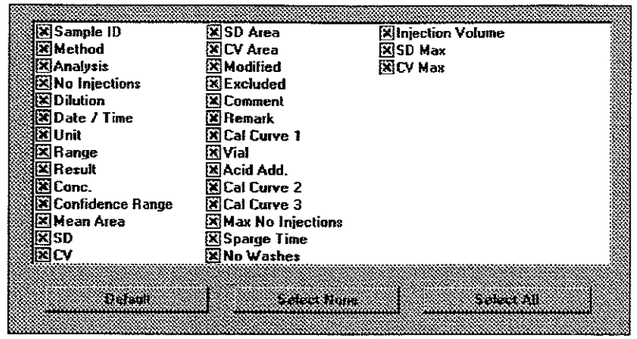
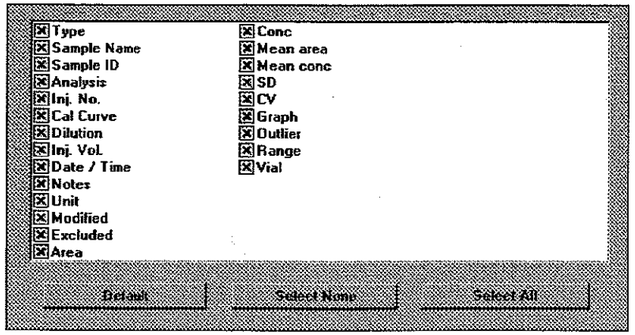
Sample Table tab



The Sample Table items

Specify the items (columns) to appear in the Sample Table. Use the Default button to select typical settings, Select All to view all the items, and Select None to clear the selections.

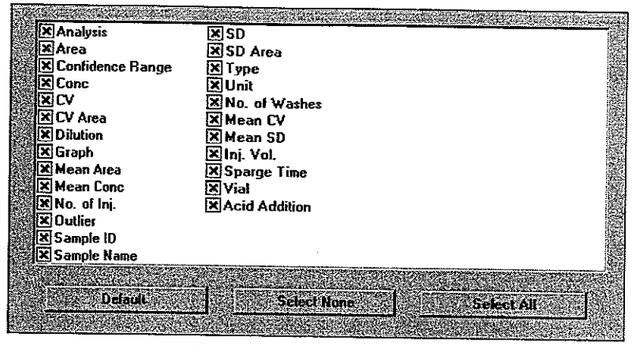
Injection Table tab



The Injection Table items

Specify the items (columns) to appear in the Injection Table. Use the Default button to select typical settings, Select All to view all the items, and Select None to clear the selections.

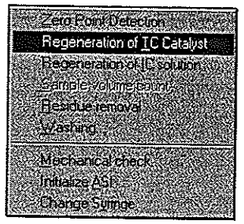
Statistics Table tab



The Statistics Table items

Specify the items (columns) to appear in the Statistics Table. Use the Default button to select typical settings, Select All to view all the items, and Select None to clear the selections.

Maintenance



The Maintenance sub-menu

Zero Point Detection

This procedure determines the zero point of the syringe. Before conducting zero point detection, place a TOC grade water-filled vial in position S1 of the turntable. Zero point detection starts after the sampling needle moves to the S1 vial. When zero point detection is completed, the ASI-5000 arm and needle return to the home positions.

Regeneration of TC Catalyst

As samples are analyzed, inorganic substances deposit on the surface of the catalyst, decreasing

sensitivity and data reproducibility. Catalyst efficiency can be restored with the injection of dilute hydrochloric acid (HCl) into the catalyst.

Before starting regeneration of the TC catalyst, place a vial containing 2N HCl in position S1. Regeneration of the TC catalyst starts after the sampling needle moves to the S1 vial. The 2N HCl is injected into the TC combustion tube several times.

The sampling needle then moves to the rinse water receptacle and the flow line from the sampling needle to the TC injection needle is washed three times with water from the rinse water receptacle.

Regeneration of IC Solution

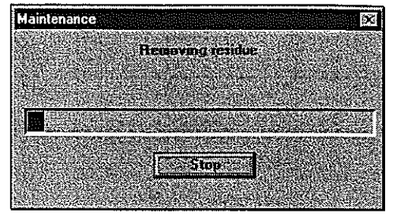
With repetitive sample analysis, the acidity of the IC solution gradually decreases. Regeneration of the IC solution pumps IC reagent to the IC reaction vessel.

Sample Volume Count

Totals the volume of injected sample (not standards) for TC analysis. This is used in combination with the External Scrubber Unit (ESU) optional accessory.

Residue Removal

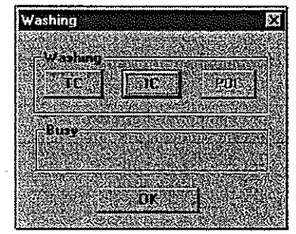
Select this command to remove residue from the flow lines and syringe. The status bar indicates the progress of the procedure.



Residue removal in progress

Washing

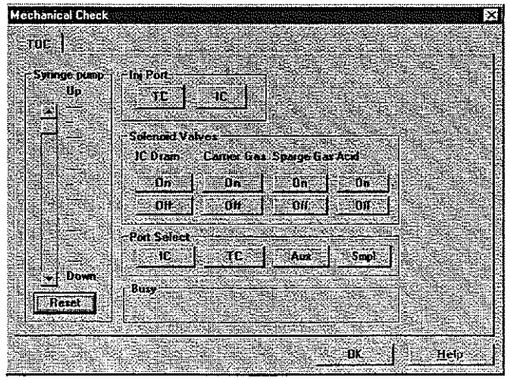
Choose whether to clean the flow lines to the TC, IC, or POC. Select OK when finished.



Select OK when finished

Mechanical Check

Select Mechanical Check to open the Mechanical Check dialog box, shown below.



The Mechanical Check dialog box

TOC Tab

Syringe Pump Slider

Use the arrows to move the syringe plunger up and down. Click RESET to move the plunger to the highest position.

Injection Port

Choose TC to move the TC sliding injection block with needle (alternates direction). Choose IC to move the IC sliding block with needle.

Solenoid Valves

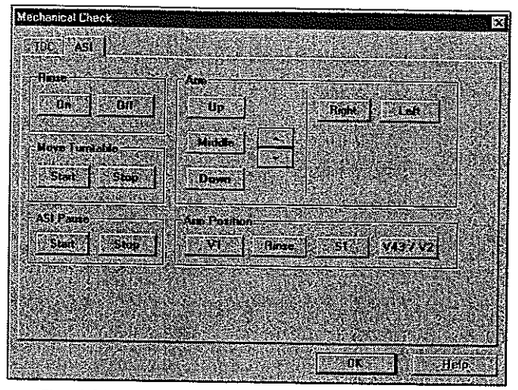
Turn the IC Drain, Carrier Gas, Sparge Gas, and Acid on and off using the ON and OFF buttons below the appropriate title.

Port Select

To open the line between the syringe and an injection port, choose the appropriate port from the buttons in this area of the dialog box. Choose IC, TC, AUX, or SMPL (Sampling Tube).

ASI Tab

The ASI Tab becomes available when ASI Used is checked on the ASI tab of the Options/Instrument Conditions dialog box.



The ASI tab of the Mechanical Check dialog box

Rinse

Use the ON and OFF buttons to start and stop ASI flow line rinsing.

Move Turntable

Use the START and STOP buttons to move the ASI turntable.

ASI Pause

When Start is selected, the ASI finds all its home positions, then returns to its home position.

Arm

Use UP, MIDDLE, and DOWN to move the arm vertically. Use the spin controls for fine vertical adjustments. The RIGHT and LEFT buttons move the arm in a horizontal direction.

Arm Position

Choose V1 to move the arm directly above Vial 1.

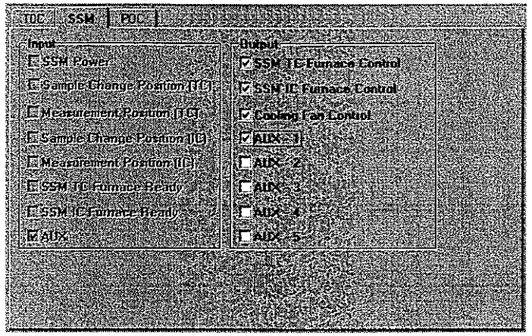
Choose RINSE to move the arm directly above the rinse water receptacle.

Choose S1 to move the arm directly above vial S1.

Choose V43/V2 to move the arm directly above either Vial 43 (when using a regular sensitivity vial) or V2 (when using a high sensitivity vial).

SSM Tab

The SSM Tab becomes available when SSM Used is checked on the SSM tab of the Instrument Conditions dialog box. Select Options/Instrument Conditions to open this dialog box.



The SSM tab of the Mechanical Check dialog box

☛ ***Note:*** *For more information about the SSM, refer to the SSM manual.*

SSM Power

A check mark in this field indicates that the SSM Power is on.

Sample Change Position (TC)

A check mark in this field indicates that the TC sample boat is in the default (sample change) position.

Measurement Position (TC)

A check mark in this field indicates that the TC sample boat has moved to the measurement position.

Sample Change Position (IC)

A check mark in this field indicates that the IC sample boat has moved to the default (sample change) position.

Measurement Position (IC)

A check mark in this field indicates that the IC sample boat has moved to the measurement position.

SSM TC Furnace Ready

A check mark in this field indicates that the SSM TC furnace temperature is ready.

SSM IC Furnace Ready

A check mark in this field indicates that the SSM IC furnace is ready.

Aux

A check mark in this position indicates the Auxiliary port connection has been made.

SSM TC Furnace Control

A check mark in this field indicates the TC Furnace control is on.

SSM IC Furnace Control

A check mark in this field indicates the IC Furnace control is on.

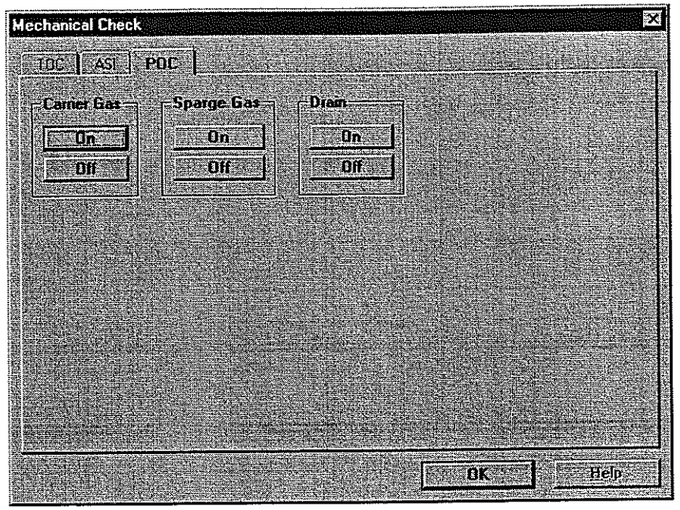
Cooling Fan Control

A check mark in this field indicates the Cooling Fan control is on.

Aux 1 – 5

A check mark in this field indicates the Auxiliary Port connections have been made.

POC Tab



The POC tab of the Mechanical Check Dialog box

The POC Tab becomes available when POC Option is checked on the TOC tab of the Instrument Conditions dialog box. (Select Options/Instrument Conditions to open this dialog box.)

Carrier Gas On/Off

Open the carrier gas valve by turning the Carrier Gas On. Turn off the Carrier gas by selecting Off.

Sparge Gas On/Off

Select the On button to open the sparge gas valve and Off to stop the flow of sparge gas.

Drain On/Off

Choose On to open the Drain Valve and Off to close the valve.

Maintenance Menu (continued)

Initialize ASI

This operation is performed when first connecting the instrument. It establishes communication between the software program and the ASI.

☛ *Note:* *Removing the needle is recommended before performing this procedure for the first time.*

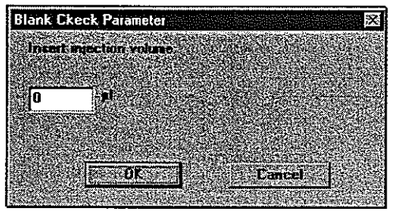
Change Syringe

This command prepares the syringe for removal. Follow the instructions on-screen to specify the new syringe volume and change the syringe.

TC Blank Settings

The TC blank check automatically determines the background level of the instrument. This is normally conducted upon installation and when changing the catalyst. A sample of reagent water is injected into the TC combustion tube and the condensed water is collected in a purified water trap. All carbon in the purified water has been removed. The purified water is then re-injected into the TC combustion tube and the area is measured. This is repeated several times.

Follow the on-screen instructions to complete the procedure.

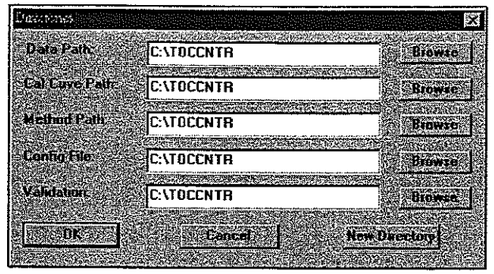


The on-screen instructions guide you through the procedure

☛ *Note:* *This check requires approximately four hours to complete.*

☛ *Note:* *This check can only be performed when high-sensitivity catalyst is in use.*

PC Configuration



The PC Configuration dialog box

Data Path

Enter a default path for data files in the *Data Path* text box. To select a path from the Select Directory dialog box, click BROWSE.

Cal Curve Path

Enter a default path for calibration curve files in the *Cal Curve Path* text box. To select a path from the Select Directory dialog box, click BROWSE.

Method Path

Enter a default path for method files in the *Method Path* text box. To select a path from the Select Directory dialog box, click BROWSE.

Config File

Enter a default path and file name for the configuration file in the *Config File* text box. To select a path and file name from the Open dialog box, click BROWSE. For more information on the configuration file, see *The prm file*, p. 4.

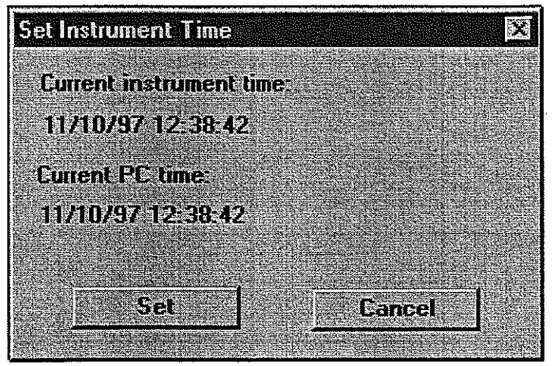
Validation

Enter a default path and file name for the validation file in the *Validation* text box. To select a path and file name from the Open dialog box, click BROWSE

New Directory

Select a new path from the Select Directory dialog box by clicking the NEW DIRECTORY button.

Set Instrument Date/Time



The Set Date/Time dialog box

To set the instrument date and time select SET.

Save Configuration

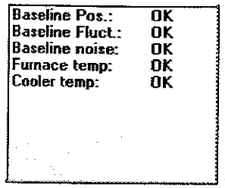
Select Save Configuration to save the Instrument Conditions (visible by selecting Options/Instrument Conditions).

The first time the TOC Control program is used, a .prm file must be specified when this command is executed. When the Save dialog box is opened using this command, the *Save File as Type* field is set to the Parameter File type (prm extension). Select a path and enter a file name for the new prm file. For more information on the settings in the prm file, see p. 4.

Instrument Status

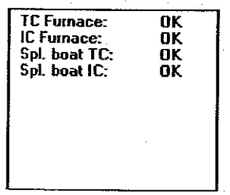
The instrument status indicates the current status of the instrument and its connected components. Alternatively, open each box individually by selecting the items from the instrument status bar.

TOC



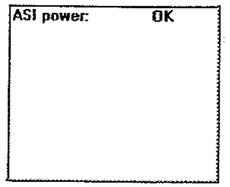
The TOC Status dialog box

SSM



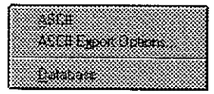
The SSM Status dialog box

ASI



The ASI Status dialog box

10. Export Menu

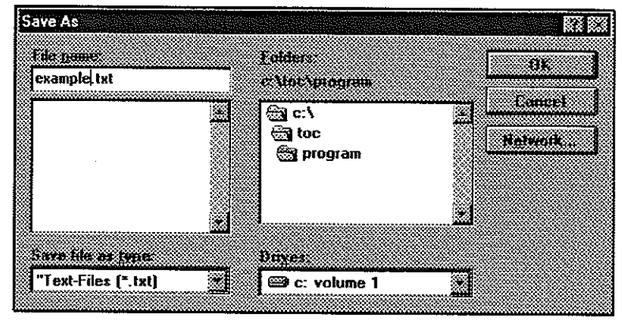


The Export menu

The Export Menu allows you to create data files in formats that are compatible with other programs.

ASCII

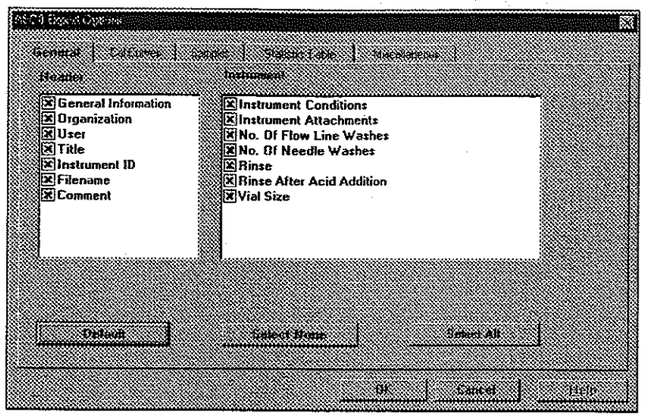
Before selecting this item, use the ASCII Export Options dialog box (see p.128) to specify which data items to export.



The Export Save As dialog box

Then, use this command to open the Export Save As dialog box. Enter a file name and specify the directory for the file (see *File/Save As* on p. 51 for a description of the Network button). Then select OK, and an ASCII text file containing the selected data items is created in the specified location.

ASCII Export Options



Select the items to export from the Export Options tabs

This command specifies the items to be exported by the ASCII command. The items are divided into tabs. Each tab has DEFAULT, SELECT ALL, and SELECT NONE buttons. Use these buttons to facilitate the selection process; the DEFAULT button selects items most commonly chosen for export.

General tab

The General Tab contains all the information from the Options/General Information dialog box (see p. 105). Also on this tab are the current Instrument Conditions. These items come from the Options/Instrument Conditions dialog box (see p. 105). In addition to these items, the Instrument Attachments shows the model numbers of the instrument and the ASI or SSM.

Cal Curves tab

Select items for export relating to the Calibration Curve. These items come from the Calibration Curve dialog box.

Samples tab

Select items for export related to the samples. The Sample information comes from the Sample Table. The Injections information is from the Injection Table.

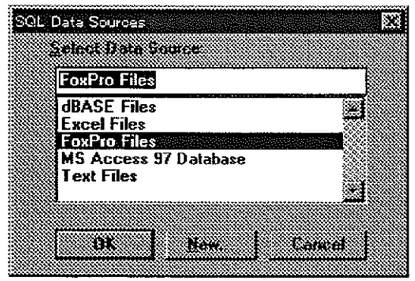
Statistic Table tab

Select items for export related to sample statistics. These items come from the View/ Statistics (Summary) window (see p.89).

Miscellaneous tab

Specify a separator (delimiter) for cell text from the drop-down box. Choices include: Tab, Comma, Colon, Semicolon, or Space. Enable the checkbox to enclose text strings in quotation marks. (This is useful for programs which require all text strings to be isolated by quotation marks.)

Database



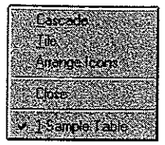
The SQL Data Sources dialog box

The Database command opens the SQL (Structured Query Language) Data Sources dialog box. Here, you can export to any commercial database which supports 16-bit ODBC (Open Database Connectivity) format, like dBase, FoxPro, MS Access, or Paradox.

Choose NEW to specify the data source name. The Add Data Source dialog box opens. Choose the appropriate driver for the database installed on your system. The ODBC setup dialog box opens. Enter the data source name, description, and database information. Choose OK to return to the SQL Data Sources dialog box.

Select the desired data source for export. Click OK. The current sample run is exported.

11. Window Menu



The Window menu

Cascade

Stack all open windows so the title bars are visible using the Cascade command.

Tile

Choose Tile to size all open windows so each occupies an equal portion of the screen.

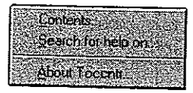
Arrange Icons

Choose Arrange Icons to neatly organize windows reduced to icons.

Close

Closes the current window.

12. Help Menu



The help menu

Contents

Select Contents to open the table of contents for the help file.

Search for help on

Select this menu command to search the help file.

About Toccntr

Select About to view software registration and version information.

Chapter Five Sample Table

The Sample Table is used to set up a data run. Use the Auto Generate, Insert Standard, Insert Control, or Insert Sample functions on the Edit menu to add new unknowns and samples to the chart.

For more information on the Auto Generate function, see p. 65. For more information on the Insert Standard function, see p.67. For more information on the Insert Sample function, see p. 68.

1. Changing Column Width

To change the column width, hold the mouse over the border on the title cell. The cursor changes to two lines with arrows in the middle. Click, then drag the cell border to the desired width.

To automatically adjust the column width to accommodate the longest entry, double-click when the cursor changes to two lines with arrows.

2. Type

The type of analysis is displayed in this column (Standard, Unknown, Control, or Trk Control).

3. Sample Name

The *Sample Name* column displays the descriptive name for the sample. The same name can be used for several samples.

4. Sample ID

The *Sample ID* column displays the descriptive identifier for the sample.

5. Method

The *Method* column displays the method file used for this sample.

6. Analysis

Displays TC, IC, or NPOC analysis types. For more information on these analysis types, see p. 4.

7. Vial

Enter/displays the vial number in the *Vial* column. This column does not appear for SSM measurement.

8. No. Injections

Displays the number of injections performed. This number is always 1 for SSM measurement.

9. Max No. of Injections

The *Max No. of Injections* column shows the maximum number of injections to be performed, if measurement must be re-conducted (because the SD and/or CV max. values were exceeded).

This column is not available for SSM measurement.

10. Sparge Time

This is the sparge time specified for the measurement (for NPOC analysis). This column does not appear for SSM measurement.

11. Dilution

This is the dilution factor specified in the method.

12. No. Washes

This is the number of rinses specified for the measurement. This does not appear for SSM measurement.

13. Injection Volume

The injection volume from the method or calibration is displayed in this column.

14. Acid Addition

The volume of acid added to the sample prior to sparging is displayed (generally for NPOC analysis).

15. SD Max

When the SD Max limit is exceeded, the instrument automatically re-injects the current sample until the measurement is within the limit or the maximum number of injections is reached. An injection that exceeds the SD Max is excluded. (This does not appear for SSM measurement.)

16. CV Max

When the CV Max limit is exceeded, the instrument automatically re-injects the current sample until the measurement is within the limit or the maximum number of injections is reached. An injection that exceeds the CV Max is excluded. (This does not appear for SSM measurement.)

17. Amount (mg)

Enter/displays the amount of sample in mg for SSM samples.

18. Volume (µl)

Enter/displays the volume of sample for SSM samples.

19. Density (mg/µl)

Displays the sample density for SSM samples.

20. Cal Curve 1, 2, and 3

These fields display the Calibration Curve file names. See *Appendix B* for more information on how the program chooses a calibration curve from among the three listed.

For SSM analysis, only one calibration curve is displayed.

21. Range

The range which was used to analyze the samples/standards is displayed here.

22. Mean Area

The *Mean Area* column displays the average of the area counts.

23. CNV

This item displays the result of the following equation:

$$\frac{\text{area of } n^{th} \text{ measurement} \times \text{weight (volume) of standard in } n^{th} \text{ measurement}}{\text{weight (volume) of standard in first measurement}}$$

The SD and CV values are calculated according to the converted area values displayed here. This column does not appear for ASI measurement.

24. Abs C

Shows the absolute carbon value for SSM measurement.

25. Conc

This is the calculated concentration of the sample in the units selected. Note that if the Confidence Range item is selected in the Sample Table tab (Options/ Display Settings), the confidence interval (calculated according to DIN38402) is shown in addition to the concentration.

26. Unit

The unit of concentration selected for the analysis is displayed here.

27. Result

The Result calculates the TOC concentration, which is either the TC measurement minus the IC measurement (TOC = TC-IC) or the POC measurement plus the NPOC measurement (TOC = NPOC + POC), depending on the measurement type selected.

28. SD

The *SD* column displays the standard deviation of the concentrations. See p. 76 for more information on the standard deviation calculation.

29. CV

The *CV* column displays the coefficient of variation of the concentrations. See p. 76 for more information on the coefficient of variation calculation.

30. SD Area

The *SD* column displays the standard deviation of the area counts. See p. 76 for more information on the standard deviation calculation.

31. CV Area

The *CV* column displays the coefficient of variation of the area counts. See p. 76 for more information on the coefficient of variation calculation.

32. Modified

An M appears in the *Modified* column if the data has been modified after it was collected.

33. Excluded

An E appears in the *Excluded* column if the data was excluded from calculations.

34. Remark

The software generates remarks for certain samples, such as Revision 23 samples.

35. Comment

A comment is displayed in this column.

36. Date/Time

The date and time at which the injection was performed displays in the *Date/Time* column.

Chapter Six Injection Table

The injection table shows detailed information about the injections from one row of the Sample Table.

To open an Injection Table, click in the Sample Table row to be examined. Then, select Injections from the View menu, or click the Injection Table button  in the Toolbar. The Injection Table opens, with three sections of injection information: the Table, the Graph, and the results of the Outlier Test.

1. Injection Table

The table columns can be customized to display only certain columns by enabling the desired items in the Options/ Display Settings/ Injections Tab.

Type

The type of sample (from the Sample Table) is shown: Standard, Unknown, Control, or Trk Control.

Sample Name, Sample ID

The name of the sample and sample ID (from the Sample Table) is shown.

Analysis

The type of analysis (TC, IC, TOC, NPOC, NPwI) used for the injection is shown (see p. 4 for a description of these analyses).

Injection No.

The injection number is shown in order of injection.

Vial

The vial number for the injection is shown. This column does not appear for SSM measurements.

Cal Curve

The calibration curve used for calculation is shown. The concentration of the injection is calculated based on this curve.

Dilution

Dilutions made, if any, are shown here. This is a multiplier for the concentration value. If no dilution was made, the multiplier is 1.0000.

Inj. Vol.

The injection volume (from the Sample Table) is displayed. This column does not appear for SSM injections.

Range

The range (from the Sample Table) is shown. If the range is automatically changed during measurement (for ASI), the new value is displayed here.

Date/Time

The Date and Time of the injection are displayed.

Notes

Remarks about the injection are made here.

T: Tailing Peak

The peak end point was not detected within a specified period of the start point (about 4.5 min for TC and 3.5 min for IC).

H: Height

The peak height exceeded the working range of the detector by a large amount. If the peak height exceeds full scale, the injection amount is reduced in an attempt to obtain the peak on-scale.

h: height

The peak exceeded the working range of the detector by a small amount. When this occurs, the

Range value is automatically adjusted and the sample is re-injected.

B: Baseline

The baseline was not stable during measurement.

F: Furnace

The furnace temperature fluctuated outside the acceptable range during measurement.

S: Solution

Auto-regeneration of the IC solution has occurred.

Unit

The unit of measurement (from the Sample Table) is displayed.

Modified

When the operator uses the Recalculate function (Edit/Recalculate), an M appears in this column, indicating that the data has been modified after measurement.

Excluded

If an injection was excluded from calculation because it exceeded the detector's linear response, or the SD Max and/or CV Max, this will be shown here as the letter "E." To manually exclude an injection, select the row, then Edit/Exclude. Save the file under its new name. To include an injection that was excluded, select the Exclude command again.

Area

The area count for the injection is displayed. At the bottom of this column, the Mean (MV) area count, Standard Deviation (SD) and Coefficient of Variation (CV) are shown. For more information on these items, see p. 76.

Conc

The calculated concentration is displayed here; the calculation is based on the displayed calibration curve and is also shown in the graph on the right. At the bottom of the column, the Mean concentration value is displayed.

Amount

The amount of sample (in mg) from the Sample Table is given here when the SSM is used. This column appears only for a SSM measurement.

Volume

The SSM volume, from the Sample Table, is given here. This column appears only for a SSM measurement.

CNV

The CNV value from the Sample Table appears here when the SSM is used.

This column appears only for a SSM measurement.

µg C

This shows the µg Carbon in a sample when the SSM is used. This column appears only for a SSM measurement.

2. Injection Graph

The Injection Table window graph shows a plot of area counts for each injection. If the graph is hidden, enable the display in the Options/ Display Settings/ Injection Table tab.

Each point on the graph represents one injection. Note that outliers are indicated differently. Five lines on the graph help with statistical interpretation: the mean, and one and two times the standard deviation above and below the mean.

The appearance of the graph can be customized, and more detailed information about the graph can be obtained. (This is also true of the Statistics (Summary) graph, and

to a lesser extent, the Peak Profile graph, Calibration Curve graph, and Baseline Profile graph.)

To customize and manipulate the graph, click on the graph with the right mouse button. The Graph menu appears.

The Graph menu

Copy

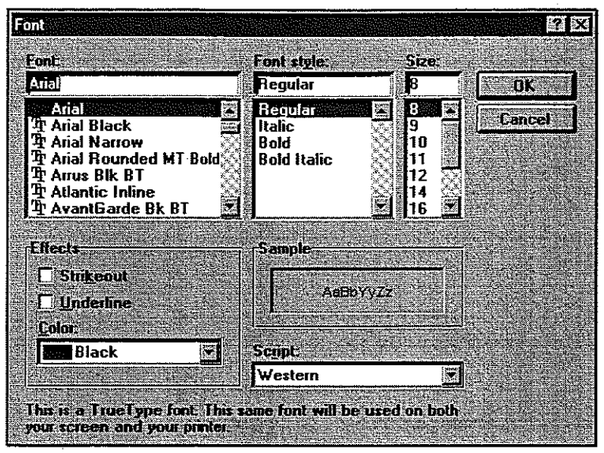
This copies the graph onto the clipboard. The bitmap can then be pasted into other applications.

Cross-hair

The Cross-hair sub-menu

From the sub-menu that appears, select Display to extend the cross-hairs and display detailed axis information at the cross-hair position. Select Lock to freeze the extended cross-hairs in position. Undo either of these actions by selecting the item again.

Fonts

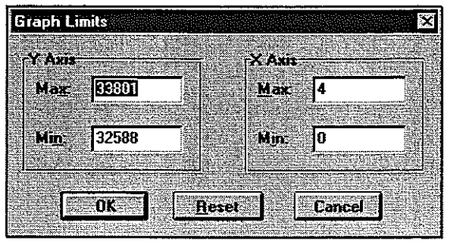


The Font dialog box

This opens the Font dialog box, where graph text style, size, and color can be changed to customize the graph's appearance.

Limits

Opens the Graph Limits dialog box, where upper and lower limits for values of the X and Y axis can be changed, so that the scale of the graph display changes.

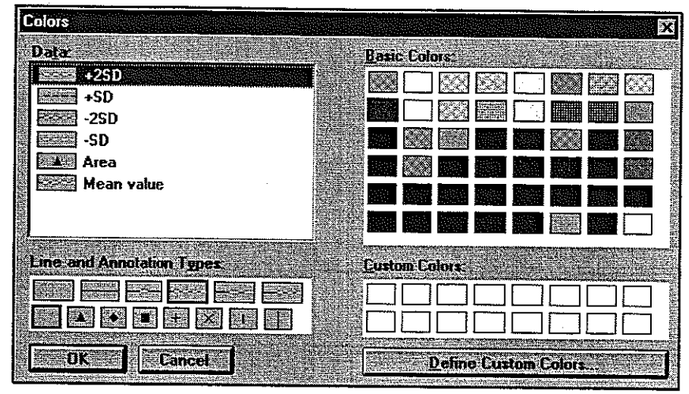


The Graph Limits dialog box

Enter new values, then select OK. The graph display changes according to the new limits. To restore the graph to its original appearance, open the dialog box, select Reset, then OK.

Line Colors

Opens the Colors dialog box, where the colors and types of annotation for the graph can be changed.



The Colors dialog box

Note: *The appearance of this dialog box varies with the graph.*

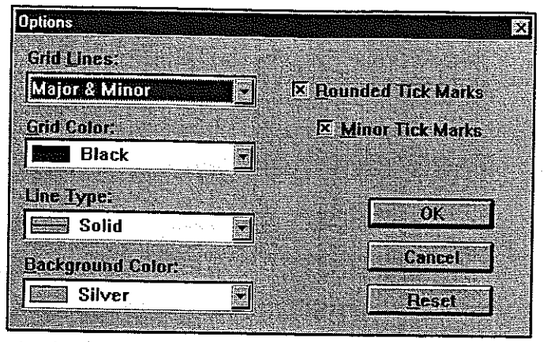
Click on one of the items to be changed in the *Data* field (for example, the Mean value line). With the item highlighted, select the new color, line type, or annotation type. Note that line types are in the first row of the bottom left box, and annotation types are in the bottom row.

To hide the line or annotation, select the first box in the appropriate row.

Select OK once the items have been customized. The graph displays with the new settings.

Options

The Options command opens the Options dialog box. Here, a grid can be selected, along with grid options and graph background color.



Customize the graph's appearance with the Options dialog box

Grid Lines

From the drop-down box, select from None, Major, or Major & Minor. The Major selection will draw the grid lines at major unit divisions. The Major & Minor selection will draw grid lines at both major and minor unit divisions.

In addition to the grid, major (rounded) and minor tick marks can be drawn to indicate unit divisions. With no grid, both major and minor tick marks can be selected. With a major grid, minor tick marks can be selected.

Grid Color

The color of the grid lines can be selected from the drop down list.

Line Type

Choose the line type for the grid lines from the drop down list.

Background Color

Choose the background color for the graph from the drop down list.

✒ *Note:* *Do not choose the same color for the grid, line colors, and background!*

Radar

Selecting this item opens the following sub-menu:

The Radar sub-menu

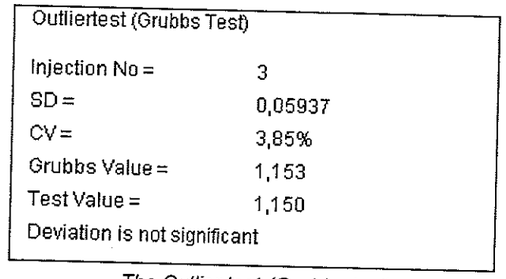
These items automatically scale the graph to maximize the display of information. The X and Y axes can be auto-scaled individually, or both axes can be adjusted.

Changing the Magnification

The graph can be magnified. To enlarge any portion of the graph, drag a box around the area of interest. The area inside the box expands to fill the graph window. Use Limits (see above) to restore the original view.

3. Outlier Test

The third portion of the Injection Table shows the results of the Outlier Test (Grubbs test).



The Outlier test (Grubbs test)

Outliers are values that lie outside the range of valid results. These values can be excluded from calculation with the Edit/Exclude command. The Grubbs test is used to determine whether a value is far enough from the mean to be considered an outlier. This test is performed in both the Injection Table and the Statistics (Summary) window.

When either of these windows is opened, an outlier test is performed on the data and the results are displayed (unless the display was turned off in the Display Options section of the Options menu). The test indicates whether any of the data points in the sample run being examined should be excluded.

The TOC Control program uses the Grubbs Test for evaluating outliers. In this method, the data points are ranked in order, from X_1 to X_n. The mean ($\overline{X}$) and standard deviation (SD) are calculated using all the data points. A value T is calculated according to the following equation:

If $X_1 < \overline{X}$: $T = \dfrac{(\overline{X} - X_1)}{SD}$

If $X_1 > \overline{X}$:: $T = \dfrac{(X_1 - \overline{X})}{SD}$

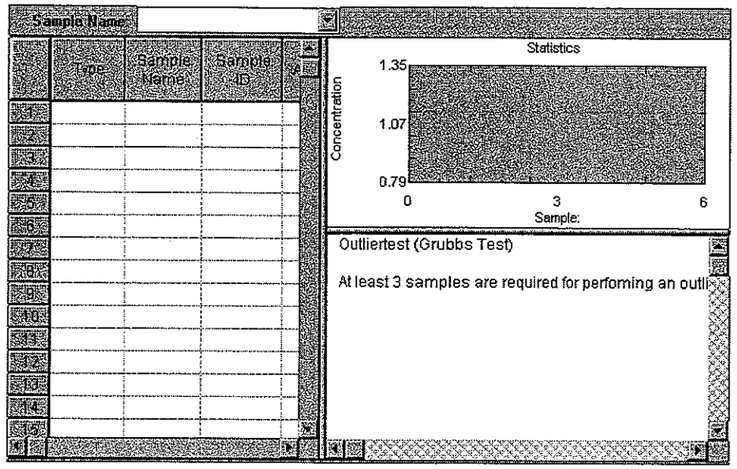
X_1 is the data point with the highest deviation from the mean value $\overline{X}$.

The value T is then compared to the Grubbs value (rM(f,P), where f= number of data points, P = 95%) from the Grubbs table. If the test value T is larger than the Grubbs value rM, the data point is considered an outlier.

Chapter Seven Statistics Summary Table

The Statistics Summary Table makes statistical comparisons among samples with the same Sample Name. This is useful, for example, for identifying outliers, or obtaining the mean area count, of all samples from a particular sampling site.

To obtain the Statistics Summary table, open a Sample Table, then select Statistics (Summary) from the View menu. The Statistics Summary table window opens.



The Statistics Summary window

At the top of the table is the Sample Name drop down list. Choose one of the Sample Names for statistical comparison. All samples with the same Sample Name will appear in the Statistics Summary window.

The window is divided into three sections: the table, the graph, and the outlier test. Each section can be resized by dragging the dividers with the mouse.

1. Statistics Table

The displayed columns can be customized by changing the Display Settings for the Statistics Table (in the Options menu).

To change the column width, hold the mouse over the border on the title cell. The cursor changes to two lines with arrows in the middle. Click, then drag the cell border to the desired width.

To automatically adjust the column width to accommodate the longest entry, double-click when the cursor changes to two lines with arrows.

Type

The type (Unknown, Control, or Trk Control) of sample is shown. This information comes from the Sample Table.

Sample Name

The Sample Name (from the Sample Table) is shown here. This should correspond to the Sample Name chosen from the drop-down list at the top of the window.

Sample ID

The Sample ID for the injections in the row (from the Sample Table) is displayed.

Analysis

The type of analysis from the Sample Table is shown.

Vial

The vial number for the sample injections is given. This column does not appear for SSM measurements.

No. of Injections

The number of injections per vial is displayed. This information is from the Sample Table.

No. of Washes

The number of sample washes performed during the injections is displayed (from the Sample Table). This column does not appear for SSM measurements.

Sparge Time

The Sparge Time, if any, from the Sample Table is shown. This column does not appear for SSM measurements.

Acid Addition

The amount of acid added (if any) is shown in µL. This information comes from the Sample Table. This column does not appear for SSM measurements.

Dilution

The dilution factor, if any, from the Sample Table is given. Note that if the dilution factor is greater than 1, the final concentration value has been multiplied by this factor.

Inj. Vol.

The injection volume for each injection is displayed (this comes from the Sample Table). This column does not appear for SSM measurements.

SD

The standard deviation is calculated for each row. Note that these values are the same as those of the Sample Table.

CV

The coefficient of variation is calculated for each row. Note that these values are the same as those of the Sample Table.

Area

The average area count for all the injections in the row is given. Note that these values are the same as those of the Sample Table. At the bottom of the column, the MV (Mean Value), SD (Standard Deviation) and CV (Coefficient of Variation) for the areas are given. This statistical information allows comparison of the area counts for all the rows in the column (all the samples with the same Sample Name).

Conc

The average concentration for all the injections in the row is given. Note that these values are the same as those of the Sample Table. At the bottom of the column, the MV (Mean Value), SD (Standard Deviation) and CV (Coefficient of Variation) for the areas are given. This statistical information allows comparison of the concentration values for all the rows in the column (all the samples with the same Sample Name).

Unit

The unit of measurement is given. This comes from the Sample Table.

Confidence Range

The confidence range used for the statistical analyses is given.

Amount [mg]

For SSM measurements, this is the sample amount in mg. This comes from the Sample Table.

Volume [µl]

This is the volume of liquid sample introduced by the SSM in µL, from the Sample Table.

Abs C

For SSM measurements, this is the absolute carbon value.

2. Statistics Graph

The Statistics Summary graph window shows a plot of concentration for each injection. If the graph is hidden, enable the display in the Options/ Display Settings/ Statistics Table tab.

Each point on the graph represents one injection. Note that outliers are indicated differently. Five lines on the graph help with statistical interpretation: the mean, and one and two times the standard deviation above and below the mean.

The appearance of the graph can be customized, and more detailed information about the graph can be obtained (see p. 142.)

3. Outlier Test

The third portion of the Statistics Summary Window shows the results of the Outlier Test (Grubbs test).

Outliertest (Grubbs Test)

Injection No =	3
SD =	0,05937
CV =	3,85%
Grubbs Value =	1,153
Test Value =	1,150

Deviation is not significant

The Outlier test (Grubbs test)

Outliers are values that lie outside the range of valid results. These values can be excluded from calculation. The Grubbs test is used to determine whether a value is far enough from the mean to be considered an outlier. This test is performed in both the Injection Table and the Statistics (Summary) window.

When either of these windows is opened, an outlier test is performed on the data and the results are displayed (unless the display was turned off in the Display Options section of the Options menu). The test indicates whether any of the data points in the sample run being examined should be excluded.