForms User's Guide

Agilent Technologies

Notices

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Agilent Technologies, Inc.
2850 Centerville Road
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Acknowledgements

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CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

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1 Introduction

EnviroForms Software

Agilent EnviroForms software allows you to produce environmental reports based on analytical data from an Agilent GC or MS ChemStation. The reports contain quantitative results for target compounds, quality control data for surrogates, blanks, matrix spikes, and calibration samples. For analyses by mass spectrometer, you can also report library search results for non-target compounds and tune evaluation data. For GC analyses, you can report Florisil and GPC calibration data and a Pesticide Identification Summary. The terminology used on the printed forms complies with the US Environmental Protection Agency's Contract Laboratory Program Statement of Work (March 1993), but can be easily customized for other applications as well.

What you need

The requirements for optimum performance of EnviroForms software are listed below.

Microsoft Windows 2000 or XP Configuration

- Either Windows 2000 Professional (Service Pack 3 (SP3), or later), or Windows XP (Service Pack 1a (SP1a) or later) must be installed as the operating system.

NOTE ChemStation software is not supported on Windows 2000 Professional Server software or on Windows NT.

- If you are upgrading from an earlier revision of the MSD ChemStation Software, you may have to change operating systems. See Upgrading from Earlier Versions in Chapter 5.
- The MSD ChemStation software requires that all disk partitions on the MSD ChemStation computer hard drives be formatted for NTFS and that active file systems are uncompressed.

- Minimize the Windows 2000 or XP desktop configuration as follows:
  - minimum desktop icons
  - no screen saver enabled
  - no background or tray applications
- Disable unused computer hardware such as USB in the BIOS
- The TCP/IP networking protocols must be installed and enabled; NetBEUI needs only to be installed if printer and/or files are to be shared.
- Microsoft Internet Explorer 5.5 or greater is required.
- Some devices which Windows 2000 or XP supports are not supported by MSD ChemStation software, for example magneto-optical drives and external CD-ROM writers. Do not use these devices.
- A Windows 2000 or XP repair disk must be created during installation, and recovery disks must be created.

Windows 2000 or XP Computer Hardware Considerations

The minimum requirements for operation of the MSD ChemStation Software are:

- A Pentium ® III computer (450 MHz or faster)
- BIOS which supports Windows 2000 with Service Pack 3 (or later) or Windows XP with Service Pack 1a (or later)
- All power-saving features of the BIOS disabled
- All power-saving programs removed
- An SVGA color monitor
- 1024 x 800 x 65,536 colors video display resolution (maximum supported resolution is 1600 x 1200 x 16,000,000 colors)
- 64 MB of RAM (additional RAM required for multiple instruments)
  - 128 MB for dual MSD acquisition
  - 256 MB for quad GC acquisition

- At least 800 MB of hard disk storage (MSD ChemStation program files use ~115 MB)
- A CD-ROM drive
- A sound card and speakers or headphones
- A Windows 2000 or XP supported mouse
- A data backup device is strongly recommended
- Printer Support
  - All DeskJet printers: These printers are not tested and are not supported.
  - LaserJet 4050 and 4100: These printers are not tested but inherit support because they were tested on older revisions. The supported drivers are PCL 5e or PCL 6, revision 5.02.
  - LaserJet 2200d and 2300dn: These printers are fully tested and are supported. The supported drivers are Post Script revision 5.02.
- MSD communication card
  - A PCI Network Interface Card for LAN-based systems
  - A PCI GPIB Control Card 82350A or 82350B for GPIB-based systems

2 Getting Started

What is Agilent EnviroForms Software?

Agilent EnviroForms software allows you to easily generate quantitative reports for your samples which include the following information:

- Quantitative results for up to 200 target compounds and, for MS data only, library search results for non-target compounds found (Form 1)
- A surrogate recovery report, which shows, for each sample, the analyte loss due to sample preparation (Form 2)
- A matrix spike report, which shows the effect of the sample matrix (water or soil) on analyte recovery (Form 3)
- A blank report, which correlates samples with their method blanks (Form 4)
- (MS data only) A tune evaluation report, which documents the calibration and performance of the GC/MS system (Form 5)
- An initial multi-point calibration report (Form 6)
- A continuing single-point calibration report (Form 7)
- An internal standard area and retention time stability report (Form 8)
- (Pesticides only) A Florisil cartridge check and GPC calibration (Form 9)
- (Pesticides only) An identification summary for single and multicomponent analytes (Form 10)

How it works

EnviroForms software manages and generates reports for lists of samples. A list of samples may include blanks, unknowns, and initial and continuing calibration samples and the analytical results for each. A sample list is associated with a list of compounds to report. A compound list contains the names of all compounds and the QA/QC parameters for reporting each compound.

EnviroForms stores sample lists and compound lists in Environmental Reporting Methods (ERMs). Each ERM can contain up to three compound lists; one each for volatiles, semi-volatiles, and pesticides. More than one sample list can be associated with each fraction. The relationships between ERMs, sample lists, and compound lists are shown in Figure 1.

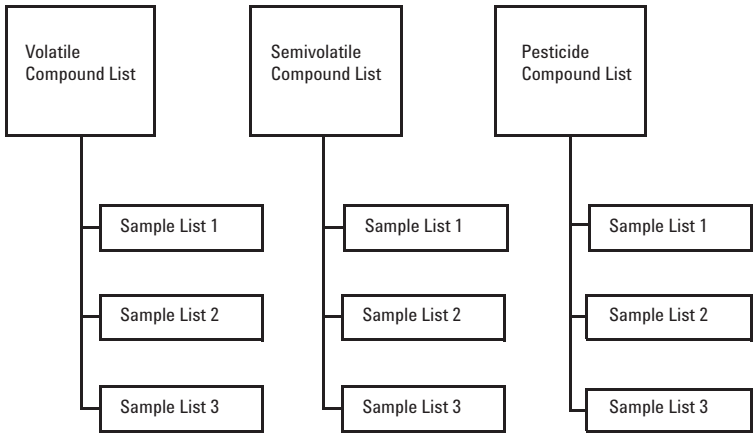


Figure 1 Environmental Reporting Method (ERM)

Forms available

You can use EnviroForms software to print the forms in Table 1 for various fractions

Table 1 Available forms

Fraction	Forms
Volatiles	Forms 1A, 2A, 2B, 3A, 3B, 4A, 5A, 6A, 7A, 8A
Semi-volatiles	Forms 1B, 1C, 2C, 2D, 3C, 3D, 4B, 5B, 6B, 6C, 7B, 7C, 8B, 8C
Pesticides	Forms 1D, 2E, 2F, 3E, 3F, 4C, 6D, 6E, 6F, 7D, 8D, 9, 10

You can customize the final printed forms by specifying the labels for some of the data that appears on the forms. Without customization, the terminology on the reports complies with the US Environmental Protection Agency's March 1993 Contract Laboratory Program Statement of Work (USEPA CLP SOW). With customization, the forms can reflect the USEPA CLP SOW Version OLM02.0 forms. Example forms can be printed using the demo data supplied with your EnviroForms software (load demo.erm, then select **Print One of Each Form** from the Help menu).

Related products

Agilent EnviroForms software is optimized for laboratories that carry out GC or GC/MS analyses with groups of 20 to 100 samples. Use one of the following alternative products if your methodology is different or if you run less than 20 or more than 100 samples in a group:

- If your methodology requires reports for single samples only, use the Custom Reports software that is part of EnviroQuant Mode of Data Analysis or Enhanced Mode of Data Analysis which is part of the MSD Productivity ChemStation software.
- If your methodology includes long-term studies using large sample groups, or where historical records must be kept, use a LIMS product such as Agilent's data systems.
- If you are a participant in the US EPA Contract Laboratory Program, use the reduced results (.rr) files generated by Environmental Data Analysis to transfer the data to the application program you use to create the required diskette deliverables.
- If you need further customization of the forms or want to output the forms electronically, purchase Microsoft Access. You can use Access to further manipulate the files or to export them in various formats. These exported files can then be used as input to a variety of software programs, such as word processing or desktop publishing applications.

Online help

You can access online help for the Environmental Forms software in any of the following ways:

- Select a topic from the Help menu.
- Click the **Help** button in any dialog box.
- The EDA Configuration panel is used to customize the operation and functionality of the Data Analysis software. The configuration may be changed at any time by selecting **File** / **EDA Configuration in Data Analysis**.

To Prepare Data for Forms Production

Input files required for forms

Use the Enviromental Data Analysis program (EDA) as described below to prepare data for forms production. This procedure assumes you have already analyzed the samples of interest, including a tune evaluation sample, calibration samples at each calibration level, blanks, surrogates, and quality control samples using the Agilent MSD Productivity ChemStation. EDA software provides both the individual data files for all samples analyzed, as well as the list of compounds in the quantitation database.

The MSD Productivity ChemStation can be configured for up to four instruments with each instrument can have one of four Data Analysis modes: Enhanced Quantitation, EnviroQuant, Aromatics in Gasoline, and Drug Analysis.

EnviroQuant (EPA) mode is specifically designed to meet the needs of laboratories performing analyses compliant with USEPA methodology.

Configure a designated instrument number for EnviroQuant (EPA) mode and then click on the desktop ICON to run either the EnviroQuant Data Acquisition or the EnviroQuant Data Analysis mofe of operation.

1 If the Environmental Data Analysis program is not already running, start it by double-clicking the EDA icon. If the Forms menu items are not already enabled, select **EDA Configuration** from the File menu, click the **Forms Menus** option, then click **OK**.

2 Establish a quantitation database entry for each target compound, and update the calibration table as described in the Environmental Data Analysis *User's Guide*.

   - When the initial calibration is acceptable, select **Response Factors to Forms File** from the InitCal menu to produce a cal.csv file for each data file in the initial calibration table (note: cal.csv file is saved under the data file).

- Select **Evaluate Data file as Continuing Cal to Forms File** from the ConCal menu to generate a cal.csv file for each continuing calibration sample.

3 Select **Make Compound List for Forms** from the InitCal menu to generate a cmpdlist.csv file. Once the list is created, you can modify reporting parameters for individual compounds as described in Chapter 4 (note: cmpdlist.csv is saved under the method file).

4 After each unknown, matrix spike, and blank sample is analyzed, quantitated, and reviewed for correctness, select **Generate Report to Forms File** from the Quant menu to create a quant.csv file for each sample. The analytical results in the quant.csv files become part of the EnviroForms sample list as described in *Chapter 3*, "Setting Up Sample Lists". If a data file is requantitated or if the results are reintegrated manually, generate a *new* quant.csv file to reflect the updated results (note: quant.csv is saved under the data file.)

5 (MS data only) Generate a tune.csv file as follows:

- For volatiles, select **Evaluate BFB to Forms File** from the Tuner menu. Select **Tuner**, click on **Evaluate BFB**, select **Evaluate BFB to Forms File** then click on **OK**. Tune evaluation data is reported on Form 5A for volatile samples. (note: Tune.csv is saved under the data file.)
- For semi-volatiles, select **Evaluate DFTPP to Forms File** from the Tuner menu. Select **Tuner**, click on **Evaluate DFTPP**, select **Evaluate DFTPP to Forms File** then click on **OK**. Tune evaluation data is reported on Form 5A for volatile samples. (note: Tune.csv is saved under the data file.)

NOTE Use Table 2 as a quick reminder of the files required by the EnviroForms software and the menu items used to generate them in the Environmental Data Analysis software.

Table 2 Files and menu items

Type of data	File produced	Menu	Menu item
Compound list	cmpdlist.csv	InitCal	Make Compound List for Forms
Initial calibration	cal.csv	InitCal	Report Calibration Table to Forms File
Continuing calibrations	cal.csv	ConCal	Evaluate Data File as Continuing Cal to Forms File
Blank, unknown, and matrix spikes samples	quant.csv	Quant	Generate Reports to Forms File
Tune evaluation (MS data only)	tune.csv	Tuner	Evaluate BFB/DFTPP to Forms File

See Also

"To Produce Environmental Forms" on page 19.

To Produce Environmental Forms

The form production process is outlined in Figure 2.

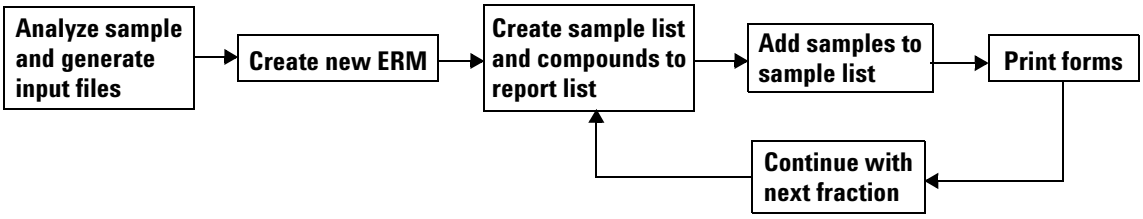


Figure 2 Producing environmental forms

1. Analyze the samples for the first fraction and generate the input files required by EnviroForms as described in *"To Prepare Data for Forms Production"* on page 16.
2. Create an environmental reporting method (ERM) for the samples of interest. See Chapter 3 for more information.
3. Create a new sample list for the group of samples to be reported. If this is the first sample list for a fraction, you are prompted to load a compound list from Environmental Data Analysis or from an existing ERM. If necessary, add or delete compounds or modify compound reporting parameters and limits. See Chapter 4 for more information.
4. Add samples to the sample list, including calibration samples, method blanks, matrix spikes, and unknown samples analyzed for this fraction. See Chapter 3 for more information.

   To speed up the process, you can set up the compound list and the ERM as described in the above steps after only *some* of the samples have been analyzed. You can then add additional samples as they are analyzed by repeating step 1 and step 3 only. But wait until the entire set of samples for a fraction is complete before *printing* any forms as described in step 5.

5 Print the desired environmental forms for this sample list as described in Chapter 5.

Wait until *all* the related samples have been analyzed and the required input files generated from EnviroQuant Data Analysis before you attempt to print *any* environmental forms, because each form requires information from several input files. Although some forms *might be* correctly generated with only some of the input files present, it is more likely that individual forms based on a partial set of input files would be incomplete or inaccurate. For example, an Organics Analysis Data Sheet (Form 1) produced before the method blank has been processed would not be able to flag compounds that were detected in the blank.

6 If you have additional fractions to include in this ERM, analyze the samples for the next fraction and generate the input files required by EnviroForms. Repeat step 3 and step 4 to set up sample lists and compound lists for this fraction, then print the forms as described in step 5.

3
Setting Up Sample Lists

Setting Up Sample Lists

Sample lists determine what samples will be reported on the environmental forms reports and specify the header information to be reported for each sample. Set up a sample list in the EnviroForms software to match a set of samples analyzed in your lab (often called a Sample Delivery Group).

Quantitative results for individual samples are copied to the sample list from the quant.csv files generated in Environmental Data Analysis. Separate sample lists are created in EnviroForms for volatile, semi-volatile, and pesticide fractions. Sample lists are associated with a compound list and reporting criteria for a fraction. A sample list can contain many samples but is limited to one set of initial calibration files. A new sample list must be created when a new initial calibration is performed for a fraction.

As described in Chapter 4, compound lists are also created for volatile, semi-volatile, and pesticide fractions within an environmental reporting method (ERM). In this way, you can specify which compounds are reported on the final printed forms for a particular group of samples.

To facilitate the process of creating a sample list, much of the header information that is often the same for all samples in a group can be specified only once. This header information is then supplied automatically and can be customized as necessary for individual samples.

To Create a New ERM

An environmental reporting method determines which samples and compounds will be reported on the volatile, semi-volatile, and pesticide environmental forms. Figure 3 describes how to set up a new environmental reporting method (ERM) for a group of samples:

The compound lists are created and managed in the Compound List Manager dialog box.

Figure 3 Creating an ERM

1. Select **Create ERM** from the File menu.
2. Type in a name for the new ERM, then click **OK**. Unless you specify otherwise, the new ERM will be stored in the \msdchem\envforms directory.
3. When the Create Sample List dialog box appears, select the fraction type for the samples (**Volatile**, **Semivolatile**, or **Pesticide**).
4. Type in a name for the Sample List or accept the default name, which is based on the fraction type and the current date, then click **OK**.
5. When the message **The Compound List is empty. Read Compound List?** appears, click the **Yes** button. You can load a compound list from either an Environmental Data Analysis method or an existing ERM. For more information on creating and customizing compound lists, see Chapter 4.
6. When you have finished creating the compound list and specifying the compound reporting parameters, click the **Edit Samples** button on the toolbar of the EnviroForms window.
7. When the message **Edit Default Sample Header values?** appears, click the **Yes** button. Specify header information to be used as

default information for all samples as described in *"To Set Default Header Information"* on page 25.

8 Create the list of samples as described in *"To Create a Sample List"* on page 30.

9 (Optional) To create sample lists for other fractions, select **Create Sample List** from the File menu. Repeat step 3 through step 8 above to define the samples and compounds for each additional fraction.

10 See Chapter 5 to generate forms for the sample lists defined in this procedure.

To Set Default Header Information

Use the following procedure to specify sample header information to be used as defaults for all samples. All these default values can be modified for individual samples as described in *"To Create a Sample List"* on page 30 and *"To Modify a Sample List"* on page 35.

1 If the Edit Default Sample Information box is already displayed, see step 2 to fill in the panel. Otherwise, select **Default Sample Values** from the Samples menu. The example in Figure 4 is for volatiles. The information requested for semivolatiles and pesticides is slightly different.

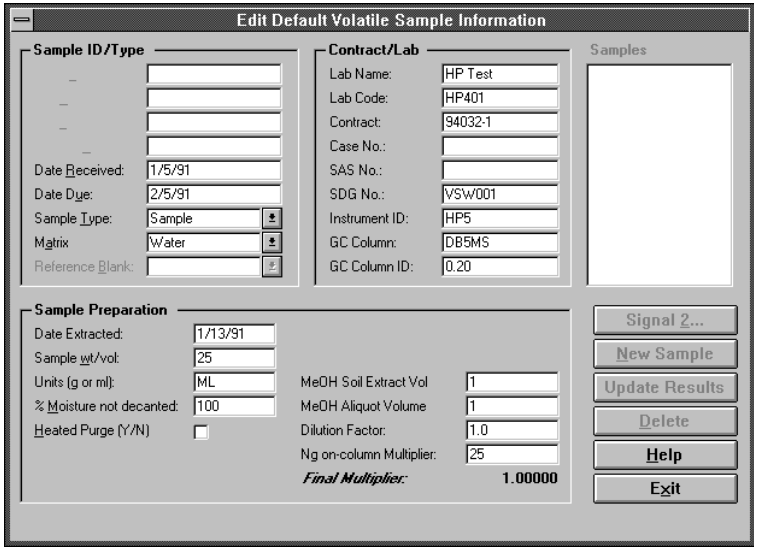


Figure 4 Default header information

2 Type in the information that you expect to be the same for most samples in the sample list, including any of the fields described on the following pages. When you have specified the desired default values, click the **Exit** button.

Sample ID / Type information

Date Received The date the samples were received by the lab.

Date Due The date the report is due or the data when data acquisition must be completed.

Sample Type One of the sample types from Table 3.

Table 3 Sample types

Sample	Description
Sample	An unknown sample to be analyzed for target compounds.
Re-Extraction	A sample that was re-extracted and reanalyzed.
Dilution	A sample analyzed at a secondary dilution.
Matrix Spike	A sample that contains known amounts of target compounds to check method reproducibility and matrix interference.
Matrix Spike Duplicate	A duplicate of the Matrix Spike sample.
Method Blank	A blank sample used to check for system contamination.
Initial Calibration	A sample used to generate the initial calibration.
Initial Continuing Calibration	The mid-level initial calibration sample that the continuing calibration will be checked against.
Continuing Calibration	The continuing calibration standard that is run and checked against the Init. Cont. Calib. Std. sample.
Tune Evaluation	(MS data only) The sample run to check the BFB or DFTPP tuning.

Matrix **Water**, **Soil Low**, or **Soil Medium**

Reference Blank The reference blank to associate with this sample. Click the arrow to the right of this field to view a list of blanks. The blanks are listed by Sample Names and Lab File Names.

Contract/Lab information

Lab Name The name of your laboratory.

Lab Code The name or number of the project for the samples. For CLP forms, use your lab code assigned by the EPA.

Contract The contract number or code. For EPA work, the contract number is included with the sample when it arrives at your lab.

Case No. The designation for the site where the sample was collected. For CLP forms, enter the case number that was included with the sample when it arrived at your lab.

SAS No. The designation for the location where the sample was collected at the site. For CLP forms, enter the SAS number that was included with the sample when it arrived at your lab.

SDG No. The name of the current sample list or sample delivery group. For CLP forms, enter the sample delivery group (SDG) number that was included with the sample when it arrived at your lab.

Instrument ID The identification of the instrument used to analyze the samples. This designation must be unique within your laboratory. This value will be overwritten for individual samples if their quant.csv file identifies the instrument.

GC Column The identification of the column used to analyze the samples. This value will be overwritten for individual samples if their quant.csv file identifies the GC column.

GC Column ID The internal diameter of the GC column in millimeters. This value will be overwritten for individual samples if their quant.csv file identifies the internal diameter of the GC column.

Sample Preparation information - All fractions

Date Extracted The date the samples were extracted.

Sample wt/vol The sample weight in grams or its volume in milliliters.

Units (g or ml) The units used for Sample wt/vol. Use G for grams or ML for milliliters.

Dilution Factor The dilution factor used for the samples. Use 1 if the samples were *not* diluted or concentrated.

Ng on-column Multiplier Used to correct for unit differences between Environmental Data Analysis and EnviroForms. For example, if you use parts-per-billion (ppb) units in EDA, but want to report parts-per-million (ppm) on the environmental forms, use a multiplier of 0.001.

Also used to correct for the expected sample volume of water samples. For example, you have set up the method to use 25 mL samples. For a standard sample, you would enter Sample wt/vol as 25 and Ng on-column Multiplier as 25. If insufficient sample amount exists for a reanalysis and less that 15 mL is used, enter 15 mL as the Sample wt/vol and 25 mL as the Ng on-column Multiplier.

Final Multiplier For display only.

Sample Preparation information - Volatiles

% Moisture not decanted The percentage of moisture not decanted, rounded to the nearest percent. Don't type in the % sign.

Heated Purge (Y/N) Click to select this box if a heated purge cycle was used. Leave this box blank if the purge cycle was *not* heated. Since the purging efficiencies are different between heated and non-heated purges, all samples in a list should be run with the same purge technique.

MeOH Soil Extract Volume The volume in microliters used to extract a soil sample.

MeOH Aliquot Volume The volume in microliters of the aliquot taken from a soil extract.

Sample Preparation information - Semivolatiles

% Moisture The percentage of moisture in the samples, rounded to the nearest percent. Don't type in the % sign.

Decanted (Y/N) Select this box if the samples were decanted. Leave this box blank if the samples were *not* decanted.

pH The pH of the samples to one decimal place accuracy.

GPC Cleanup (Y/N) Select this box if the samples were cleaned up with GPC. Leave this box blank if the samples were *not* cleaned up with GPC.

Extract Vol. The volume of the concentrated extract in microliters.

Injection Volume The injection volume in microliters.

Sample Preparation information - Pesticides

% Moisture The percentage of moisture in the samples, rounded to the nearest percent. Don't type in the % sign.

Decanted (Y/N) Select this box if the samples were decanted. Leave this box blank if the samples were *not* decanted.

pH The pH of the samples to one decimal place accuracy.

Extraction Type **SepF** for separatory funnel, **Cont** for continuous liquid-liquid, or **Sonc** for sonication.

GPC Cleanup (Y/N) Select this box if the samples were cleaned up with GPC. Leave this box blank if the samples were *not* cleaned up with GPC.

Sulfur Cleanup Select this box if the samples were cleaned up with sulfur. Leave this box blank if the samples were *not* cleaned up with sulfur.

Concentrated Extract Vol. The volume of the concentrated extract in microliters.

Injection Volume The injection volume in microliters.

To Create a Sample List

Use the following procedure to create a new sample list for the current ERM (shown in the title bar of the EnvForms program window). You must create a sample list for each fraction in an ERM. You must create a *new* sample list whenever you perform a new initial calibration on your system. Only one initial calibration is allowed per sample list.

1 If the Edit Sample Information box is already displayed, skip to step 8 to begin adding samples. Otherwise, select **Create Sample List** from the File menu (Figure 5).

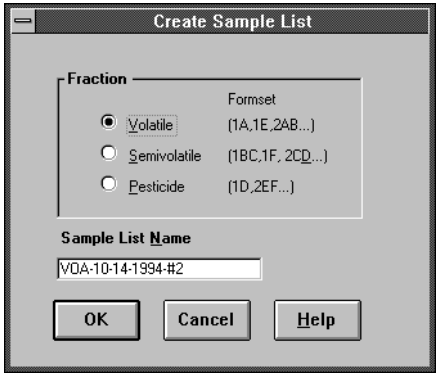


Figure 5 Create sample list

2 Select the fraction type for the samples (**Volatile**, **Semivolatile**, or **Pesticide**).

3 Type in a name for the Sample List or accept the default name, which is based on the fraction type and the current date, then click **OK**.

4 When the message **The Compound List is empty. Read Compound List?** appears, click the **Yes** button. You can load a compound list from either an Environmental Data Analysis method or an existing ERM.

5 When you have finished creating the compound list, click the **Edit Samples** button on the toolbar of the EnviroForms window or select **Enter-Edit Sample** from the Samples menu.

6 To specify default header information for the sample list, see *"To Set Default Header Information"* on page 25. Once specified, the default header information will appear for each sample you add to the sample list. The header information can be modified for individual samples as described later in step 13.

7 When the Edit Sample Information box appears, use it to set up the sample list as described in Steps 8 through 16. The box shown in Figure 6 is for volatiles. The information requested for semivolatiles and pesticides is slightly different.

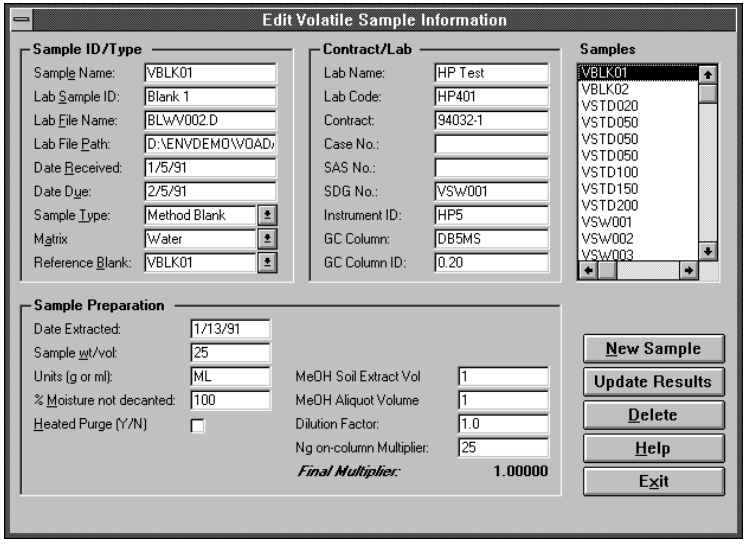


Figure 6 Edit sample information

8 To start the sample list, read in the quantitative results for the first sample by clicking the **Quant File** button (Figure 7).

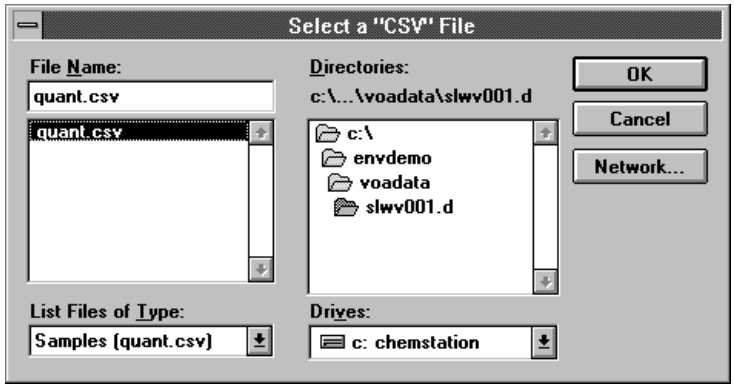


Figure 7 Selecting a data file

9 When the list of data files appears, select the file of interest for this sample by double-clicking the name of its data file in the list on the right side of the panel. The .csv files generated for this sample are displayed on the left side of the panel.

10 Use the list box in the lower left corner of the screen to select the type of .csv file appropriate to the sample type (Table 4).

Table 4 .csv file usage

File type	Description
Use cal.csv	For initial or continuing calibration samples.
Use quant.csv	For samples, blanks, and matrix spikes.
Use tune.csv	(MS data only) For the tune evaluation sample.

11 Click the .csv file in the list, then click **OK**. As with any Windows file selection box, you can also load the file by double-clicking the file name of interest.

12 If necessary, modify any of the default header information for the current sample by clicking the field of interest and typing

in the desired values. The following parameters usually have to be modified for each sample:

Sample Name Unique name to identify the individual sample.

Lab Sample ID The name this sample is known by within your lab (up to eight characters).

Lab File Name The name of the data file created when the sample was analyzed, including the .d extension. You can leave this field blank if the sample analysis is not yet complete.

Lab File Path The full path name for the directory where the data file is located. For example, data files acquired on an MS ChemStation are often stored in c:\msdchem\1\data.

Sample Type Select a type from Table 5 for this sample.

Table 5 Sample types

Sample type	Description
Sample	An unknown sample to be analyzed for target compounds.
Re-Extraction	A sample that was re-extracted and reanalyzed.
Dilution	A sample analyzed at a secondary dilution.
Matrix Spike	A sample that contains known amounts of target compounds to check method reproducibility and matrix interference.
Matrix Spike Duplicate	A duplicate of the Matrix Spike sample.
Method Blank	A blank sample used to check for system contamination.
Initial Calibration	A sample used to generate the initial calibration.
Initial Continuing Calibration	The mid-level initial calibration sample that the continuing calibration will be checked against.

Table 5 Sample types (continued)

Sample type	Description
Continuing Calibration	The continuing calibration standard that is run and checked against the Init. Cont. Calib. Std. sample.
Tune Evaluation	(MS data only) The sample run to check the BFB or DFTPP tuning.

13 Repeat step 8 through step 12 for each sample you wish to include in this sample list. As you move to the next sample, you are prompted to confirm that you want to save changes to the current sample.

14 (GC data with two signals only) To modify sample information for a different signal, click the **Signal 1 2** button. The sample information for signal 2 will be displayed. You can modify the Lab File Path, the Contract/Lab information, and the Sample Preparation information. You *cannot* select a quant file, add a new sample, or delete a sample. Use the same button, now labeled **Signal 2 1**, to return to the sample list for the first signal.

15 When all the changes have been made to the sample list, click the **Exit** button. You are prompted to confirm saving changes to the last sample you modified.

See Also

"To Modify a Sample List" on page 35

"To Display or Print Sample Information" on page 37

To Modify a Sample List

1 If the sample list you want to edit is the one currently displayed in the title bar of the EnvForms window, skip to step 2. Otherwise:

- To load a different sample list in the same ERM, click the **Sample List** button on the toolbar of the EnvForms program window.
- To load a sample list in a *different* ERM, select **Open ERM** from the File menu. You are prompted to select a sample list.

2 Click the **Edit Samples** button on the toolbar of the EnvForms program window to display the Edit Sample Information dialog box.

3 You can change the sample list in any of the following ways:

- To change header information for any of the samples, select a sample by clicking it in the list of samples. You can then modify any of the fields on the panel by clicking the field, then typing in a new value. The sample information fields are described in *"To Set Default Header Information"* on page 25 and *"To Create a Sample List"* on page 30 earlier in this chapter. You are prompted to save the changes when you select another sample to edit or try to exit the panel.
- To add a sample, click the **New Sample** button and fill in the information as described earlier in this chapter.
- To delete a sample, select the sample by clicking it in the list, then click the **Delete** button. You are prompted to confirm deletion of the current sample.
- To update the quantitative results for a sample from the same data file name, click the **Refresh Results** button.

4 (GC data with two signals only) To modify sample information for a different signal, click the **Signal 1 2** button. The sample information for signal 2 will be displayed. You can modify the Lab File Path, the Contract/Lab information, and the Sample Preparation information. You *cannot* select a

quant file, add a new sample, or delete a sample. Use the same button, now labeled **Signal 2 1**, to return to the sample list for the first signal.

5 When all the changes have been made to the sample list, click the **Exit** button. You are prompted to confirm saving changes to the last sample you modified.

To Display or Print Sample Information

You can display and print the information in the sample list in various ways as described below. These procedures are for viewing data only; see *"To Modify a Sample List"* on page 35 if you want to make any changes.

1 If the sample list you want to view is the one currently displayed in the title bar of the EnvForms window, skip to step 2. Otherwise:

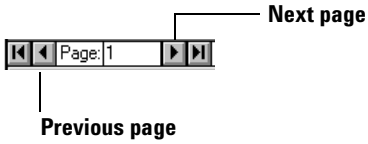
   - To load a different sample list in the same ERM, click the **Sample List** button on the toolbar of the EnvForms program window.
   - To load a sample list in a *different* ERM, select **Open ERM** from the File menu. To see an example of each listing, use the sample data provided in demo.erm.

2 Select an item (Table 6) from the Utilities menu.

Table 6 Utilities

Name	Displays
Display Sample Information	Header information for a selected sample.
Display Sample List	List of samples, including the Lab File ID, EPA Sample ID, Lab Sample ID, date acquired, data received, and date due for each sample.
Display Header Summary	Header information for all samples in the list in a single table.
Display Sample Group Summary	List of samples grouped by sample type, including data file names and the date and time each file was acquired.

3 The first page of the table appears on the screen. Use the page arrow buttons at the lower left part of the window to view more data.



4 To print the list to the Windows default printer, select **Print** from the File menu or click the **Print** button.

5 To exit the display window, select **Close** from the File menu or click the **Close** button.

4
Setting Up Compound Lists

Setting Up Compound Lists

Compound lists determine what compounds will be reported on the environmental forms reports for a particular sample list within an environmental reporting method. A compound list also defines the parameters for reporting the results for each compound, such as compound type (Target, Matrix, Surrogate, ISTD), detection limits, and cutoff values for flagging data (minimum response factor, minimum relative standard deviation, and maximum response factor deviation).

The initial compound list comes from the cmpdlist.csv file generated from Environmental Data Analysis as described in Chapter 2. Compound lists are stored as part of an environmental reporting method (ERM) in EnviroForms. From within EnviroForms, a compound list can be modified and printed as described in this chapter.

You may want to vary the reporting parameters in the compound list and save different versions of the list in different ERMs. When these different compound lists are applied to the same sample list, you can produce more than one set of reports for the same samples. For example, you might want to have a more stringent set of quality control parameters for in-house use, or you might want to produce forms with only a few key compounds of interest, in addition to full reports.

To Load or Select a Compound List

The current environmental reporting method and sample list are displayed in the title bar of the EnviroForms program window. To modify the compound list for the current sample list, skip to the next section. Otherwise, follow the directions below to load or select a different compound list to associate with the current sample list and ERM. When you create a new sample list or ERM as described in Chapter 3, you are *automatically* prompted to load a compound list.

1 If the Load Compound List box is already displayed, skip to step 2. Otherwise, select **Load Compound List** from the Edit menu (Figure 8).

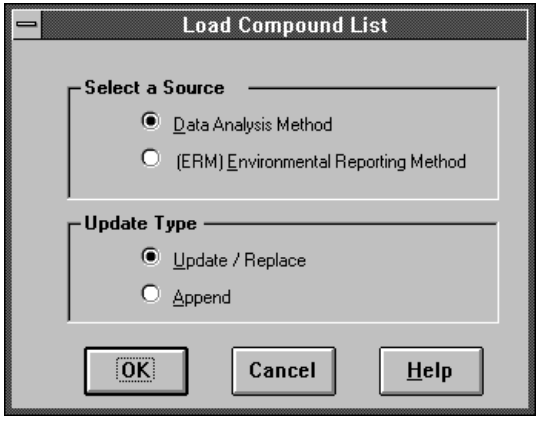


Figure 8 Load compound list

2 Select a Source for the compound list, either a **Data Analysis Method** or an existing **Environmental Reporting Method**.

3 Select the Update Type, either **Update / Replace** or **Append**, then click **OK**.

4 When the file select dialog box appears, select a cmpdlist.csv file in the method directory of interest for a Data Analysis method or the appropriate .erm file for an Environmental Reporting Method, then click **OK**. As with any Windows file selection dialog box, you can also load the file by double-clicking the file name of interest.

See Also

"To Modify a Compound List" on page 43

To Modify a Compound List

Use this procedure to modify the compound list associated with the current sample list (displayed in the title bar of the EnviroForms program window). To modify the compound list for a *different* sample list or ERM, load that sample list or ERM as described in Chapter 3. To associate a *different* compound list with the current sample list and ERM, see *"To Load or Select a Compound List"* on page 41.

1 If the Compound List Manager box (Figure 9) is already displayed, skip to step 2. Otherwise, click the **Edit Compound List** button on the toolbar of the EnviroForms window or select **Edit Compound List** from the Edit menu. When you create a new sample list or ERM as described in Chapter 3, you are *automatically* prompted to load and modify a compound list.

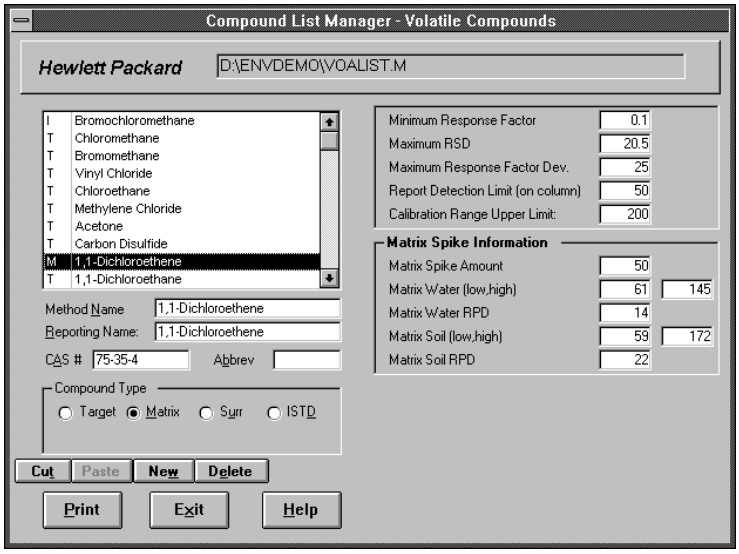


Figure 9 Compound list manager

The reporting parameters for the first compound are displayed. Note that the compounds will be reported on the forms in the order they appear in the compound list. To change the order of the compounds, see step 5.

2 Modify the reporting parameters for the current compound if necessary.

- Select a **Compound Type** of either **Target**, **Matrix**, **Surr**, or **ISTD**. Notice that additional fields appear on the panel when you select the **Matrix** or **Surr** compound types.
- Modify any reporting parameter by clicking a field to select it, then type in the new information.
- To clear *all* fields for the current compound, click the **New** button, then type in the new information for each field.
- For more information, see the description of the compound reporting parameters at the end of this section or in online help.

3 To modify the reporting parameters for a different compound, click the compound of interest in the list. The reporting parameters for the selected compound are displayed and can be modified as described in step 2. You are asked to confirm saving changes to the previous compound before the parameters for the next compound are displayed.

4 To remove a compound from the list, select the compound by clicking it, then click the **Delete** button. You are prompted to confirm deletion of the current compound.

5 To change the order that compounds appear in the list, select the compound you want to move by clicking it, then click the **Cut** button. Select the new position in the list and click **Paste**. The compound is inserted in the list *above* the current selection.

6 To add a compound to the list, use the **Cut** and **Paste** buttons. If you have already cut a compound as described in step 5, select a position in the list for the new entry and click **Paste**. The compound is inserted in the list *above* the current selection.

If you haven't already cut a compound as described in step 5, cut and paste a compound to its original position, then paste the entry again where you want the new entry to appear in the list.

Change the compound name simply by entering the new compound name in the already highlighted **Name** field. Change other parameters as necessary by clicking a field to select it, then type in the new information.

NOTE If you plan to change *all* parameters for the new compound, click the **New** button to clear all the values from the old compound, then type in the new values.

7 (GC data with two signals only) To modify the compound information for a different signal, click the **Signal 1 2** button. The compound information for signal 2 will be displayed. When you are done, use the same button (now labeled **Signal 2 1**) to return to the compound list for the first signal.

8 (Optional) Click the **Print** button to print the compound list. See "To Display or Print a Compound List" on page 51 to view or print the list after you have exited the Compound List Manager dialog box.

9 When all the changes have been made to the compound list, click the **Exit** button. You are prompted to confirm saving changes to the last compound you modifed.

Compound reporting parameters

The compound reporting parameters are described below. Most of the information in these fields is filled in from Page 2 of the Edit Compounds dialog box in the EnviroQuant Data Analysis (EDA) software. The equivalent parameter name in EDA is given when it differs.

Name The name of the compound as it appears in the quantitation database of the Environmental Data Analysis Software.

Reporting Name The name of the compound as it is to appear on the environmental form.

CAS Number (optional) Chemical Abstracts Service Number used on Forms 1A and 1B. You can enter any text here as a proprietary registry number.

Abbrev Surrogates and internal standards require three-letter compound name abbreviations on their respective forms: Forms 2A, 2B, 2C, and 2D for surrogates and Forms 8A and 8B for internal standards. Use upper case letters enclosed in parentheses–(BEN) for benzene, for example. Called A1 in EDA.

Compound Type Select a compound type option from Table 7.

Table 7 Compound type options

Compound type	Description
Target	A compound whose presence or absence in a sample must be reported.
ISTD	**Internal standard.** A compound added to the sample extract in a known concentration prior to analysis. All concentration calculations for target compounds are made relative to the response of an internal standard. Internal standards are also used to establish the retention time stability of a chromatographic system. The expected retention time of a target compound is typically adjusted relative to the actual retention time of an internal standard. This practice ensures accurate detection of target compounds.
Matrix	**Matrix spike compound.** This compound type includes special Matrix Spike fields on the right side of the dialog box. A matrix spike is a compound that is added to an aliquot of a matrix (water or soil) and carried through the entire analytical procedure in order to measure the recovery properties of that procedure for that matrix.
Surr	**Surrogate compound.** This compound type includes special Surrogate fields on the right side of the dialog box. A surrogate is a compound that is added (prior to sample preparation) to every blank, unknown sample, matrix spike, matrix spike duplicate, and standard, in order to evaluate analytical efficiency by measuring the recovery of the surrogate compound. Surrogate compounds are chosen to have chemical properties similar to those of the target compounds. Surrogates are compounds not normally found in environmental media.

Mix A (Pesticides only) Used to specify compounds for Form 7E. Select this field if the compound is present in calibration mix A.

Mix B (Pesticides only) Used to specify compounds for Form 7E. Select this field if the compound is present in calibration mix B.

Minimum Response Factor The minimum acceptable response factor for the compound. Values below this minimum are flagged on Forms 6A and 6B (initial calibration) and Forms 7A and 7B (continuing calibration). Called Signal level minimum in EDA.

Maximum RSD The maximum acceptable standard deviation of the response factors in the initial calibration. Values above this maximum are flagged on Forms 6A and 6B (initial calibration). Called Maximum in EDA.

Maximum Response Factor Dev. The maximum percentage deviation of the response factor that is acceptable in the daily or continuing calibration. Values above this maximum are flagged on Forms 7A and 7B (continuing calibration). Called N4 in EDA.

Report Detection Limit (on column) The minimum detection limit for the compound in soil and water. Compounds detected at a concentration below this value or not at all are flagged on Forms 1A and 1B. Called N6 in EDA.

Calibration Range Upper Limit The highest calibration level used in instrument units. Used to calculate the E flag (exceeds calibration) for Form 1.

Surrogate Table 8 lists the parameters for Surrogate compound types.

Table 8 Surrogate types

Type	Description
Amount	The amount of surrogate compound added to the sample prior to sample preparation. The units are the same as those used for quantitation.
Recoveries (low, high)	The lower and upper bounds for the acceptable percentages of surrogate compound recovery, for water and for soil.

Matrix Spike Table 9 lists the parameters for Matrix Spike compound types.

Table 9 Matrix spike types

Type	Description
Amount	The amount of matrix spike compound added to the sample prior to sample preparation. The units are the same as those used for quantitation.
Recoveries (low, high)	The lower and upper bounds for the acceptable percentages of matrix spike compound recovery, for water and for soil.
RPD	The maximum acceptable value for relative percent deviation for each matrix type.

Additional fields for pesticides only (all compound types)

Florisil Check Indicate with a check mark whether or not a Florisil check was performed. If the check was performed, enter the information described in Table 10.

Table 10 Florisil check

Entry	Description
Amount	The amount of compound used for the Florisil check. The units are the same as those used for quantitation.
Recoveries (low, high)	The lower and upper bounds for the percentages of compound recovered in the Florisil check.

GPC Check Indicate with a check mark whether or not a GPC check was performed. If the check was performed, enter the information described in Table 11.

Table 11 GPC check

Entry	Description
Amount	The amount of compound used for the GPC check. The units are the same as those used for quantitation.
Recoveries (low, high)	The lower and upper bounds for the percentages of compound recovered in the GPC check.

Performance Evaluation Indicate with a check mark whether or not a performance evaluation was performed. If the evaluation was performed, enter the amount of compound used.

Resolution Check Indicate with a check mark whether or not a resolution check was performed.

Calibration Nominal Amount The concentration of a compound in the calibration check standard (Form 7E).

NOTE

Use Table 12 as a quick reminder of the corresponding compound reporting parameters between Environmental Data Analysis (EDA) and EnviroForms. The compound information from the Edit Compound—Page 2 dialog box of the Environmental Data Analysis program (EDA)—is copied into the compound list in EnviroForms when you load a compound list from a Data Analysis method, as described in "To Load or Select a Compound List" on page 41.

Table 12 Parameter correspondence

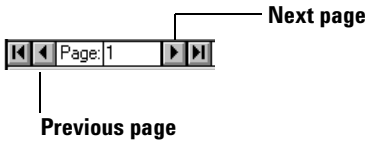
EDA - Edit compound page 2	EnviroForms - Compound list manager	For compound types
Signal level Minimum	Minimum Response Factor	Target, Matrix, Surr, ISTD
Maximum	Maximum RSD	Target, Matrix, Surr, ISTD
N4	Max Response Factor Dev.	Target, Matrix, Surr, ISTD
N6	Report Detection Limit (on column)	Target, Matrix, Surr, ISTD
Calibration Range Upper Limit		
Surrogate amount	Surrogate Amount	Surrogate only
Matrix A (conc) LOW	Surrogate Water Low	Surrogate only
Matrix A (conc) HIGH	Surrogate Water High	Surrogate only
Matrix B (conc) LOW	Surrogate Soil Low	Surrogate only
Matrix B (conc) HIGH	Surrogate Soil High	Surrogate only
A1	Abbrev	Surrogate only
Matrix spike amount	Matrix Spike Amount	Matrix spike only
Matrix A (conc) LOW	Matrix Water Low	Matrix spike only
Matrix A (conc) HIGH	Matrix Water High	Matrix spike only
Matrix A (conc) %Dev	Matrix Water RPD	Matrix spike only
Matrix B (conc) LOW	Matrix Soil Low	Matrix spike only
Matrix B (conc) HIGH	Matrix Soil High	Matrix spike only
Matrix B (conc) %Dev	Matrix Soil RPD	Matrix spike only

To Display or Print a Compound List

1 If the compound list you wish to view is already loaded, skip to step 2. Otherwise, load the compound list of interest as described in "To Load or Select a Compound List" on page 41.

2 Select **Display Compound List** from the Utilities menu. A table of the compound list and the compound parameters appears on the screen.

3 Click the page arrow buttons at the lower left part of the window to view different pages of the table.



4 To print the list to the Windows default printer, select **Print** from the File menu or click the **Print** button.

5 To exit the display window, select **Close** from the File menu or click the **Close** button.

5
Printing Forms

Printing Forms

Once you have set up lists of samples and compounds as described in Chapter 3 and Chapter 4, you are ready to generate the environmental forms.

The following forms (Table 13) are available depending on the fraction analyzed:

Table 13 Available forms

Environmental form		Volatiles	Semi-volatiles	Pesticides
1	Organics Data Analysis Sheet	1A	1B, 1C	1D
2	System Monitoring Compounds (surrogates)	2A, 2B	2C, 2D	2E, 2F
3	Matrix Spike/Matrix Spike Duplicate Recovery	3A, 3B	3C, 3D	3E, 3F
4	Method Blank Summary Report	4A	4B	4C
5	Tune Evaluation (MS data only)	5A (BFB)	5B (DFTPP)	1D
6	Initial Calibration Data	6A	6B, 6C	6D, 6E, 6F
7	Continuing Calibration Check	7A	7B, 7C	7D
8	Internal Standard Area and Retention Time Summary Report	8A	8B, 8C	8D
9	Pesticide Florisil Check and GPC calibration			9
10	Pesticide Identification Summary- Single and MultiComponent Analytes			10

Example forms

Example forms can be printed by selecting **Print One of Each Form** from the Help menu. You can use data in an ERM you have created or use the demo data supplied with your EnviroForms software (load demo.erm).

Available formats

You can customize the final printed forms by specifying the labels for some of the data that appears on the forms. See *"To Customize Labels Used on Forms"* on page 59 in this chapter. Without customization, the terminology on the reports complies with the US Environmental Protection Agency's March 1993 Contract Laboratory Program Statement of Work (USEPA CLP SOW).

To Generate Environmental Forms

1 If the sample list you want to generate forms for is the one currently displayed in the title bar of the EnvForms window, skip to step 2. Otherwise:

- To load a different sample list in the same ERM, click the **Sample List** button on the toolbar of the EnvForms program window.
- To load a sample list in a *different* ERM, select **Open ERM** from the File menu. You are prompted to select a sample list.

2 (Optional) To change the labels for some data on the forms, see "To Customize Labels Used on Forms" on page 59 in this chapter.

3 Click the **Preview Forms** button on the toolbar of the EnvForms program window or select **Preview-Print Forms** (Figure 10) on the Forms menu.

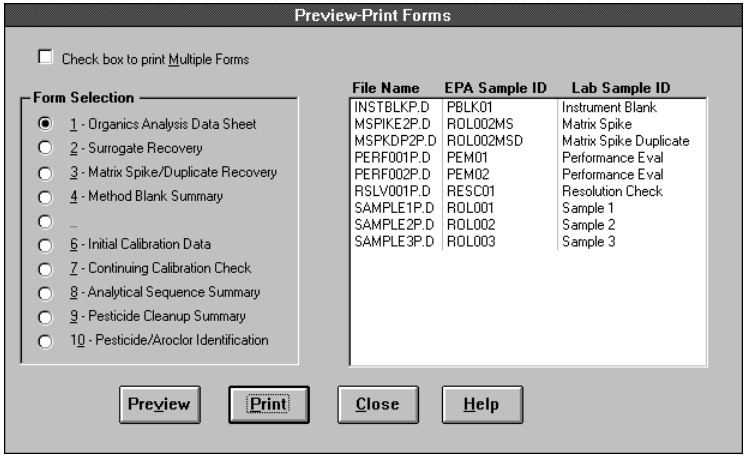


Figure 10 Preview-Print Forms

4 Select the forms and samples to print:

a Single form, single sample

- Leave the check box in the upper left corner of the panel blank to generate a single form for a selected sample.
- Select the form from the left side of the screen.
- Select the sample of interest from the right side of the screen (except for Forms 2 and 5, which don't require sample selection).

b Multiple forms, all samples

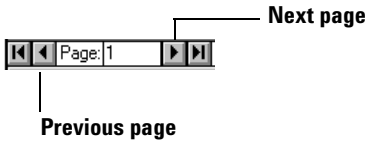
- Select the check box in the upper left corner of the panel blank to generate one or more forms for all the samples in the sample list.
- Select the forms from the left side of the screen.

5 To print the form or forms selected in step 4, click the **Print** button.

Wait until *all* the related samples have been analyzed and the required input files generated from EnviroQuant Data Analysis before you attempt to print *any* environmental forms, because each form requires information from several input files. Although some forms *might be* correctly generated with only some of the input files present, it is more likely that individual forms based on a partial set of input files would be incomplete or inaccurate. For example, an Organics Analysis Data Sheet (Form 1) produced before the method blank has been processed would not be able to flag compounds that were detected in the blank.

6 (Single form only) To preview a form on the screen before printing, select the form and sample as described in step 4, then click the **Preview** button. The form appears on the screen. The information is presented for display only; you can't modify the data at this point. You can view different parts of the form or print the form.

- Use the page arrow buttons at the lower left part of the window to view different pages of the form.



- To print the form to the Windows default printer, select **Print** from the File menu or click the **Print** button.

- To exit the display window, select **Close** from the File menu or click the **Close** button.

7 Repeat step 4 through step 6 to generate other forms for the same sample list. Click the **Exit** button when you are done.

8 Repeat step 1 through step 7 to generate forms for other sample lists.

To Customize Labels Used on Forms

You can customize the final printed forms by specifying the labels for some of the data that appears on the forms.. Without customization, the terminology on the reports complies with the US Environmental Protection Agency's March 1993 Contract Laboratory Program Statement of Work (USEPA CLP SOW).

1 Select **Customize Formset** (Figure 11) from the Forms menu in the EnviroForms window.

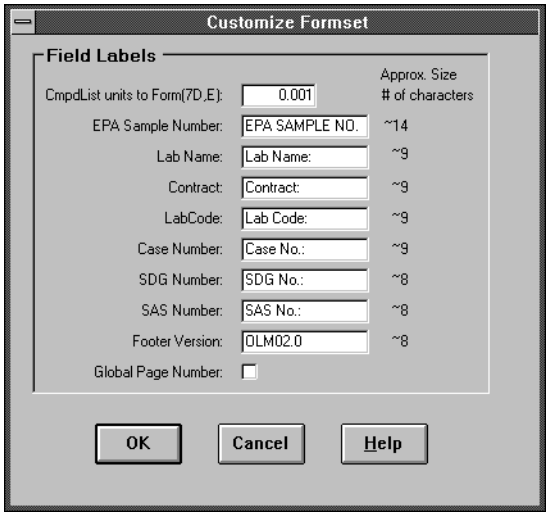


Figure 11 Customize Formset

2 Type in new values for any labels you want to change; click **OK** when done.

CmpdList units to Form (7D, E) Type in the multiplier used to convert instrument units to reporting units. For example, type 0.001 to convert from ppb to ppm.

Footer Version Change to OLM02.0 as shown in Figure 11 to customize forms for USEPA CLP SOW Version OLM02.0.

Global Page Number Select this field to consecutively number the pages when you generate multiple forms as described in *"To Generate Environmental Forms"* on page 56.

6
Calculations for VOAs Analysis

Calibration

The calibration curve for volatiles analysis is constructed using one of the following schemes (Table 14 and Table 15).

Table 14 Calibration using 5.0 mL samples

Calibration level µg/L = ng/mL	Analyte concentration µg/L = ng/mL	Analyte on column ng per 5.0 mL	Int std concentration µg/L = ng/mL	Int std on column ng per 5.0 mL
10	10	50	50	250
20	20	100	50	250
50	50	250	50	250
100	100	500	50	250
200	200	1000	50	250

Reference SOW, D-22/VOA, Section 5.5.1

Table 15 Calibration using 25.0 mL samples

Calibration level µg/L = ng/mL	Analyte concentration µg/L = ng/mL	Analyte on column ng per 5.0 mL	Int std concentration µg/L = ng/mL	Int std on column ng per 5.0 mL
1	1 to 5	25 to 125	20	500
2	2 to 10	50 to 250	20	500
5	5 to 25	125 to 625	20	500
10	10 to 50	250 to 1250	20	500
25	25 to 125	620 to 3125	20	500

Problem compounds such as ketones are at the higher level. During calibration, the volume purged is held constant at 5.0 or 25.0 mL. The calibration equations are then expressed in terms

of concentration in the actual water sample. Remember that 1.0 µg/L = 1.0 ng/mL. The calibration is not expressed in terms of nanograms-on-column.

Relative response factors (RRF) are computed using Equation 1. Again, concentrations are used, not nanograms-on-column.

$$RRF = \frac{A_x \times C_{is}}{A_{is} \times C_x} \quad \textbf{(1)}$$

where:

A_x	=	Response of the analyte (area)
C_{is}	=	Concentration of the internal standard (µg/L = ng/mL)
A_{is}	=	Response of the internal standard (area)
C_x	=	Concentration of analyte (µg/L = ng/mL)

Reference SOW, D-27/VOA, Section 7.4.3

Equation 1 can be recast to solve for C_x, the concentration of the unknown analyte.

$$C_x = \frac{A_x \times C_{is}}{A_{is} \times RRdF} = C_{qnt} \quad \textbf{(2)}$$

The quantitation report gives C_{qnt}, the concentration of the analyte if exactly 5.0 or 25.0 mL of the sample were purged.

The total amount of internal standard added to the sample in the purge tube (I_s) and desorbed onto the GC column is given in Equation 3.

$$I_s = C_{is} \times M_{noc} \quad \textbf{(3)}$$

where:

C_{is}	=	Concentration of the internal standard (µg/L = ng/mL)
M_{noc}	=	Ng on-column Multiplier (5 or 25 mL)

Water Samples

The SOW specifies using Equation 4 to determine the concentration of an analyte in the unknown sample. Note that I_s (the number of nanograms of internal standard desorbed onto the GC column) is specified rather than C_{is} (the concentration of the internal standard).

$$\mu g/L = \frac{A_x \times I_s \times Df}{A_{is} \times RRF \times V_0} \quad \textbf{(4)}$$

where:

A_x	=	Response of the analyte (area)
I_s	=	Amount of internal standard added (nanograms-on-column)
Df	=	Dilution factor
A_{is}	=	Response of the internal standard (area)
RRF	=	Relative response factor
V_0	=	Volume purged (5 or 25 mL)

Reference SOW, D-42/VOA, Section 10.3

Edit Volatile Sample Information panel

EnviroForms software uses the values set in the Sample Information panel (Figure 12). In this example, the user default value for Ng on-column Multiplier (M_{noc}), has been set to 25.0 mL. The values entered for MeOH Soil Extract Vol and MeOH Aliquot Volume are for soil and are ignored when the sample type is water.

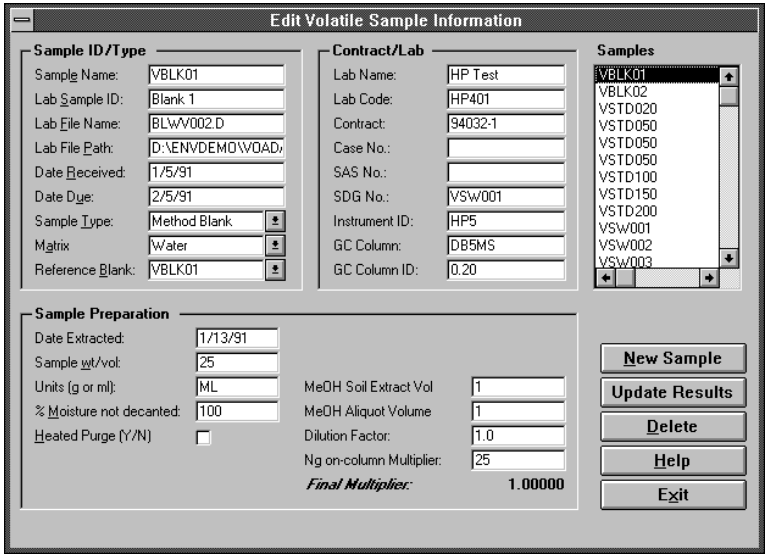


Figure 12 Sample Information

The actual volume purged (V_{hdr}) is the value set in the Sample wt/vol field of the Sample Information panel for the individual sample. Since the matrix in this example is water, MeOH Soil Extract Vol and MeOH Aliquot Volume are not used.

The equation used to calculate the concentration of a volatiles water sample is derived from Equation 4 by substituting (C_{is} X M_{noc}) for I_s to give Equation 5.

$$\mu g/L = \frac{A_x \times C_{is} \times M_{noc} \times Df}{A_{is} \times RRF \times V_0} \quad \textbf{(5)}$$

Further substitution of C_{qnt} for the elements of Equation 2 on the right hand side of Equation 5 gives Equation 6, the equation used by EnviroForms software to calculate the concentration of a VOAs water sample.

$$\mu g/L = \frac{C_{qnt} \times M_{noc} \times Df}{V_0} \quad \textbf{(6)}$$

where:

C_{qnt}	=	Concentration from the quant report (µg/L = ng/mL)
M_{noc}	=	Ng on-column Multiplier (5 or 25 mL)
Df	=	Dilution factor
V_0	=	Volume actually purged from the Sample Information pane (5 or 25 mL)

Low Soil

Calibration is performed as described for a water sample. The SOW specifies using Equation 7 to determine the concentration of an analyte in a low soil sample.

$$\mu g/Kg = \frac{A_x \times I_s}{A_{is} \times RRF \times W_s \times D} \quad \textbf{(7)}$$

where:

A_x	=	Response of the analyte (area)
I_s	=	Amount of internal standard added (ng)
A_{is}	=	Dilution factor
RRF	=	Relative response factor
W_s	=	Wet weight of sample added to the purge tube (g)
D	=	Fractional solids ((100 - % Moisture)/100)

Reference SOW, D-43/VOA, Section 10.3

The calculations used by EnviroForms software for the low soil VOAs sample can be derived from Equation 7 by substituting (C_{is} X M_{noc}) for I_s then substituting C_{qnt} for the elements of Equation 2 in Equation 7 to give Equation 8.

$$\mu g/Kg = \frac{C_{qnt} \times M_{noc}}{W_s \times D} \quad \textbf{(8)}$$

where:

C_{qnt}	=	Concentration from the quant report (µg/L = ng/mL)
M_{noc}	=	Ng on-column Multiplier (5 or 25 mL)
W_s	=	Wet weight from the Sample Information panel (4 g)
D	=	Fractional solids ((100 - % Moisture)/100)

Percent moisture is the value entered in the % Moisture field in the Sample Information panel for the sample. Note that no dilution factor is used in Equation 7 and Equation 8.

When Form 1 is printed for a low soil sample, the Soil Extract Volume and Soil Aliquot Volume fields are blank. The dilution factor is 1 by default.

Medium Soil

A VOAs medium soil sample is handled quite differently from the water or low soil sample. Typically, the medium soil analysis is used if a 1 gram low soil analysis gave saturated peaks. A nominal 4.0 gram sample of the soil is extracted with 9.0 mL of methanol and 1.0 mL of the system monitoring compounds (10,000 µL total methanol). Of this 10.0 mL solution, 100 µL is transferred into 4.9 mL of reagent water in a 5 mL syringe giving a total of 5.0 mL of sample to be purged. As with water samples, 10 µL of the internal standard solution is added prior to transferring the 5.0 mL in the syringe into the purging vessel.

The SOW specifies using Equation 9 to determine the concentration of an analyte in a medium soil sample.

$$\mu g/Kg = \frac{A_x \times I_s \times V_t \times 1000 \mu L/mL \times Df}{A_{is} \times RRF \times V_a \times W_s \times D} \quad \textbf{(9)}$$

where:

A_x	=	Response of the analyte (area)
I_s	=	Amount of internal standard added (ng)
V_t	=	MeOH soil extract volume (mL)
Df	=	Dilution factor (see definition in SOW)
A_{is}	=	Response of the internal standard (area)
RRF	=	Relative response factor
V_a	=	Methanol aliquot volume purged (µL)
W_s	=	Wet weight of sample extracted with methanol (g)
D	=	Fractional solids ((100 - % Moisture)/100)

Reference SOW, D-43/VOA, Section 10.3

The 1000 µL/mL term in the numerator is needed when V_t is expressed in mL.

The Df for medium soil samples is defined as 1.00 when exactly 10 mL of methanol is used to extract the soil samples and V_a is between 10 and 100 µL. If the methanolic extract is diluted, then Df will be calculated based on that dilution.

Reference SOW, D-37/VOA Section 8.2.2.5

The calculations used by EnviroForms software for the medium soil VOAs sample can be derived by substituting (C_{is} X M_{noc}) for I_s in Equation 9, expressing V_t in µL instead of mL, and then substituting C_{qnt} for the terms in Equation 2 to give Equation 10.

$$(\mu g)/(Kg) = \frac{C_{qnt} \times M_{noc} \times V_t \times Df}{V_a \times W_s \times D} \quad \textbf{(10)}$$

where:

C_{qnt}	=	Concentration from the quant report (µg/L)
M_{noc}	=	Ng on-column Multiplier (5 or 25 mL)
V_t	=	MeOH soil extract volume in the Sample Information panel (10,000 µL)
Df	=	Dilution Factor in the Sample Information panel
V_a	=	MeOH Aliquot Volume in the Sample Information pane (100 µL)
W_s	=	Sample wt/vol in the Sample Information panel (4 g)
D	=	Fractional solids ((100 - % Moisture)/100)

Percent moisture is the value entered in the % Moisture field in the Sample Information panel for the sample.

VOA CRQLs

The CRQLs that SOW C-2 specifies are based on a detection limit of 50 nanograms-on-column for each analyte in the method when the sample size is 5.0 mL. The SOW gives a table that converts the 50 nanograms-on-column detection limit to the nominal CRQL concentration of the analyte in the original sample. This is 10 µg/L for water, 10 µg/Kg for low soil, and 1250 µg/Kg for medium soil.

In the Compound List Manager dialog box, Figure 13 on the next page, you can enter these values as Report Detection Limit (on column). These values are also entered on Page 2 of the quantitation database. Report Detection Limit (on column) in EnviroForms Compound List Manager is field N6 on Page 2 of the quantitation database in Environmental Data Analysis.

Compound List Manager for Volatiles

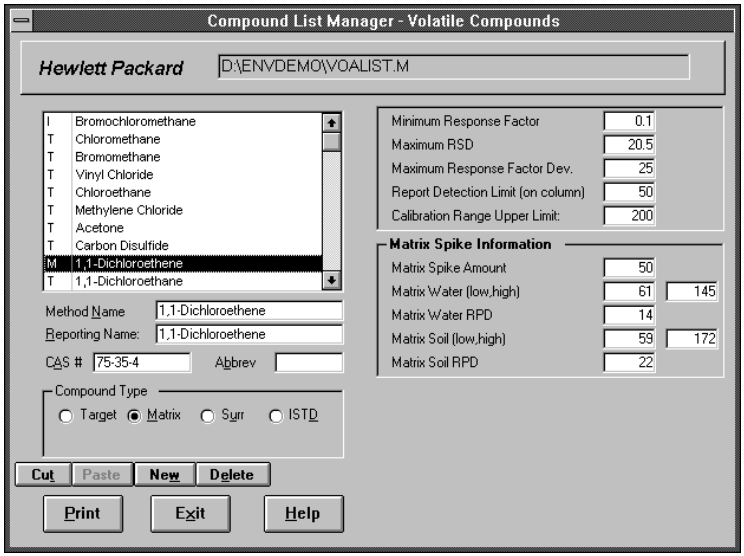


Figure 13 Compound List Manager

Water

Given that the volatile water CRQL is 10 µg/L in a 5.0 mL sample, Equation 6 can be solved for that C_{qnt} that gives 10 µg/L. Obviously, C_{qnt} = 10 µg/L gives a CRQL of 10 µg/L. This is 50 nanograms-on-column divided by M_{noc}, the default Ng on-column Multiplier.

Low soil

Given that the low soil CRQL is 10 µg/Kg in a 5.0 mL sample, Equation 8 can be solved for that C_{qnt} that gives 10 µg/Kg. In this case, W_s is the nominal value of 5 g. Again, C_{qnt} = 10 µg/L gives a the correct CRQL of 10 µg/Kg for a low soil.

Medium soil

Given that the medium soil CRQL is 1,250 µg/Kg in a 5.0 mL sample, Equation 10 can be solved for that C_{qnt} that gives 1,250 µg/Kg by setting all other terms to their nominal value (4 grams of sample, 0 % moisture, 10,000 µL methanol extract volume, and 100 µL methanol aliquot volume) and solving for C_{qnt}. Again, C_{qnt} = 10 µg/L gives the correct CRQL of 1,250 µg/Kg for a medium soil. When rounded off, this becomes 1,300 µg/Kg.

CRQL calculations

If the analyte is not found, EnviroForms software will calculate a C_{crql} using Equation 11 and substitute that for C_{qnt} into Equation 6, Equation 8, or Equation 10 as appropriate.

$$C_{crql} = \frac{DL_{noc}}{M_{noc}} \quad \textbf{(11)}$$

where:

C_{crql}	=	Value of C_{qnt} to give the CRQL concentration
DL_{noc}	=	Value of Report Detection Limit (on column) in the Compound List
M_{noc}	=	Ng on-column Multiplier (5 or 25 mL) in the Sample List

The value for Report Detection Limit in the Compound List can be treated as an information-only field. The important field is the Ng on-column field in the Sample List.

Each sample can give a different CRQL. The CRQL is dependent on the actual sample size, the actual dry weight of the soil, the dilution factor, and the methanol volumes used when the sample is treated as a medium soil sample.

J flags

The J flag will be assigned whenever C_{qnt} is < (DL_{noc} / M_{noc}).

Ng on-column Multiplier

This field appears on the Edit Sample Information screen and is used to convert ng/mL to ng/µL as needed in Equation 6, Equation 8, and Equation 10. Set M_{noc} to 5 if the LOW standard is reporting µg/L. Set M_{noc} to 1 if the LOW standard is reporting nanograms-on-column.

Further Concerns

Dilutions and surrogates

The equations are set up to apply the Dilution Factor set in the Sample Information panel to all concentrations. This works out correctly if the surrogates are added to the original sample and the sample is subsequently diluted and reanalyzed.

If samples are prescreened to determine if a dilution is needed, there can be problems with the calculated values for the surrogates concentration.

For example, prescreening indicates that the sample needs a 1:5 dilution. The analyst dilutes the sample, adds the surrogates to the diluted sample, and proceeds with the extraction or purging. A dilution factor of 5 is entered into the Sample Information panel. All analyte values will be corrected to the concentration in the original sample, but all surrogate concentrations will be five times too high.

The best workaround for this is to set a quant dilution factor of 0.2 and apply it to only the surrogates. Then the number in the quant report will be one-fifth of what it should be. The dilution factor used in EnviroForms software will then correct this to the proper concentration. Small dilution factors can give errors because the formats used in CSV.MAC to write out QUANT.CSV are limited to two decimal places. The formats in CSV.MAC may need to be changed to overcome this.

Heated purge

A calibration set up with a heated purge is a different calibration from a non-heated purge. The purging efficiencies will be quite different. As such, heated purge calibrations should exist in a different ERM from the multipoint calibration that does *not* use a heated purge.

Calibrating soils

The calibrations for a soil are always Sample Type = Calibration, Matrix Level = Water, and Percent Moisture =100.

Production run

A production run consists of all injections into a given system while the multipoint curve is valid. An ERM can continue as long as the initial multipoint curve is valid. You do not need to create a new ERM for each days work.

7
Calculations for SVs Analysis

Calibration

The calibration curve for semivolatiles (SVs) analysis is constructed using 2.0 µL injections of solutions at the following concentrations (1.0 µg/mL = 1.0 ng/mL). See Table 16.

Table 16 SV calibration

Calibration level, µg/mL	Analyte concentration, µg/µL	Analyte injected, ng per 2 µL	Int std concentration, ng/µL	Int std injected, ng per 2 µL
10	10	20	20	40
25	25	50	20	40
40	40	80	20	40
60	60	120	20	40
80	80	160	20	40

Reference SOW, D-38/SV, Section 3.2

It is not totally clear if the SOW prefers calibrations be set up using the calibration level and response or if they are to be set up using nanograms-on-column and response. In the first case, the continuing calibration will give quant reports with concentrations of 25. In the second case, continuing calibrations will give quant reports with concentrations of 50. It is recommended that the SVs analysis be set up reporting nanograms-on-column.

Nine of the analytes will not be present in the 10 ppm standard due to the difficulty of detection of these analytes when less than 50 nanograms is injected on the GC column.

Each sample will have 100 µg of the surrogates added at the beginning of the analysis. If the surrogate exhibits a 100% recovery, the value will be above the high point of the calibration. The surrogate recovery is expected to be less than 100%, so this should not present a problem.

The Pesticide/Arochlor analytes can be included at a concentration of less than 10 ng/µL in the continuing calibration standard (25 ng/µL) to facilitate confirmations of these analytes. If the Pesticide/Arochlor analytes are in the continuing calibration mix, they are not reported on Form 7, but instead are included in any quantitation reports for the continuing calibration standard.

The relative response factors (RRF) are computed using Equation 12. The SOW is quite emphatic in stressing that the concentration terms are expressed in concentration, not amount on column; however, the RRF is the same number if the concentrations are expressed in either concentration (ng/µL) or nanograms-on-column.

$$RRF = \frac{A_x \times C_{is}}{A_{is} \times C_x} \quad \textbf{(12)}$$

where:

A_x	=	Response of the analyte (area)
C_{is}	=	Concentration of the internal standard (ng/µL)
A_{is}	=	Response of the internal standard (area)
C_x	=	Concentration of analyte (ng/µL)

Reference SOW, D-43/SV, Section 5.4

Equation 1 in Chapter 6 (RRFs for VOAs) expresses the concentration in ng/mL = mg/L in the original sample. Equation 12 for Semivolatiles expresses the concentration in terms of ng/mL in the concentrated 1.0 mL extract, which in this case is also numerically equal to the concentration in the original sample (assuming 100% extraction efficiency).

The amount of internal standard injected on column (ng) is given in Equation 13:

$$I_s = C_{is} \times V_i = C_{is} \times M_{noc} \quad \textbf{(13)}$$

where:

C_{is}	=	Concentration of the internal standard (ng/µL)
V_i	=	Volume of standard purged (2 µL)
M_{noc}	=	Ng on-column Multiplier (2 µL)

The term M_{noc} is the value that you entered for the Ng on-column Multiplier. This value will be either 1 or 2 µL depending on whether your calibration is set up in terms of concentration in the extract or nanograms-on-column. The latter case is preferable; the concentration should be expressed in terms of nanograms-on-column.

Water Samples

The SOW specifies using Equation 14 to determine the concentration of an analyte in a semivolatiles water sample.

$$\mu g/L = \frac{A_x \times I_s \times V_t \times Df}{A_{is} \times RRF \times V_0 \times V_i} \quad \textbf{(14)}$$

where:

A_x	=	Response of the analyte (area)
I_s	=	Amount of internal standard added (40 nanograms-on-column)
V_t	=	Concentrated extract volume (1,000 µL)
Df	=	Dilution factor (see definition in SOW)
A_{is}	=	Response of the internal standard (area)
RRF	=	Relative response factor
V_0	=	Original sample volume extracted (1,000 mL)
V_i	=	Volume of concentrated extract injected (2.0 µL)

Reference SOW, D-52/SV, Section 8.2

The equation used to calculate the concentration of a semivolatiles water sample is derived from Equation 14 by substituting ($C_{is} \times M_{noc}$) for I_s to give Equation 15.

$$\mu g/L = \frac{A_x \times C_{is} \times M_{noc} \times V_t \times Df}{A_{is} \times RRF \times V_0 \times V_i} \quad \textbf{(15)}$$

Equation 12 can be rearranged to give Equation 16.

$$C_x = \frac{A_x \times C_{is}}{A_{is} \times RRF} = C_{qnt} \quad \textbf{(16)}$$

Substituting C_{qnt} into Equation 15 for the elements of Equation 16 gives Equation 17, which EnviroForms software uses to calculate the concentration of an analyte in an unknown semivolatiles water sample.

$$\mu g/L = \frac{C_{qnt} \times M_{noc} \times V_t \times Df}{V_0 \times V_i} \quad \textbf{(17)}$$

where:

C_{qnt}	=	Concentration from the quant report (µg/L = ng/mL) **or** Nanograms-on-column from the quant report
M_{noc}	=	Ng on-column Multiplier (1 or 2 µL)
V_t	=	Concentrated extract volume in Sample Information panel (1,000 µL)
Df	=	Dilution factor in Sample Information panel (see definition in SOW)
V_0	=	Original sample volume extracted (1,000 mL)
V_i	=	Volume of concentrated extract injected (2.0 µL)

When you enter sample information from within EnviroForms software, you must set the Ng on-column Multiplier (M_{noc}) to agree with the way you set up the calibration.

The value that you enter for M_{noc} is 2 if C_{qnt} is reporting standards at 10, 25, 40, 60, and 80 ng/µL. It is 1 if C_{qnt} is reporting standards at 20, 50, 80, 120, and 160 nanograms-on-column.

The RRFs reported are independent of the way you set up the calibration. Equation 12 has C_{is} in the numerator and C_x in the denominator. Since C = nanograms-on-column / volume injected, the ratio C_{is} / C_x is the same if C is expressed in ng/mL or if it is expressed in terms of nanograms-on-column.

Soil Samples

Calibration is performed as described for a water sample. The SOW specifies using Equation 18 to determine the concentration of the analyte in an unknown soil sample. Although the SOW specifies a Soil Low and Soil Medium sample preparation, the SOW specifies only a single equation for determining the concentration of analytes in an unknown Semivolatiles Soil/Sediment sample.

$$\mu g/Kg = \frac{A_x \times I_s \times V_t \times Df}{A_{is} \times RRF \times V_i \times W_s \times D} \quad \textbf{(18)}$$

where:

A_x	=	Response of the analyte (area)
I_s	=	Amount of internal standard added (40 nanograms-on-column)
V_t	=	Concentrated extract volume (1,000 µL)
Df	=	Dilution factor (see definition in SOW)
A_{is}	=	Response of the internal standard (area)
RRF	=	Relative response factor
V_i	=	Volume of concentrated extract injected (2.0 µL)
W_s	=	Wet weight of sample extracted (g)
D	=	Fractional solids ((100 - % Moisture)/100)

Reference SOW, D-53/SV, Section 8.2

The equation that EnviroForms software will use to calculate the concentration of a Semivolatiles Soil Sample is derived from Equation 18 by first substituting (C_{is} X M_{noc}) for I_s , then substituting C_{qnt} for the elements of Equation 16 to give Equation 19.

$$\mu g/Kg = \frac{C_{qnt} \times M_{noc} \times V_t \times Df}{V_i \times W_s \times D} \quad \textbf{(19)}$$

where:

C_{qnt}	=	Concentration from the quant report (µg/L = ng/µL) **or** Nanograms-on-column from the quant report
M_{noc}	=	Ng on-column Multiplier (1 or 2 µL)
V_t	=	Concentrated extract volume in Sample Information panel (1,000 µL)
Df	=	Dilution factor in Sample Information panel (see definition in SOW)
V_i	=	Volume of concentrated extract injected (2.0 µL)
W_s	=	Wet weight of sample extracted in Sample Information panel (g)
D	=	Fractional solids ((100 - % Moisture)/100)

If a dilution is used, it is mandatory that additional internal standard spiking solution be added to the extract to bring the concentration of the internal standards up to 20 ng/µL prior to analysis.

The value that you enter for M_{noc} is 2 if C_{qnt} is reporting standards at 10, 25, 40, 60, and 80 ng/µL. It is 1 if C_{qnt} is reporting standards at 20, 50, 80, 120, and 160 nanograms-on-column.

Percent moisture is the value entered in the % Moisture field in the Sample Information panel for the sample.

SV CRQLs

The CRQLs that the SOW specifies are based on a detection limit of 20 nanograms-on-column. Eight semivolatile analytes have a CRQL based on 100 nanograms-on-column.

Reference SOW, C-4

The SOW gives a table that converts the 20 or 100 nanograms-on-column detection limit to the nominal CRQL concentration of the analyte in the original sample. This is 10 or 50 µg/L for water, 330 or 1700 (333 or 1666) µg/Kg for low soil preparation, and 10,000 or 50,000 mg/Kg for medium soil preparation.

In the Compound List Manager dialog box, you can enter these values as Report Detection Limit (on column). These values are also entered on Page 2 of the quantitation database. Report Detection Limit (on column) in Compound List Manager is field N6 on Page 2 in the quantitation database in Environmental Data Analysis.

Water

Given that the semivolatile water CRQL is 10 µg/L, Equation 17 can be solved for that C_{qnt} that gives 10 µg/L. Set all terms to their nominal value for a water sample (M_{noc} = 2 µL, V_t = 1,000 µL, Df = 1, V_i = 2 µL, and V_0 = 1000 mL) and solve for C_{qnt}. A C_{qnt} = 10 µg/L gives the correct CRQL of 10 µg/L in a water sample.

When the calibration is set up to report standards at 10, 25, 40, 60, and 80 ng/µL, M_{noc} must be set to 2 and Report Detection Limit (on column) must be set to 20 or 100. Thus, the C_{qnt} term used when no analyte is found is the value of (DL_{noc}/M_{noc}).

When the calibration is set up to report standards at 20, 50, 80, 120, and 160 nanograms-on-column, M_{noc} must be set to 1 and Report Detection Limit (on column) (DL_{noc}) must be set to 10 or 50. Then the C_{qnt} term used when no analyte is found is again the value of (DL_{noc}/M_{noc}).

Low soil

Given that the low soil CRQL is 333 µg/Kg in the original sample, Equation 19 can be solved for that C_{qnt} that gives 333 mg/Kg. Set all terms to their nominal value for a low soil preparation (M_{noc} = 2 µL, V_t = 1,000 µL, V_i = 2 µL, W_s = 30 g, and D = 1) and solve for C_{qnt}. A C_{qnt} = 10 µg/L gives correct CRQL of 333.33 µg/Kg in a low soil sample. When rounded off, this is reported as 330 µg/Kg.

When the calibration is set up to report standards at 10, 25, 40, 60, and 80 ng/µL, M_{noc} must be set to 2 and Report Detection Limit (on column) (DL_{noc}) must be set to 20 or 100. Thus the C_{qnt} term used when no analyte is found is the value of (DL_{noc}/M_{noc}).

When the calibration is set up to report standards at 20, 50, 80, 120, and 160 nanograms-on-column, M_{noc} must be set to 1 and Report Detection Limit (on column) (DL_{noc}) must be set to 10 or 50. Then the C_{qnt} term used when no analyte is found is again the value of (DL_{noc}/M_{noc}).

Medium soil

Given that the medium soil CRQL is 10,000 µg/Kg in the original sample, Equation 19 can be solved for that C_{qnt} that gives 10,000 µg/Kg. Set all terms to their nominal value for a medium soil preparation (M_{noc} = 2 µL, V_t = 1,000 µL, V_i = 2 µL, W_s = 1 g, and D = 1) and solve for C_{qnt}. A C_{qnt} = 10 µg/L gives the correct CRQL of 10,000 µg/Kg in a medium soil sample.

When the calibration is set up to report standards at 10, 25, 40, 60, and 80 ng/µL, M_{noc} must be set to 2 and Report Detection Limit (on column) must be set to 20 or 100. Thus, the C_{qnt} term used when no analyte is found is the value of (DL_{noc}/M_{noc}).

When the calibration is set up to report standards at 20, 50, 80, 120, and 160 nanograms-on-column, M_{noc} must be set to 1 and Report Detection Limit (on column) (DL_{noc}) must be set to 10 or 50. Then the C_{qnt} term used when no analyte is found is again the value of (DL_{noc}/M_{noc}).

CRQL calculations

If the analyte is not found, EnviroForms software will calculate a C_{crql} using Equation 20 and substitute that for C_{qnt} into Equation 17 or Equation 19 as appropriate.

$$C_{crql} = \frac{DL_{noc}}{M_{noc}} \quad \textbf{(20)}$$

where:

C_{qnt} = Value of C_{qnt} to give the CRQL concentration

If standards are reported as 10, 25, 40, 60, and 80:

DL_{noc} = Report Detection Limit (on-column) = 20 or 100 in the Compound List

M_{noc} = Ng on-column Multiplier (1 or 2 µL) in the Sample List

If standards are reported as 20, 50, 80, 120, and 160:

DL_{noc} = Report Detection Limit (on-column) = 10 or 50 in the Compound List

M_{noc} = Ng on-column Multiplier (µL) in the Sample List

The value for Report Detection Limit in the Compound List can be treated as an information only field. The important field is the Ng on-column Multiplier field in the Sample List. You must adjust the Report Detection Limit (on-column) numbers (DL_{noc}) to match how the standards are reported.

Each sample can give a different CRQL. The CRQL is dependent on the actual sample size, the actual dry weight of the soil, the final extract volumes, using GPC cleanup, and the dilution factor.

J flags

The J flag will be assigned any time that C_{qnt} is < (DL_{noc}/M_{noc}). The Report Detection Limit (on-column) must be set to 20 or 100 if M_{noc} = 2. If M_{noc} = 1, Report Detection Limit (on-column) must be set to 10 or 50.

Other Factors

EnviroForms software uses some other factors in its calculations that affect the numbers reported on the Forms. See Figure 14.

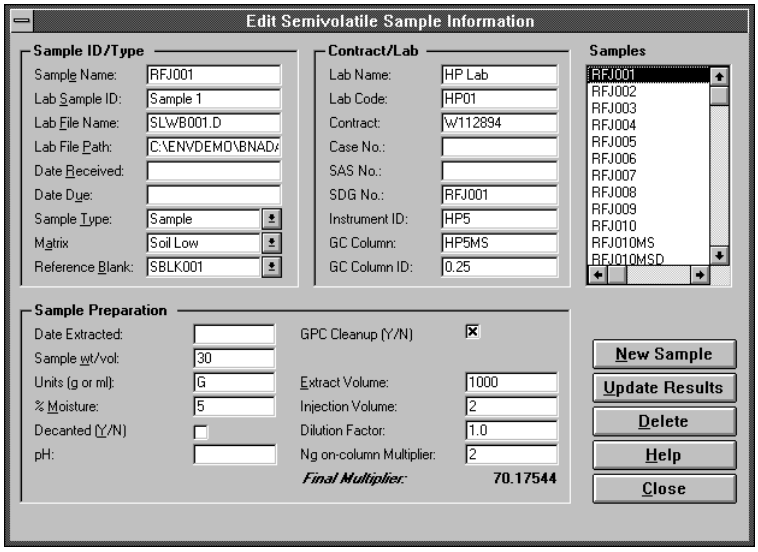


Figure 14 Semivolatile sample information panel

Ng on-column Multiplier

This appears on the Edit Sample Information screen and is used to convert ng/mL to ng/µL as needed in Equation 24 and Equation 26. Set M_{noc} to 0.001 if the LOW standard is labeled as 5.0 ng/mL or to 1.000 if the LOW standard is labeled as 0.005 ng/mL.

GPC Cleanup (Y/N)

This appears only on the Edit Semivolatiles Sample Information screen. The value Y or N appears on Form 1. If Y appears on Form 1, the value reported by Equation 17 and Equation 19 is

multiplied by 2. The SOW states that you can concentrate a GPC extract to 500 µL rather than 1000 µL to account for the 5.0 mL lost in the GPC cleanup. If you do this, you must be sure to set V_t to 500 µL for each sample.

Reference SOW, D-30/SV, Section 3.6.1

Further Concerns

Dilutions and surrogates

The equations are set up to apply the Dilution Factor set in the Sample Information panel to all concentrations. This works out correctly if the surrogates are added to the original sample and the sample is subsequently diluted and reanalyzed.

If samples are prescreened to determine if a dilution is needed, there can be problems with the calculated values for the surrogate concentrations.

For example, prescreening indicates that the sample needs a 1:5 dilution. The analyst dilutes the sample, adds the surrogates to the diluted sample, and proceeds with the extraction or purging. A dilution factor of 5 is entered into the Sample Information panel. All analyte values will be corrected to the concentration in the original sample; but all surrogate concentrations will be five times too high.

The best workaround for this is to set a Quant dilution factor of 0.2 and apply it to only the surrogates. Then the number in the quant report will be one-fifth of what it should be. The dilution factor used in EnviroForms software will then correct this to the proper concentration. Small dilution factors can give errors because the formats used in CSV.MAC to write out QUANT.CSV are limited to two decimal places. The formats in CSV.MAC may need to be changed to overcome this.

Calibrating soils

The calibrations for a soil are always Sample Type = Calibration, Matrix Level = Water, and Percent Moisture =100.

Production run

A production run consists of all injections into a given system while the multipoint curve is valid. An ERM can continue as long as the initial multipoint curve is valid. You do not need to create a new ERM for each days work.

8
Calculations for Pesticide Analysis

Calibration

The calibration curve for pesticides (PEST) analysis is different from volatiles and semivolatiles in that external standard calibrations are used. The calibration curve is constructed using the levels in Table 17.

Table 17 Pesticide calibration

Calibration level	Analyte concentration, ng/mL	Analyte on column, pg per 1 µL injection
LOW	5, 10, 20, 50	5, 10, 20, 50
MED	3 x LOW	3 x LOW
HIGH	30 x LOW	30 x LOW

Reference SOW, D-37/PEST, Section 3.3

The calibration factors are computed using Equation 21.

$$CF = \frac{A_x}{C_{inj}} = \frac{A_x}{C_x \times M_{noc}} \quad \textbf{(21)}$$

where:

CF = Calibration factor (response per nanogram injected)

A_x = Response of the analyte (area or peak height)

C_{inj} = Nanograms injected, nanograms-on-column

C_x = Analyte concentration in standard (ng/mL = pg/µL)

M_{noc} = Ng on-column Multiplier (= 0.001)

Reference SOW, D-48/PEST, Section 9.2.2

The term (M_{noc}= 0.001) is needed if the standards are expressed in terms of ng/mL in the standard solution. A 1.0 µL injection of the 5 ng/mL LOWstandard solution will deliver 5 picograms on column. Since the CF must be expressed in terms of response per nanogram injected, the conversion factor is needed to convert the 5 picograms injected to 0.005 nanograms injected. If the pesticide standards are expressed in terms of µg/mL or ng/µL, i.e. the LOW standard is labeled 0.005 ng/µL instead of 5 pg/µL, the conversion factor is set to 1.0.

The SOW states that manual injections must be 2.0 µL. If autosamplers are used, injections can be 1.0 µL. The same volume must be used for all standards, blanks, and samples.

Reference SOW, D-38/PEST, Section 4.1

Equation 21 can be recast to give Equation 22.

$$\frac{A_x}{CF} = C_x \times M_{noc} \quad \textbf{(22)}$$

Water Samples

The SOW specifies using Equation 23 to determine the concentration of an analyte in a pesticide water sample.

$$\mu g/L = \frac{A_x \times V_t \times Df}{CF \times V_0 \times V_i} \quad \textbf{(23)}$$

where:

A_x	=	Response of the analyte (area)
V_t	=	Concentrated extract volume (10,000 µL)
Df	=	Dilution factor (see definition in SOW)
CF	=	Calibration factor for the MED level (area per ng injected)
V_0	=	Original sample volume extracted (1,000 mL)
V_i	=	Volume of concentrated extract injected (µL)

Reference SOW, D-52/SV, Section 13.5.1

The equation used to calculate the concentration of an analyte in a pesticide water sample is derived from Equation 23 by first substituting (C_{is} X M_{noc}) for (A_x/CF) to give Equation 24.

$$\mu g/L = \frac{C_{qnt} \times M_{noc} \times V_t \times Df}{V_0 \times V_i} \quad \textbf{(24)}$$

where:

C_{qnt}	=	Concentration from the quant report (ng/mL = pg/µL)
M_{noc}	=	Ng on-column Multiplier (= 0.001)
V_t	=	Concentrated extract volume (10,000 µL)
Df	=	Dilution factor from Sample Information panel (see definition in SOW)

CF = Calibration factor for the MED level (area per ng injected)

V_0 = Original sample volume extracted (1,000 mL)

The nanogram-on-column term (M_{noc} = 0.001) is needed if a quantitation report shows the LOW standard at 5.0 ng/mL. If the quantitation report shows the LOW standard at 0.005 ng/µL, the nanogram-on-column term is set to 1.

Soil Samples

Calibration is performed as described for a water sample. The SOW specifies using Equation 25 to determine the concentration of the analyte in an unknown soil sample. The SOW specifies using only what appears to be a Medium Soil sample preparation.

Reference SOW, D17/PEST, Section 6.2

$$\mu g/Kg = \frac{A_x \times V_t \times Df}{CF \times V_i \times W_s \times D} \quad \textbf{(25)}$$

where:

A_x	=	Response of the analyte (area)
V_t	=	Concentrated extract volume (10,000 µL)
Df	=	Dilution factor (see definition in SOW)
CF	=	Calibration factor for the MED level (area per ng)
W_s	=	Wet weight of sample extracted (30 g)
D	=	Fractional solids ((100 - % Moisture)/100)

Reference SOW, D-53/SV, Section 13.5.2

The equation that EnviroForms software will use to calculate the concentration of an analyte in a pesticide soil sample is derived from Equation 25 by first substituting (C_{is} X M_{noc}) for (A_x/CF) to give Equation 26.

$$\mu g/Kg = \frac{C_{qnt} \times M_{noc} \times V_t \times Df}{V_i \times W_s \times D} \quad \textbf{(26)}$$

where:

C_{qnt}	=	Concentration from the quant report (ng/mL = pg/µL)
M_{noc}	=	Ng on-column Multiplier (= 0.001)
V_t	=	Concentrated extract volume (10,000 µL)
Df	=	Dilution Factor in Sample Information panel (see definition in SOW)
V_i	=	Volume of concentrated extract injected (µL)
W_s	=	Wet weight of sample extracted (30 g)
D	=	Fractional solids ((100 - % Moisture)/100)

1000 Converts 5.0 ng/mL to 0.005 ng/µL

The nanogram-on-column term (M_{noc} = 0.001) is needed if a quantitation report shows the LOW standard at 5.0 ng/mL. If the quantitation report shows the LOW standard at 0.005 ng/µL, the nanogram-on-column term is set to 1.

Percent moisture is the value entered in the % Moisture field in the Sample Information panel for the sample.

Pesticide CRQLs

Single component analytes

The CRQLs that the SOW specifies for the single component pesticides are based on detection limits of 5 to 50 picograms on column (0.005 to 0.050 nanograms-on-column). The SOW gives a table that converts the 5, 10, or 50 picograms on column detection limit to the nominal CRQL concentration of the analyte in the original sample. This is 0.05, 0.10 or 0.50 µg/L for water and 5, 10, or 50 µg/Kg for soil samples.

Reference SOW, C-8

Multi-component analytes

The CRQLs that the SOW specifies for the multi-component pesticides are based on detection limits of 100, 200, or 500 picograms on column. The SOW gives a table that converts the 100, 200, or 500 picograms on column detection limits to the nominal CRQL concentration of the analyte in the original sample. This is 1.0, 2.0, or 5.0 mg/L for water and 33.0, 67.0, or 170.0 mg/Kg for soil samples.

Reference SOW, C-8

In the Compound List Manager dialog box, you can enter these values as Report Detection Limit (on column). These values are also entered on Page 2 of the quantitation database. Report Detection Limit (on column) in EnviroForms Compound List Manager is field N6 on Page 2 of the quantitation database in Environmental Data Analysis. The value for Report Detection Limit (on column) can be treated as an information only field. The important field is the Ng on-column Multiplier field in the Sample List. You must adjust the Report Detection Limit (on column) numbers (DL_{noc}) to match how the standards are reported.

Water

Given that the pesticide water CRQL is 0.05 µg/L, Equation 24 can be solved for that C_{qnt} that gives a water sample concentration of 0.05 µg/L. Set all other terms to their nominal value (V_0 = 1,000 mL, V_i = 1.0 µL, V_t = 10,000 µL, M_{noc} = 0.001, Df = 1) and solve for C_{qnt}. A C_{qnt} = 5 ng/mL = 5 pg/µL gives the correct CRQL of 0.050 µg/L for a pesticide water sample.

The term (M_{noc} = 0.001) is needed when the on column detection limit is expressed in terms of picograms-on-column.

Soil

Given that the pesticide soil CRQL is 1.7 µg/Kg, Equation 27 can be solved for that C_{qnt} that gives a soil sample concentration of 1.7 µg/Kg. Set all other terms to their nominal value (V_i = 1.0 µL, W_s = 30 g, V_t = 10,000 µL, M_{noc} = 0.001, Df = 1), and solve for C_{qnt}. A C_{qnt} = 5 ng/mL = 5 pg/µL gives the correct CRQL of 1.7 (1.66) µg/Kg for a pesticide soil sample.

The term (M_{noc} = 0.001) is needed when the on column detection limit is expressed in terms of picograms-on-column.

CRQL calculations

If the analyte is not found, EnviroForms software will calculate a C_{crql} using Equation 27 and substitute that for C_{qnt} in Equation 24 or Equation 26 as appropriate.

$$C_{crql} = \frac{DL_{poc}}{M_{noc}} \quad \textbf{(27)}$$

where:

C_{crql} = Value of C_{qnt} to give the CRQL concentration

DL_{poc} = Report Detection Limit (on-column) (= 5, 10 ... 500 picograms)

M_{noc} = Ng on-column Multiplier (= 0.001) in the Sample List

The value for Report Detection Limit in the Compound List can be treated as an information-only field. The important field is the Ng on-column Multiplier field in the Sample List. Each sample can give a different CRQL. The CRQL is dependent on the actual sample size, the actual dry weight of the soil, the final extract volumes, and the dilution factor.

J flags

The J flag will be assigned any time that C_{qnt} is < (DL_{noc}/M_{noc}). If the LOW standard is reporting analytes at 5.00 ng/mL, the on column detection limits will be 5, 10, 50, 100, 200, or 500. If the LOW standard is reporting analytes at 0.005 ng/µL, the term $M_{noc} = 1$, and you must then enter the on column detection limits as 0.005, 0.010, 0.050, 0.100, 0.200, or 0.500.

Other Factors

EnviroForms software uses some other factors in its calculations that affect the numbers reported on the Forms.

Ng on-column Multiplier

This is set on the Edit Sample Information screen and is used to convert ng/mL to ng/µL as needed in Equation 24 and Equation 26. Set M_{noc} to 0.001 if the LOW standard is labeled as 5.0 ng/mL, or to 1.000 if the LOW standard is labeled as 0.005 ng/mL.

GPC Cleanup (Y/N)

This appears on the Edit Sample Information screen. The value Y or N appears on Form 1. If Y appears on Form 1, the value reported is multiplied by 2. The SOW states that you can concentrate a GPC extract to 5.0 mL rather than 10 mL to account for the 5.0 mL lost in the GPC cleanup. If you do this, you must be sure to set V_t to 5,000 µL for each sample.

Further Concerns

Dilutions and surrogates

The equations are set up to apply the Dilution Factor set in the Sample Information panel to all concentrations. This works out correctly if the surrogates are added to the original sample and the sample is subsequently diluted and reanalyzed.

If samples are prescreened to determine if a dilution is needed, there can be problems with the calculated values for the surrogates concentration.

For example, prescreening indicates that the sample needs a 1:5 dilution. The analyst dilutes the sample, adds the surrogates to the diluted sample, and proceeds with the extraction or purging. A dilution factor of 5 is entered into the Sample Information panel. All analyte values will be corrected to the concentration in the original samples, but all surrogate concentrations will be five times too high.

The best workaround for this is to set a quant dilution factor of 0.2 and apply it to only the surrogates. Then the number in the quant report will be one-fifth of what it should be. The dilution factor used in EnviroForms software will then correct this to the proper concentration. Small dilution factors can give errors because the formats used in CSV.MAC to write out QUANT.CSV are limited to two decimal places. The formats in CSV.MAC may need to be changed to overcome this.

Calibrating soils

The calibrations for a soil are always Sample Type = Calibration, Matrix Level = Water, and Percent Moisture = 100.

Production run

A production run consists of all injections into a given system while the multipoint curve is valid. An ERM can continue as long as the initial multipoint curve is valid. You do not need to create a new ERM for each days work.

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