GENERAL OPERATING INFORMATION

The DU Series 600 Spectrophotometer user interface operates on the principle of windows. A "mouse" is used to move an arrow around a window. Action is initiated when a mouse button is clicked on.

The instrument contains several analysis modes, which are selected from the Main window by using the mouse to position an arrow on the mode name and clicking on the left mouse button. When the mode is selected, an analysis window for the mode is displayed. Analysis parameters can be input in the analysis window or can be recalled from a stored method.

The analysis modes have an associated Method window, which is used to recall stored methods and to input the parameters to develop new methods. The methods, sample data, calculated results, and standard data can be stored, in a designated file. These files are located in the main instrument or in an optional external disk.

3.1 Analysis Windows

Analysis windows are displayed during normal operation. These windows are used to select parameters, collect data and calculate results. A typical analysis window is shown in Figure 3-1.

	Fired Wave ReadSample		h Meth	od Par	ameters	S	aveClear	Print	HEL⊃ Quit
>	Results f Read aver			1 0 Read mo	ode: [Abs]		name: A:\F g device:		•
·	Sample I	D	Fact	350.0 or 56.00	Facto	440.0 or 230.0	λ 5 Factor	20.0 6.500	
	1 2 43F 43T 46J 48K		Abs 0.2790 0.3647 0.6747 0.67413 1.0447 0.9504	RBSU 1 t RG/M1 15.6221 28.4213 37.7840 35.9108 58.5056 53.2240	Abs 0.1535 0.0971 0.2244 0.2421 0.3162 0.3767	Result ng/ml 35.2955 22.3246 51.6012 55.6869 72.7205 86.6482	Abs 6.3152 6.3784 1.0832 6.6864 1.4383 1.3868	Result ng/n1 2.6490 2.4596 7.8407 4.4613 9.2369 8.9698	
	BLANK Match off		OFF] Re			486.0 nm .0813 Abs		DATE TEMP /30/91 N/A	CELL 1

Figure 3-1. Typical Analysis Window

The manual uses the following nomenclature when referring to analysis windows:

1 - Window

The entire display, or any portion of the display that is enclosed with a box. More than one window can be displayed at a time.

2 - Window Name

All analysis windows have a name on the top line of the window. An example of each analysis window is provided in this manual. A listing of these windows is provided at the end of the Table of Contents.

3 - Help Messages

"HELP" is displayed on the top line of the window, to the right of the window name. Click on "HELP" to display Help windows.

4 - Permanent Menu Bar

A list of commands is always displayed at the bottom of the display. A permanent menu bar command is referred to in these instructions with the use of double angle brackets, i.e. << BLANK>>. Status information is provided on the right-hand side of the permanent menu bar.

5 - Window Menu Bar

A list of commands is located at the top of each window, directly below the window name. The specific commands change with each window. A window menu bar command is referred to in these instructions with the use of single angle brackets, i.e. <Print>. Commands that can be used are identified by color.

6 - File Names

The files where the method, standard data, and/or results data are stored are listed directly under the window menu bar.

7 - Parameters

The analysis parameters are listed near the top of a window. Parameters are referred to in these instructions with the use of quotes, i.e. "Wavelength". The values for parameters that can be changed are displayed in a different color than the parameter name.

8 - Data Column Labels

Some column labels can be changed, such as the units for calculated results. Labels that can be changed are displayed in the same color as parameters that can be changed.

9 - Scrolling Arrows

Click on the arrows to display data that is not displayed because of insufficient room. The window shown in Figure 3-1 has both up and down arrows and right and left arrows. Many windows have only up and down arrows.

3.2 General Operating Procedure

When the DU Series 600 Spectrophotometer is powered up, it performs a series of diagnostic tests. When these tests are completed satisfactorily, the Power Up Diagnostics window, Figure 3-2, is displayed.

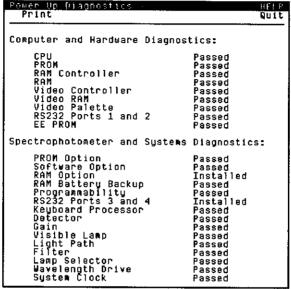


Figure 3-2. Power Up Window

If all power up tests pass, remove the Power Up Diagnostics window from the display by using the mouse to move the arrow to <Quit> and clicking on the left mouse button. The Main window, Figure 3-3, is displayed. The Main window is used to select an operating mode.

NOTICE

If any power up test fails, refer to the Troubleshooting section for instructions.

Programmability is an option and may not be installed on all instruments.

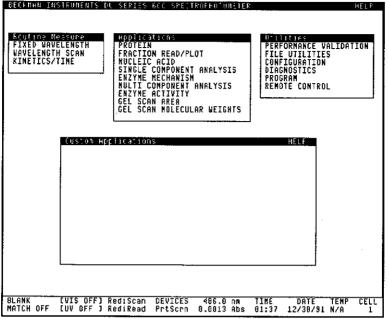


Figure 3-3. Main Window

The following are general operating instructions. Specific instructions for each analysis mode are provided in the respective section in this manual.

- To select an analysis mode from the Main window, use the mouse to move the arrow to the desired mode. Press the left mouse button to click on the analysis mode. An analysis window, such as shown in Figure 3-1, is displayed.
- 2. Analysis parameters are listed on the window. The mouse is used to input different values for the parameters. More information on parameter input is given in section 3.7.
 - As an alternative, a stored method can be recalled or a new method can be developed. Either of these is done by clicking on <Method>, located on the menu bar at the top of the window to display the Method window. A typical Method window is shown in Figure 3-16.
- 3. When the desired parameters are displayed, place a cuvette of blank solution in the sample compartment and click on <<BLANK>>. (<<BLANK>> is located in the permanent menu bar.)

- 4. Place the first sample in the sample compartment and click on <Read-Samples>. (<ReadSamples> is located on the menu bar at the top of the window.) As an alternative, the right mouse button can be used to take a sample reading, with the cursor in any position.
- 5. To print the data, click on **<Print>**. All information in the window is printed, even if only partial information is displayed, because of insufficient room. If the window contains graphic data, it is printed on the device selected in the Printer and Plotter Configuration window. If the window contains no graphic data, it is printed on the printer, if installed and operational. The permanent menu bar is not printed.

To stop printing while the DU-600 is transferring the information to the printer, the Stop Printing window is placed at the top of the display. To stop printing, click on [QUIT]. Reset the paper to the top of a new page before starting another printout.

To stop printing after the Stop Print window is removed, click on <<DEVICES>> to display the Device Control window. Click on [STOP PRINTING], then <Exit> to remove the Device Control window from the display. Reset the paper to the top of a new page before starting another printout.

- 6. To clear all data from the window, with the option of storing the data, click on **SaveClear>**. If the data are stored, no additional data can be placed in the data file.
- 7. When the analysis is complete, click on <Quit> to return to the Main window. (<Quit> is located on the menu bar at the top of the window.) An opportunity is given to store the method and/or sample data.

1 -

3.3 Help Messages

Help windows are displayed by clicking on "HELP", displayed to the right of the window name. Typical Help windows are displayed in Figures 3-4 and 3-5. If a Help window similar to Figure 3-4 is displayed, click on the desired selection to display a Help window similar to Figure 3-5. Click on <Exit> to remove the Help windows from the display.

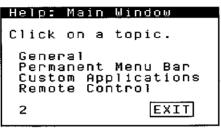


Figure 3-4. Help Window

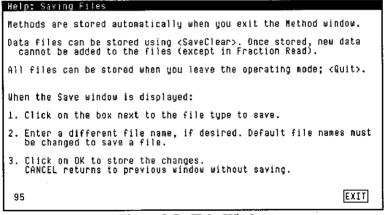


Figure 3-5. Help Window

3.4 The Mouse

The mouse, Figure 3-6, is used to move an arrow to desired locations on the DU Series 600 Spectrophotometer display. When the arrow is in a desired location, click on the left mouse button to initiate action. The items that can be clicked on include window menu bar commands, file names, parameters, sample data, and permanent menu bar commands.

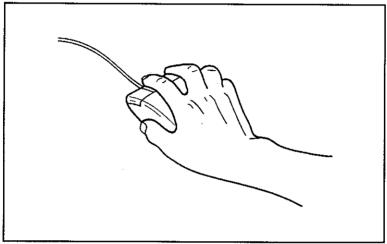


Figure 3-6. Mouse

The left mouse button is used the most frequently to click on a command or parameter. However, the mouse buttons have other uses:

- To take a reading The right mouse button can be used to initiate a reading, with the cursor in any position, as an alternate to <ReadSamples> in the window menu bar.
- 2. To input lower case letters When the alphanumeric keypad is displayed for character input, click on the right mouse button, rather than the left button, to input lower case letters.
- 3. To use Trace Trace is a feature that is used to find the ordinate and abscissa values from graphic data. Trace is a window menu bar command (<Trace>) that is clicked on in the normal manner. After <Trace> is clicked on, the mouse is used to move the arrow to the desired location on the graph and the center mouse button is clicked on to position a line on the graph. Then the right and left mouse buttons can be used to move the line to the right and left, respectively.

The Hour Glass

Most of the time the arrow appears on the window. However, when an action is initiated that cannot be completed quickly, the arrow is changed into an hour glass. The hour glass can be moved across the window in the same manner as the arrow, and the mouse buttons can be clicked on, but no action occurs until the arrow returns. Typical actions that cause the hour glass to be displayed include printing a window and performing complex data calculations.

The Diskette Symbol

When the optional disk drive is accessed, the arrow is changed into a diskette symbol. The diskette symbol cannot be moved and no action can be taken until disk access is completed.

3.5 Permanent Menu Bar

The permanent menu bar, Figure 3-7, is always displayed at the bottom of the display. Commands that can be used at any time during the operation of the instrument are listed on the left-hand side of the permanent menu bar. Current nanometer position and reading are displayed in the middle. Status information is displayed on the right-hand side. If a source burns out during operation, an error message is displayed under the commands on the left-hand side.

BLANK (VIS OFF) Rediscan DEVICES 486.0 nm TIME DATE TEMP CELL MATCH OFF (UV OFF) Rediread Priscrn 0.0013 Abs 81:37 12/30/91 M/A 1

Figure 3-7. Permanent Menu Bar

The permanent menu bar commands are:

BLANK

Take a reading at the analytical and background wavelength(s) and set the value 0.000 absorbance and 100%T. In the Wavelength Scan mode, only, make a background scan.

MATCH OFF/ON

If an Auto Cell Holder is used for the analysis, zero readings can be taken on each of the cuvettes. When Match is enabled, the zero readings are subtracted from all subsequent readings for the appropriate cell. Operational information is provided in Manual 517314.

VIS OFF/ON

Turn the visible source on or off.

UV OFF/WAIT/ON

Turn the UV source on or off. The UV source requires about 30 seconds to light after being turned on. During this time <<UV WAIT>> is displayed.

NOTICE

Do not blank the instrument or take sample readings while <<UV WAIT>> is displayed, even in the visible region. When the UV source lights, readings at all wavelengths are affected.

RediScan

Enter the RediScan mode. This is described in section 4.3.

RediRead

Enter the RediRead mode. This is described in section 4.2.

DEVICES

Display the Device Control window, Figure 3-8. The window is used to stop sending information to the printer or plotter after printing has begun; to position the transport at a cell position for the Auto Cell Holder, a millimeter position, or the home position to align; to control the temperature controller; and to move the aspirator arm on the batch sampler. When the desired action has been taken, click on **Exit>** to remove the window from the display.

The information input in the Device Control window is overridden if the device is automatically controlled as part of an analysis.

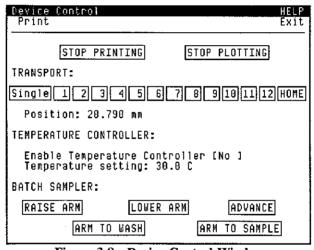


Figure 3-8. Device Control Window

PrtScrn

Print an exact copy of the entire display on the Dot Matrix Printer. Information that is not displayed because of insufficient room will not be printed. The X-Y Plotter cannot be used for this printout.

NOTICE

There is also a **Print>** command in the menu bar at the top of most windows, which is used to print the window in which it appears and also prints the continuation of data that are not displayed.

The status information includes:

Nanometer Position

The current nanometer position.

Absorbance/Transmittance Reading

The current reading, in either absorbance or transmittance, determined by the reading mode in the selected analysis mode. This field is blank until the instrument is blanked.

TIME

The current time. The time is set in the configuration mode, using the Clock Configuration window.

DATE

The current date. The date is set in the configuration mode, using the Clock Configuration window.

TEMP

The current temperature, if the Temperature Controller is being used. When the Temperature Controller is controlling temperature, "on" is displayed under the temperature. If the Temperature Controller is not installed or is not turned on, "N/A" is displayed. The Temperature Controller is turned on using the Device Control window, Figure 3-9.

CELL

If the Transport Accessory is installed, the Auto Cell Holder cell number that is in the beam is displayed. If the Transport Accessory is not installed, "N/A" is displayed.

3.6 Window Menu Bars

Across the top of analysis windows is a menu bar specific to the window. This is referred to in the manual as a window menu bar or simply a menu bar. The following are some of the commands that typically appear in the menu bar.

<ReadSamples>

Take a sample reading. In some modes, and with some sampling accessories, this command causes the window shown in Figure 3-9 to be displayed. Sample readings are started when [START] is clicked on and are stopped when [QUIT] is clicked on.

Insert sample(s) Click on START when ready Click on QUIT to stop START QUIT

Figure 3-9. Read Samples Window

In most cases, clicking on the right mouse button, with the cursor in any position, performs the same function as <ReadSamples> and [START].

<Window Name>

Most operating modes have more than one analysis window. The other windows are displayed by clicking on the window name, displayed in the menu bar.

<Method>

Display the Method window to select a stored method or create a new method.

<SaveClear>

Clear all data from the window, without leaving the analysis mode. Before the data are removed, the Save Clear window, Figure 3-10, is displayed, allowing the data to be stored. To store the data, click on the box to darken it, verify that the desired file name is displayed and click on [OK]. To change the file name, click on it to display the Results File Directory window, which is described in section 3.9. To change the storage location, click on the displayed location to toggle between [A:\] and [B:\].



Figure 3-10. Save Clear Window

NOTICE

The user can select to have the save box darkened automatically each time the Quit window is displayed. This selection is made on the User Interface window in the Configuration mode, which is described in section 2.4.

<Print>

Print the data displayed on the window. Alphanumeric data are printed on the Dot Matrix Printer. Sample data and other information that are not displayed on the screen because of insufficient room are printed. If the X-Y Plotter is installed, graphic data can be printed on either the Dot Matrix Printer or the X-Y Plotter. This is selected in the Printer and Plotter Configuration window.

<Exit>

Remove the window.

<Quit>

Leave an operating mode and return to the Main window. If the method, standards file or results file has changed, the Quit window, Figure 3-11, is displayed. To store any of the information, click on the associated box to darken it, verify that the desired file name is displayed and click on [OK]. To change a method file name, click on it to display the alphanumeric keypad and input the desired file name. To change a data file name, click on it to display the Results File Directory window, which is described in section 3.9. To change the storage location, click on the displayed location to toggle between [A:\] and [B:\].

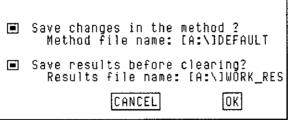


Figure 3-11. Quit Window

NOTICE

The user can select to have the save boxes darkened automatically each time the Quit window is displayed. This selection is made on the User Interface window in the Configuration mode, which is described in section 2.4.

3.7 Parameter Input

Parameters that pertain to a particular analysis window are listed near the top of the window. The Method window contains a complete listing of analysis parameters. The selected value can be changed for any parameter where the displayed value is a different color than the parameter. For example: the parameter, "Wavelength", is a different color that the value, "500".

There are several types of parameter input. These include:

Numeric Input

When a parameter is clicked on that requires a numeric input, the numeric keypad, Figure 3-12, is displayed. The limits of the input are displayed at the bottom of the keypad. Input the desired value and click on [OK] to accept the value and remove the numeric keypad. Examples of parameters that require numeric input include the wavelength, number of samples, and read average time.

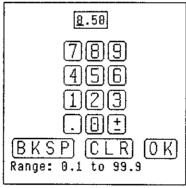


Figure 3-12. Numeric Keypad

As an alternative, the optional keyboard can be used to input numbers. When the numbers are input, they are displayed in the box at the top of the keypad. When the desired number(s) are displayed, press enter on the keyboard (or click on [OK] on the keypad) to accept the value and remove the keypad.

Alphanumeric Input

When a parameter is clicked on that requires an alphanumeric input, the alphanumeric keypad, Figure 3-13, is displayed. The maximum number of characters that can be input is indicated by the space provided for the input. Input the desired information and click on

[OK] to accept the information and remove the alphanumeric keypad. Examples of parameters that require alphanumeric input include file names, concentration units and sample identifications.

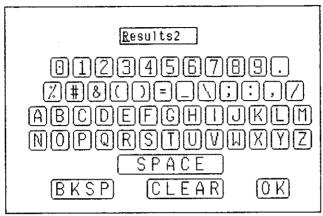


Figure 3-13. Alphanumeric Keypad

As an alternative, the optional keyboard can be used to input this information. When the characters are input, they are displayed in the box at the top of the keypad. When the desired characters are displayed, press enter on the keyboard (or click on [OK] on the keypad) to accept the information and remove the keypad.

Option Selection

If a parameter has a variety of options, a selection window is displayed when the parameter is clicked on. In some cases, the word "VIEW" is displayed and clicked on to get the selection window. A typical selection window is shown in Figure 3-14.

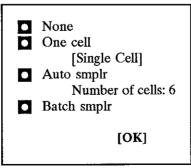


Figure 3-14.
Sampling Device Window

Each of the options on the selection window is preceded by a box. Click on the box to darken it to select the desired option. A second click on the box removes the darkened area. Some selection windows accept only one choice. Others allow multiple selections. When the selection(s) are made, click on [OK] to input the option and remove the selection window.

Bracketed Options

Some parameters require a selection from only two or three options, such as "yes" or "no". The selection for these types of parameters is displayed with brackets, such as [Yes]. When the selection in brackets is clicked on, the selection changes to the other option. For example, click on [Yes] to display [No]. Examples of parameters that have bracketed options include the selection of absorbance or transmittance readings and the use of a background wavelength.

Parameters that Cannot Change

If the selected value for an analysis parameter is displayed in the same color as the parameter, the value cannot be changed. There are several reasons that a parameter cannot be changed. They include:

- 1. The method in use has been protected. After a method is developed, it can be protected, so that the analysis must be done with the selected parameters.
- 2. Parameters used for sample collection must be the same as for the related standards. For example, if the standard curve was calculated using an analytical wavelength of 500 nm, the wavelength for the sample analysis must be 500 nm.
- 3. Data collection is complete. For example, the temperature cannot be changed if data were previously collected.

3.8 Method Development and Use

Parameter setup for analyses that are repeated often can be simplified by storing the analysis parameters in a method file. Each analysis mode (with the exception of the Fraction Read mode) has a Method window associated with it. The Method window is used to setup, store and retrieve analysis parameters. A typical Method window is shown in Figure 3-15.

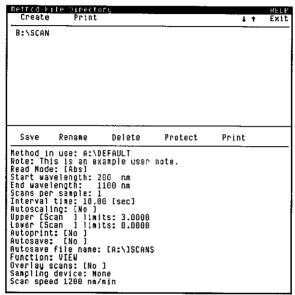


Figure 3-15. Typical Method Window

Each Method window is divided into two parts. The top part is the Method File Directory; the bottom part lists the analysis parameters for the "Method in use".

Creating a Method

To create a new method:

- 1. With the Main window displayed, click on the desired analysis mode. The first window for the analysis mode is displayed.
- 2. Click on <Method> to display the Method window for the analysis mode. The analysis parameters are listed in the lower part of the window.

- 3. If the method to be created is similar to an existing method, click on the existing method name in the directory at the top of the Method window. The existing parameters are displayed on the lower part of the window.
- 4. Click on <Create> to display the Create window, Figure 3-16.

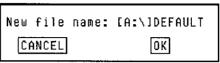


Figure 3-16. Create Window

Input the new method file name and location in this window.

- a. To input the location, click on the displayed location to toggle between [A:\] and [B:\].
- b. To input the new file name, click on the name that is displayed following "New file name" to display the alphanumeric keypad. Input the new name, then click on [OK] to remove the keypad.
- c. Click on [OK] to remove the Create window and accept the new file name.
- d. The new method file name is displayed following "Method in use".
- 5. To input comments about the method, click on "Note" and use the alphanumeric keypad to input a message with a maximum of 40 characters.
- 6. To input the analysis parameters, click on the displayed value(s) and input the desired value(s). Detailed instructions for parameter input are provided in section 3.7.
- 7. After the desired parameters are displayed on the Method window, the method can be used or stored, and if stored, protected.

To use or to store the method, click on **Exit>**. The method is stored automatically and the appropriate analysis window is displayed with the parameters for the method.

To store the method without removing the Method window, click on <Save>. This allows more than one method to be created without leaving the Method window.

Protected Methods

After a method has been developed and stored, it can be protected. The parameters for a method that has been protected cannot be changed, as long as the protection remains.

To protect a method:

- 1. Display the desired method name on the Method window, following "Method in use".
- 2. Click on <Protect> to display the Set Protection window, Figure 3-17.

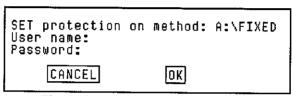


Figure 3-17. Set Protection Window

3. Input the assigned "User name" and "Password", then click on [OK]. If both are accepted, the protection is implemented and the window is removed from the display. **PROTECTED** is displayed following the method name on the Method window.

To remove protection:

Protection is removed using the same steps. If a protected method is displayed following "Method in use", when <Protect> is clicked on, the Remove Protection window shown in Figure 3-18, is displayed. To delete the protection, input the assigned "User name" and "Password", and click on [OK].

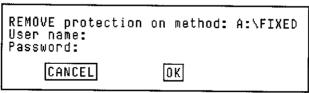


Figure 3-18. Remove Protection Window

Placing the Method Name on the Main Window

The method can be listed on the Main window in the area entitled "Custom Applications". To place it there, use the File Utilities mode to copy the method file from the appropriate method directory to the "CUST_APP" directory. Up to 30 methods can be listed on the Main window.

Using a Stored Method

To use a stored method listed in the "Custom Applications" area on the Main window, click on the desired method name. The appropriate analysis window with the values for the method is displayed.

NOTICE

When a method listed in the "Custom Applications" area is selected, the parameters can be modified on the applications window or the Method window. However, the changes cannot be stored. To store the changes, recall the method from the applications mode, make the changes, store the method, then move it to the Custom Applications directory.

To use a stored method not listed on the Main window:

- 1. With the Main window displayed, click on the desired analysis mode. The first window for the analysis mode is displayed.
- 2. Click on <Method> to display the Method window for the analysis mode.
- 3. The Method File Directory for the analysis mode is displayed at the top of the Method window. Click on the desired method name. The parameters are displayed on the lower part of the window.
- 4. If the method is protected, the protection is indicated to the right of the method name on the lower part of the window. If the method is not protected, any of the parameters can be modified.
- 5. Click on **Exit** to display the appropriate analysis window with the values for the method.

Renaming a Method File

- 1. Display the desired method name, following "Method in use", on the Method window.
- 2. Click on <Rename> to display the Rename window, Figure 3-19.



Figure 3-19. Rename Window

- 3. Click on the name following "New file name" and input the desired file name. Then click on [OK] to rename the file and remove the window from the display.
- 4. The file is stored with the new name when either <Save> or <Exit> (to remove the Method window) is clicked on.

Deleting a Method File

- 1. Display the desired method name, following "Method in use", on the Method window.
- 2. Click on < Delete > to display the Delete window, Figure 3-20.

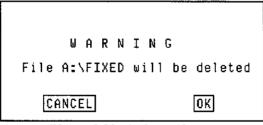


Figure 3-20. Delete Window

3. Verify that the desired file name is displayed, then click on [OK] to delete the file and remove the window from the display.

3.9 Stored Data

The instrument has the capability of storing the data it collects either in internal memory (drive A) or on the optional external disk drive (drive B). Data from most modes are stored in "Results Files". However, some modes have special types of data files, such as "Standard Files" in the protein analysis mode. All types of data files operate the same.

Data files are renamed, copied to another location, moved to another location and deleted using the File Utilities mode. Instructions are provided in section 8.

The following options are available for data storage:

1. Not storing the data.

The data are removed from the window by clicking on either <SaveClear> or <Quit> to display the appropriate window. The data are deleted if the box next to the file name is *not* darkened. The Save Clear window is shown in Figure 3-10. The Quit window is shown in Figure 3-11.

- Designating a file name for data storage before the data are collected.
 The file name is input by clicking on "Results file", displayed with the other parameters on the analysis window.
- 3. Collect the data and then decide whether to store the data.
 When the data are removed from the window by clicking on either <SaveClear> or <Quit>, the appropriate window is displayed.
 The data are stored if the box next to the file name is darkened.

Naming a File

When "Results file" is clicked on from an analysis window, or when the file name is clicked on from the Save Clear or Quit window, the Results File Directory window specific for the analysis mode is displayed. A typical Results File Directory window is shown in Figure 3-21.

To name a new results file:

- 1. To input the location, click on the location that is displayed following "Selected file" to toggle between [A:\] and [B:\].
- 2. To input the new file name, click on the name that is displayed following "Selected file" to display the alphanumeric keypad.

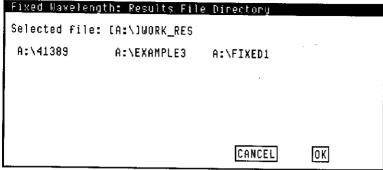


Figure 3-21. Results File Directory Window

- 3. Input the new file name, then click on [OK] to remove the keypad.
- 4. Click on [OK] to remove the window and accept the new file name.
- 5. The new file name is displayed following "Results file".

Recalling Data

Data files that are stored in the instrument can be recalled in the mode where they were created. The stored information can be used to recalculate results in the same way that the data was manipulated after it was collected. With the exception of the Fraction Read mode, data cannot be added to an existing file.

To recall data:

- 1. With the Main window displayed, click on the desired analysis mode. The first window for the analysis mode is displayed.
- 2. Verify that no data are displayed on the window. If data are displayed, click on <SaveClear>.
- Click on the file name following "Results file". The Results File Directory window is displayed.
- 4. Click on the desired file name, listed in the directory to place the name after "Results file name". Click on [OK] to remove the Results File Directory window and display the data in the appropriate analysis window.

GETTING STARTED

The DU Series 600 Spectrophotometer user interface operates on the principle of windows. The "mouse" is used to position an arrow on the window. When the arrow points to the desired position, the left button on the mouse is pressed to initiate the desired action. In these instructions, the positioning of the arrow and pressing the left mouse button is called "clicking on".

4.1 Power Up

Power Up Diagnostics Window

When the DU Series 600 Spectrophotometer is powered up, the Power Up Diagnostics window, Figure 4-1, is displayed. If all tests passed, use the mouse to move the arrow so that it points to "Quit", located near the top right-hand corner of the window, and press the left mouse button.

Power Up Diagnostics Print			Quit
			quic
Computer and Hardware	Diagnost	ics:	
CPU PROM RAM Controller RAM Video Controller Video RAM Video Palette RS232 Ports 1 and EE PROM		Passed Passed Passed Passed Passed Passed Passed Passed Passed	
Spectrophotometer and	Systems	Diagnostic	s:
PROM Option Software Option RAM Option RAM Battery Backup Programmability RS232 Ports 3 and Keyboard Processor Detector Gain Visible Lamp Light Path Filter Lamp Selector Wavelength Drive System Clock	4	Passed Passed Installed Passed	

Figure 4-1. Power Up Window

Getting Started 4-1

NOTICE

If any of these tests fail, refer to the Troubleshooting instructions in section 11.1 of this manual.

Programmability is an option and may not be installed on all instruments.

The "Quit" command is located in the menu bar at the top of the Power Up Diagnostics window. Most windows have a menu bar associated with them. Commands in the menu bar at the top of a window are referred to in these instructions with single angle brackets, i.e. <Quit>.

Main Window

When the Power Up Diagnostics Window is removed, the Main window, Figure 4-2, is displayed. The desired operating mode is selected from the Main window. The Fixed Wavelength, Wavelength Scan and Kinetics/Time modes are standard on all instruments. All other modes are optional, and are only displayed if they are installed on the instrument.

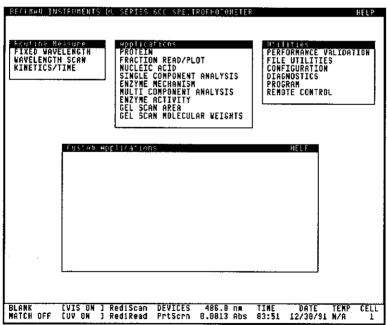


Figure 4-2. Main Window

Sources

The commands to turn the sources on and off are located in the Permanent Menu bar, which is always located at the bottom of the display. Commands in the permanent menu bar are referred to in the instructions with double angle brackets, i.e. <<VIS OFF>>.

To turn on the visible source, click on <<VIS OFF>> to display <<VIS ON>>. The visible source lights immediately.

To turn on the UV source, click on <<UV OFF>> to display <<UV WAIT>>. The UV source requires about 30 seconds to warm up before it lights. When the source lights the command is changed to <<UV ON>>. Do not blank while <<UV WAIT>> is displayed.

The instrument should be allowed to warm up for at least 30 minutes before blanking and taking sample readings. Any reading taken with the sources turned off is invalid.

To turn off the sources, click on <<VIS ON>> and/or <<UV ON>>. When the source is turned back on, a new blank will be required.

Data Collection Modes

The DU Series 600 Spectrophotometer has five data collection modes: RediReadTM Mode, RediScanTM Mode, Fixed Wavelength, Wavelength Scan and Kinetics/Time. They are described in the following sections.

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4.2 RediReadTM Mode

The RediRead window is used to take fixed wavelengths readings at one or more wavelengths quickly and easily. This window can be displayed whenever the instrument is not collecting data, regardless of the operating mode of the instrument. Data collected in this mode cannot be stored.

1. Click on <<RediRead>>, located in the permanent menu bar at the bottom of the display, to display the RediRead window, Figure 4-3.

RediRead ReadSample	ReadBlank	: Print	HELP Exit
500.0nm 0.1	278 A		
Read avg ti Sample Wav		Read Mode: Reading	[Abs]
2 500 3 500		0.0109 A 0.0481 A 0.1091 A 0.1278 A	

Figure 4-3. RediRead Window

- 2. Set the parameters:
 - a. Click on the wavelength value displayed and input the desired wavelength.
 - b. Click on "Read avg time" and input the desired read average time.
 - c. Verify that the desired reading mode is displayed, [Abs] or [%T]. Click on the mode to change it.
- 3. Place a cuvette of solvent in the cell holder and click on <ReadBlank>. (If the instrument has previously been blanked at the selected wavelength using <<BLANK>>, it is not necessary to blank in the RediRead mode. <ReadBlank> in the RediRead mode does not affect the blank stored using <<BLANK>>.)
- 4. Place a cuvette of sample solution in the cell holder and click on <ReadSample>. The reading is displayed in the table on the window.

- 5. Repeat step 4 for all the samples. The parameters input in step 2 can be changed at any time.
 - Readings from 11 samples are displayed on the window. When the sample 12 is read, the data is written over the data for sample 1.
- 6. To print the window, click on <**Print>**. Only the data that are displayed are printed.
- 7. To remove the RediRead window, click on <Exit>.

4.3 RediScanTM Mode

The RediScan window is used to make a wavelength scan at 1200 nm/min on a sample with minimum parameter setup. Data collected using this window cannot be stored; the Wavelength Scan mode must be used for data storage.

1. Click on <<RediScan>>, located in the permanent menu bar at the bottom of the display, to display the RediScan window, Figure 4-4.

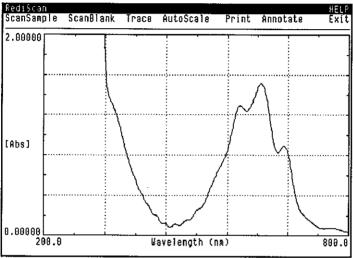


Figure 4-4. RediScan Window

- 2. Verify that the proper ordinate label is displayed, [Abs] or [%T]. Click on the label to change it.
- 3. Verify that the desired wavelength limits are displayed. To change them, click on the displayed value and input the desired value. The sample will be scanned over the displayed wavelength range, only.
- 4. Place a cuvette of solvent in the cell holder and click on <ScanBlank>. (If the instrument has previously been blanked in the Wavelength Scan mode at 1200 nm/min over the selected range, it is not necessary to blank in the RediScan mode.)
- Place a cuvette of sample solution in the cell holder and click on ScanSample>. The scan data is displayed.

- 6. The following functions are available to reformat the data:
 - a. The data can be autoscaled by clicking on <AutoScale>.
 - b. Individual axis limit values can be changed by clicking on them and inputting the desired value.
- 7. To display the wavelength and ordinate readings at any point in the spectrum, click on <Trace>. Then move the mouse to the point of interest in the spectrum and click on the center mouse button to place a vertical line on the spectrum. The values at the place where the vertical line is placed are displayed in the lower right-hand side of the window. To move the vertical line to either the right or left, click on the right or left mouse button, respectively.
- 8. To annotate the data, click on <Annotate>. Then, click on the graph to position a cross and input information from the alphanumeric keypad or keyboard. Up to four annotations can be placed on the graph. The annotations are printed with the window, but are not stored with the data.
- 9. To print the wavelength scan in the window, click on <Print>.
- 10. Repeat steps 5 to 8 for all the samples.
- 11. To remove the RediScan window, click on **Exit>**.

4.4 Fixed Wavelength

The Fixed Wavelength mode is used to collect data from a series of samples at up to 12 wavelengths. The data can be multiplied by user-input factor(s) to calculate a result at each wavelength. Any of the sampling devices can be used to simplify sample handling. Data can be stored for later recall.

To select the analysis parameters:

1. With the Main window displayed, click on "FIXED WAVELENGTH" to display the Fixed Wavelength window, Figure 4-5.

Fixed Wavelergi ReadSamples	h Method	Parameters	SaveClear	Print	HEL? Quit
Results file: Read average t		ead mode: [Abs]	Method name: A:\FI Sampling device: N		†
Sample ID		0.0 56.00 Factor	440.0 λ 5 230.0 Factor	20.0 6.500	
1 2 43F 43T 46J 48K	0.2790 15 0.3647 20 0.6747 37 0.6413 35 1.0447 58	.4213 0.0971 .7840 0.2244 .9108 0.2421 .5056 0.3162	mg/ml 35.2955 0.3152 22.3246 0.3784 51.6912 1.0832 55.6869 0.6864 72.7205 1.4303	Result ng/nl 2498 24596 7.0407 4.4613 9.2969 8.9698	

Figure 4-5. Fixed Wavelength Window

2. Click on <Parameters> to display the Parameters window, Figure 4-6.

Fixed Wavelend ClearAll	ith: Para Print	meters	Exit
Wavelength	Factor	Units	Use
350.0 440.0 520.0 200.0 400.0 350.0 550.0 600.0 750.0	56.90 230.0 6.500 1.000 1.000 1.000 1.000 1.000 1.000 1.000	mg/ml	Cyes] Cyes] Cyes] CNo] CNo] CNo] CNo] ENo]

Figure 4-6. Parameters Window

- a. Listed in the Parameters window are 12 wavelength values, with a factor and units that correspond to each wavelength. To change any of these values, click on the displayed value to display a keypad. Input the desired value on the keypad, then click on [OK] to accept the input and remove the keypad.
- b. The fourth column in the Parameters window is the "Use" column. Each wavelength that is to be used in the analysis must have a "Yes" displayed. If a "No" is displayed for a desired wavelength, click on the "No" to display a "Yes".
- c. When all the desired values are displayed, click on **Exit>** to remove the Parameters window. The input values are immediately displayed on the Fixed Wavelength window.
- 3. Readings can be taken in either absorbance or transmittance. The selection is displayed following "Read mode" in the parameter listing near the top of the window. To change the read mode, click on the displayed option.

To take readings:

- 1. Place a cuvette of solvent in the instrument. Click on <<BLANK>>.
- If desired, click on the next displayed sample number and input up to an 11-digit alphanumeric sample identification. If a sample identification is not input, the instrument numbers the samples consecutively.

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- 3. Place a cuvette of sample solution in the cell holder and click on <ReadSamples>.
- 4. Data from up to 3 wavelengths are displayed at one time. To display data at other selected wavelengths, click on the right and left arrows, located on the right-hand side of the analysis parameters.
- 5. Repeat steps 2 to 4 until all samples have been read.
- 6. To print the sample data, click on <Print>.
- 7. When the analysis is complete, click on **Quit>**. To store the method and/or results, click on the displayed file name(s) and input the desired file name(s). Then click on **[OK]** to store the data and return to the Main window.

The complete capabilities of the Fixed Wavelength mode are described in section 5 of this manual.

4.5 Wavelength Scan

The Wavelength Scan mode is used to collect, manipulate and store scan data.

To select the analysis parameters:

1. With the Main window displayed, click on "WAVELENGTH SCAN" to display the Wavelength Scan window, Figure 4-7.

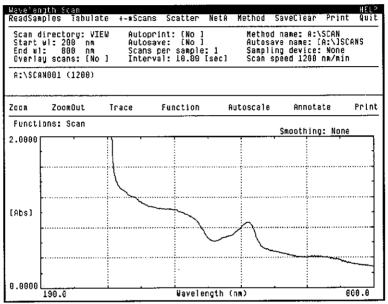


Figure 4-7. Wavelength Scan Window

- 2. Twelve parameters are listed near the top of the window.
 - a. Locate the "Start wl" and "End wl" parameters. To change the values, click on the displayed value and input the desired values.
 - b. Verify that the following parameters are as follows:

Overlay scans: [No]
Autoprint: [No]
Autosave: [No]
Scans per sample: 1
Sampling device: None
Scan speed: 1200 nm/min

If any of the parameters are different than those listed, click on the displayed value and input the listed value.

3. The ordinate label and limits are displayed on the graphic portion of the window. To change any of these values, click on the displayed value and input the desired value.

To take readings:

- 1. Place a cuvette of solvent in the cell holder. Click on <<BLANK>>.
- 2. Place a cuvette of sample solution in the cell holder and click on <ReadSamples>.
- 3. The following functions are available to reformat the data:

Autoscale - Automatically scales the ordinate axis.

Limit changes - The limits on either axis can be changed by clicking on the displayed value and inputting the desired value.

Zoom - The "zoom" feature is used to expand any portion of the graph. Click on <Zoom>, then click on two points on the graph to place crosses at the opposite corners of the area to be enlarged. When the second cross is clicked on, the graph is replotted. This can be repeated as often as desired. To return to the original plot, click on <ZoomOut>.

- 4. To smooth the data, click on "Smoothing" and select the desired number of points to use for the calculation. If too few points are used, the data may appear to be noisy. If too many points are used, real peaks can be lost.
- 5. To display a derivative or log scan, peak pick, valley pick and/or point pick, click on <Function> to display the Function Selection window. To select a function, click on to darken the box preceding the selection. Then click on <Exit> to remove the Function selection window from the display. The data are replotted using the selected function(s).
- 6. To display the wavelength and ordinate readings at any point in the spectrum, click on <Trace>. Then move the mouse to the point of interest in the spectrum and click on the center mouse button to place a vertical line on the spectrum. The values at the place where the vertical line is placed are displayed in the lower right-hand side of the window. To move the vertical line to either the right or left, click on the right or left mouse button, respectively.

- 7. To annotate the data, click on <Annotate>. Then, click on the graph to position a cross and input information from the alphanumeric keypad or keyboard. The annotation is printed with the window, but is not stored with the data.
- 8. To print the sample data, click on < Print>.
- 9. To store data before scanning another sample, click on <SaveClear>. Click on the displayed file name, input the desired file name, then click on [OK]. The data are stored and the graphic area is cleared.
- 10. To scan additional samples, repeat steps 2 to 9, above.
- 11. When all the samples have been scanned, click on <Quit>. To store the method and/or displayed scan, click on the displayed file name(s) and input the desired file name(s). Then click on [OK] to store the data and return to the Main window.

The complete capabilities of the Wavelength Scan mode are described in section 6 of this manual. These include selection of different analysis parameters, overlaid scans, repetitive scanning, scatter correction, spectral manipulation (addition, subtraction and multiplication), and net absorbance.

4.6 Time Drive

The Kinetics/Time mode is used to collect, manipulate and store time drive data. This mode is also used to calculate the rate of kinetic reactions.

To select the analysis parameters for time drive:

1. With the Main window displayed, click on "KINETICS/TIME" to display the Plotting window, Figure 4-8.

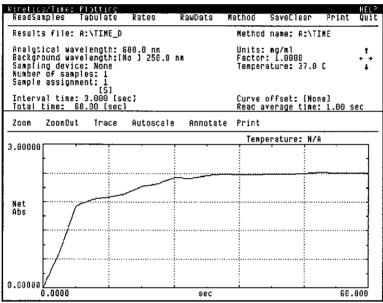


Figure 4-8. Plotting Window

- 2. Fourteen parameters are listed near the top of the window.
 - a. Locate "Analytical wavelength". To change the wavelength, click on the displayed value and input the desired wavelength.
 - b. Locate "Interval time", which determines the frequency of data collection. To change the displayed value, click on it and input the desired value.
 - c. Locate "Total time", which determines when data collection is stopped. To change the displayed value, click on it and input the desired value.

d. Verify that the following parameters are as follows:

Background wavelength: [No]

Sampling device: None Number of samples: 1 Sample assignment: [S] Read average time: 0.5 sec

If any of the parameters are different than those listed, click on the displayed value and input the listed value.

3. The absorbance limits are displayed on the graphic portion of the window. To change the limits, click on the displayed value and input the desired value.

To take readings:

- 1. Place a cuvette of solvent in the cell holder. Click on <<BLANK>>.
- 2. Place the sample in the cell holder and click on <ReadSamples>. The Read Samples window is displayed. Click on [START].
- 3. The data are displayed as they are collected. If no data appear on the graph, the data probably do not fall within the axis limits.
- 4. After data collection is complete, the following functions are available to reformat the data:

Autoscale - Automatically scales the ordinate axis.

Limit changes - The limits on either axis can be changed by clicking on the displayed value and inputting the desired value.

Zoom - The "zoom" feature is used to expand any portion of the graph. Click on <Zoom>, then click on two points on the graph to place crosses at the opposite corners of the area to be enlarged. When the second cross is clicked on, the graph is replotted. This can be repeated as often as desired. To return to the original plot, click on <ZoomOut>.

- 5. To annotate the data, click on <Annotate>. Then, click on the graph to position a cross and input information from the alphanumeric keypad or keyboard. The annotation is printed with the window, but is not stored with the data.
- 6. To print the sample data, click on **<Print>**.

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- 7. To display the tabulated data, click on <Tabulate>.
- 8. Before analyzing another sample, click on **SaveClear**. To store the data, if desired, click on the displayed file name and input the desired file name, then click on [OK]. The data are stored and the graphic area is cleared.
- 9. To analyze additional samples, repeat steps 2 to 8, above.
- 10. When all the samples have been analyzed, click on <Quit>. To store the method and/or displayed data, click on the displayed file name(s) and input the desired file name(s). Then click on [OK] to store the data and return to the Main window.

The complete capabilities of the Kinetics/Time mode are described in section 7 of this manual. These include selection of different analysis parameters, analysis of multiple samples, and rate calculations.

4.7 Recalling Stored Files

Method File

If a method was stored in one of the operating modes, it can be recalled by clicking on the file name following "Method name", listed with the analysis parameters at the top of the analysis window. When the file name is clicked on, the Method window is displayed. The stored method files are displayed near the top of the window. To select a stored file, click on the file name. The parameters will be listed in the lower portion of the window. Then click on <Exit> to remove the method window and display the analysis parameters on the analysis window.

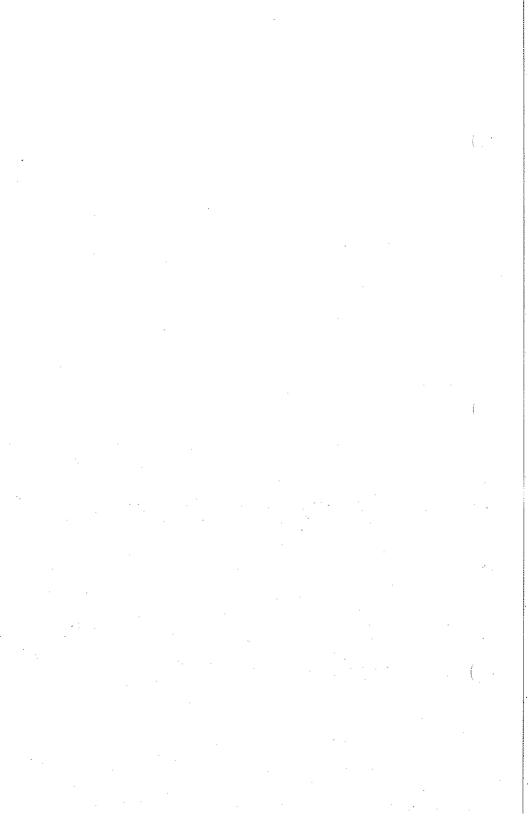
Results File - Fixed Wavelength and Kinetics/Time

If a results file was stored in the Fixed Wavelength or Kinetics/Time mode, it can be recalled by clicking on the file name following "Results file" on the analysis window. When the file name is clicked on, the directory is displayed. To select a stored file, click on the file name, then click on [OK] to remove the directory and display the data on the analysis window.

Scan File - Wavelength Scan

If a scan file was stored, it can be recalled by clicking on "VIEW", following "Scan directory" on the Wavelength Scan window. When the file name is clicked on, the directory is displayed. To select a stored file, click on the file name, then click on [OK] to remove the directory and display the data on the Wavelength Scan window.

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FIXED WAVELENGTH

The Fixed Wavelength mode is used to collect data in either absorbance or transmittance at up to 12 wavelengths. The reading at each wavelength can be multiplied by a user input factor to calculate a final result.

5.1 Calculations

The result is calculated using the equation:

Result = Reading x Factor,

where the reading is in either absorbance or transmittance. The result is a concentration value if the reading is taken in absorbance.

NOTICE

Use of this mode to calculate concentration requires that the slope of the standard curve is constant and known, and that the y-intercept is zero. Concentration calculations, derived from a standard curve with multiple standards, are possible using the optional Single Component Analysis mode.

5.2 Parameter Setup

Click on "FIXED WAVELENGTH" from the Main window to start the analysis. The Fixed Wavelength window, Figure 5-1, is displayed. The Fixed Wavelength window is used to select analysis parameters, collect sample data and display stored sample data.

tmed kaveleng: eadSamples	Method	Para	neters	Sa	veClear	Print	80 i i
Results file: Read average t	A:\⊌ORK_RE: iae: 0.50	Read Rod	e: [Abs]		ame: A:\D device: (Yes]		1
Sample ID	λ 20 Factor	1.800	λ 2 Factor	50.0 1.000	λ 3 Factor	90.9 1.000	
1	Abs	Result Rg/al	Abs	Result mg/ml	ADS	Result mg/ml	

Figure 5-1. Fixed Wavelength Window

Use the Method window to setup the analysis parameters:

- Click on <Method> to display the Method window, Figure 5-2. The Method window is used to setup analysis parameters, recall stored methods and create new methods. General information on method windows is provided in section 3.8.
- 2. To recall a stored method, click on the desired method name in the listing at the top of the Method window.
- 3. The analysis parameters are displayed on the lower part of the Method window. Input the desired analysis parameters:

Method in use - This displays the name of the method that has been selected. If the method is protected, **PROTECTED** is displayed following the method name. If the method is protected, the analysis parameters cannot be changed. To input a new method name, click on <Create>.

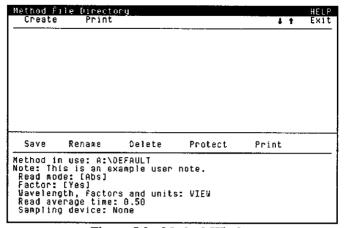


Figure 5-2. Method Window

Note - Click on to input a 40-character message that is used to describe the method or procedure.

Read mode - Toggle between [Abs] and [%T] to select readings in absorbance or transmittance, respectively.

Factor - Toggle betweem [Yes] and [No] to specify whether a factor and units are input for each wavelength for results calculations.

Wavelength, factors and units - Click on "VIEW" to display the Parameters window, Figure 5-3. The Parameters window is used to input analysis wavelength(s), a concentration factor for each wavelength and the concentration units for each wavelength.

Fixed Wavelend ClearAll	ith: Para Print	meters	Exit
Wavelength	Factor	Units	Use
200.0 250.0 350.0 400.0 450.0 550.0 650.0 700.0	1.986 1.998 1.908 1.908 1.908 1.808 1.800 1.800 1.608 1.608 1.608	mg/ml	Yes] Yes] Yes] Yes] Yoo] ENO]

Figure 5-3. Parameters Window

Fixed Wavelength 5-3

- a. Input the desired values for wavelengths, factors and units by clicking on the respective location and inputting the desired values. Up to 12 wavelengths can be input.
- b. Enable or disable each wavelength by clicking on [Yes]/[No] in the "Use" column.
- c. When all the desired values are input, click on **Exit** to accept the values and remove the window from the display.

Sampling device - Display the Sampling Device window to select the sampling device. Detailed information on the sampling devices is provided in Manual 517314.

Read average time - The time, in seconds, that data are collected and averaged to take a reading. Twenty sets of data are collected every second.

- 3. To store the analysis parameters in the selected method file, click on <Save>.
- 4. Click on **Exit** to display the Fixed Wavelength window with the parameters from the selected method.

To input the desired parameters on the Fixed Wavelength window:

- 1. The analysis parameters are listed near the top of the window. To change any of these, click on the parameter and input the desired value. A description of the parameters is provided above.
- 2. To change the number of wavelengths, the wavelength value, factor or concentration units, click on <Parameters> to display the parameters window, Figure 5-3. As an alternative, the wavelength, factor and concentration units, displayed in the table on the Fixed Wavelength window, can be changed by clicking on them and inputting the desired values. The Parameters window must be used to change the total number of enabled wavelengths.

5.3 Sample Analysis

After the desired parameters are displayed on the Fixed Wavelength window, samples can be run.

1. Place a cuvette of solvent in the cell holder. Click on <<BLANK>>. The instrument blanks on the solvent.

<u>Auto Cell Holder</u> - Place the cuvette of solvent in the cell position that is in the light beam. Click on <<BLANK>>.

<u>Sipper/Batch Sampler</u> - Aspirate and read the solvent by pressing {FILL/BLANK}.

- If desired, click on the file name following "Results file" and input the desired file name. As an alternative, the file can be named after the data are collected.
- 3. If desired, click on the next displayed sample number to display the alphanumeric keypad. Input up to an 11-character alphanumeric sample identification using the mouse, the optional keyboard or the optional Bar Code Accessory. If a sample identification is not input, the instrument numbers the samples consecutively.

NOTICE

The sample number can be input only for the next sample to be analyzed. These values cannot be changed for samples that have already been analyzed.

4. Place a cuvette of sample solution in the cell holder. Click on < Read-Samples >. (As an alternative, click on the right mouse button with the cursor in any position.)

<u>Auto Cell Holder</u> - Place the cuvettes of sample solution into the input number of cell positions in the sampler. Click on **<ReadSamples>**.

<u>Sipper</u> - Aspirate and read each sample solution by pressing {FILL/READ}. Flush or return each sample solution before reading the next.

ISCO Sampler - Load the tubes of sample solutions into the batch sampler, starting with the position directly under the aspirator arm. Click on <ReadSamples>. The sample solutions are read until the last position of the red rack is read.

<u>Gilson Sampler</u> - Program the Sample Controller with the rack type, number of tubes and orientation of the tubes. Load the samples in the programmed configuration. Click on <ReadSamples>. The analysis stops when the programmed number of tubes are read.

- 5. Data from up to 3 wavelengths are displayed at one time. To display data at other selected wavelengths, click on the right and left arrows, located on the right-hand side of the analysis parameters.
- 6. Repeat steps 3 to 5 until all samples have been read. A typical Fixed Wavelength window is shown in Figure 5-4.

ixed Naveleno eadSamples	th Method	Par	ameters	S	aveClear	Print	HEL Quí
Results file: Read average		Read no	de: [Abs]		name: A:\ g device:		-1
Sample ID	Factor	350.0 56.08	λ Facto	440.0 r 230.0	λ Facto	520.0 r 6.500	
	Abs	Result	Abs	Result ng/ml	Abs	Result mg/ml	
1 2	0.3647	15.6221 20.4213	0.1535 0.0971	35.2955 22.3246	0.3152 0.3784	2.0499 2.4596	
43F 43T	0.6413	37.7848 35.9108	0.2244 0.2421	51.6012 55.6869	1.0832 0.6864	7.0487 4.4613	
46J 48K 7		58.5056 53.2240	0.3162 0.3767	72.7205 86.6482	1.4303 1.3800	9.2969 8.9698	
ſ							

Figure 5-4. Fixed Wavelength Window

- 7. To display sample data that has scrolled off the window, click on the arrows, located on the right-hand side of the analysis parameters, to scroll through the data.
- 8. To print the sample data, click on < Print>. All sample data, even that which are not displayed because of insufficient room on the display, are printed.

NOTICE

When analyzing at more than three wavelengths, the condensed print mode on the printer is suggested for the optimum data formatting. 9. To clear all sample data from the window or to store the data, then clear the window, click on **SaveClear>**. The Save Clear window is displayed so the sample data can be stored.

NOTICE

Do not store the data until all sample data have been collected. After the data are stored, no additional data can be placed in the Results file.

10. When the analysis is complete, click on <Quit>. The Quit window is displayed so the method and/or sample data can be stored. Then the Main window is displayed.

5.4 Example Analyses

EXAMPLE 1

Create a method to collect data on chromate samples at 500 nm with a read average time of 1.0 second. Multiply the readings by a factor of 125 to calculate the concentration in units of $\mu g/mL$.

SOLUTION

The Method window shown in Figure 5-5 was used to create this method. The name of the method is CHROMATE and it is stored on the A drive.

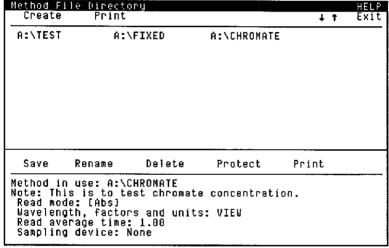


Figure 5-5. Method Window for Chromate Analysis

EXAMPLE 2

Run the method developed in EXAMPLE 1. Analyze four samples, with sample numbers of 41389.1, 41389.2, 41389.3 and 41389.4. Store the data in a file on the optional B drive named 41389.

SOLUTION

The method named "A:\CHROMATE" was recalled into the Fixed Wavelength window, shown in Figure 5-6. The results file was named "B:\41389". Sample readings were taken by clicking on <ReadSamples>.

med Wavelen adSamples	Method	Parameters	SaveClear	Print	Gui
lesults file: lead average	B:\41389 time: 1.00	Read mode: [Abs]	Method name: A:\CHR Sampling device: No		† + 1
Sample IĐ	Factor	500.0 125.0			
	Abs	Result			
41389.1	0.1835	ug/mL 22 9426			
41389.2	0.2176	22.9426 27.2048			
41389.3	0.2722	34,0193			
41389.4	0.2132	26.6459			
5					

Figure 5-6.
Sample Data for Analysis of CHROMATE Method

EXAMPLE 3

Using the Fixed Wavelength window, setup and run an analysis of samples at the following wavelengths: 230, 260, 280 and 320 nm. Use the sipper for the analysis. Do not store the data.

SOLUTION

The parameters were input into the Parameter window by clicking on <Parameters> from the Fixed Wavelength window. The results file was named "WORK_RES" because the data were not stored. The data are shown in Figure 5-7. Part of the data at 320 nm is not displayed. Click on the right arrow to display the remainder of the data.

Fixed Waveleng ReadSamples	th Method	Par	ameters	S	aveClear	Pri	HELP nt Quit
Results file: Read average			de: [Abs]		name: A:\ g device:		, †
Sample ID	Factor	230.0	λ Factor	268.0 1.000	Facto	280.0 r 1.000	Fact
	Abs	Result ag/ml	Abs	Result ng/ml	Abs	Result	Abs
1 2 3 4 5 6	0.3015 0.6146 0.8658 0.1963 1.5613	0.3015 0.8146 0.8658 0.1963 1.5613	0.2865 0.5928 0.8924 0.2041 1.6238	9.2965 0.5928 0.8924 6.2041 1.6238	0.2824 0.5692 0.9189 0.2074 1.6190	0.2624 0.5692 0.9169 0.2074 1.6190	8.2711 8.4563 8.7929 8.2847 1.4864

Figure 5-7. Analysis of Samples at 4 Wavelengths

5.5 Data Output

Data are output to the Communications port whenever an Output Data Type is selected in the Communications Configuration window. The type of data output is selected: "raw and calculated", "raw", or "calculated". General information on data output is provided in section 9.3.

In the Fixed Wavelength mode, the order of the output for each data type is shown below. The "User ID" is input in the Communications Configuration window. The "Method ID" is the method name. A < carriage return > and < line feed > are sent at the end of every line.

Raw and Calculated

The data output for each sample includes the sample number followed by the reading and calculated result for each wavelength. The following is the output obtained when the data in Figure 5-4 were collected.

User ID: [DU600		*			
Method ID	: A:\FIXED					
Date: 10\0	09\91					
Time: 10:	18					
1	0.2790	15.6221	0.1535	35.2955	0.3152	2.0490
2	0.3647	20.4213	0.0971	22.3246	0.3784	2,4596
43F	0.6747	37.7840	0.2244	51.6012	1.0832	7.0407
43T	0.6413	35.9108	0.2421	55.6869	0.6864	4.4613
46J	1.0447	58.5056	0.3162	72.7205	1.4303	9.2969
48K	0.9584	53,2248	0.3767	86,6482	1.3800	8.9698

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Raw

The data output for each sample includes sample number followed by the reading at each wavelength. The following is the output obtained when the data in Figure 5-4 were collected.

User ID: D	J600		
Method ID:	A:\FIXED		
Date: 10\09	9\91		
Time: 10:18	-		
1	0.2790	0.1535	0.3152
2	0.3647	0.0971	0.3784
43F	0.6747	0.2244	1.0832
43T	0.6413	0.2421	0.6864
46J	1.0447	0.3162	1.4303
48K	0.9584	0.3767	1.3800

Calculated

The data output for each sample includes the sample number followed by the result at each wavelength. The following is the output obtained when the data in Figure 5-4 were collected.

```
User ID: DU600
Method ID: A:\FIXED
Date: 10\09\91
Time: 10:18
                15.6221
                         35.2955
                                   2.0490
2
                20.4213 22.3246
                                   2,4596
43F
                37.7840 51.6012
                                   7.0407
                35.9108
43T
                         55,6869
                                   4.4613
46J
                58.5056 72.7205
                                   9.2969
                53.2248 86.6482
48K
                                   8.9698
```

5.6 Files

Two file types are created in the Fixed Wavelength mode: method files and data files. The method files are stored in the FIX_METH directory with the .APX extension. Method files are ASCII files and cannot be converted to the Lotus format.

The data files are stored in the FIX_DATA directory with the .DUF extension. They contain analysis parameters and sample data.

5.7 ASCII Format

The ASCII file for the Fixed Wavelength mode consists of two parts: analysis parameters and sample data, in the same format as the Fixed Wavelength window.

The analysis parameter, "Mode", is either 0 (absorbance) or 1 (transmittance).

The sample data include: sample identification and the reading and calculated result at each wavelength.

The following ASCII file was converted from the sample data displayed in Figure 5-4.

Mode:	0		•			
Numbe	r of waveler	ngths: 3				
Wavel	ength Units	Factor				
350	.0000 mg/ml	56.0000				
440	.0000 mg/ml	230.0000				
520	.0000 mg/ml	6.5000				
1	1.2308	68.9246	0.9970	229.3057	0.6357	4.1318
2	1.6560	92.7359	0.7138	164.1711	0.5403	3.5118
43F	1.5952	89.3310	1.2345	283.9270	1.0218	6.6416
43T	1.4123	79.0914	1.2133	279.0618	0.9941	6.4615
46J	2.0417	114.3350	1.2609	290.0163	0,7257	4.7174
48K	1.7491	97.9472	1.2632	290.5295	0.8627	5.6073

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5.8 Lotus Format

The Lotus file for the Fixed Wavelength mode consists of two parts: analysis parameters and sample data, in the same format as the Fixed Wavelength window.

The analysis parameter, "Mode", is either 0 (absorbance) or 1 (transmittance).

The sample data start in row 9 and are stored in the following columns:

Column A Sample identification

Column B Reading at the first wavelength Column C Result at the first wavelength

Columns D, E Reading and result at the second wavelength, etc.

The following Lotus file was converted from the sample data displayed in Figure 5-4.

```
2
3
4
5
    Number of wavelengths:
    Wavelength
                               Units
                          350
                                  mg/ml
                                              56
                                             230
                           440
                                  mg/ml
                          520
                                  mg/ml
              0.278965
                       15.62207
                                0.153458 35.29548 0.315226 2.048974
10
11
              0.364666
                       20.42131 0.097063 22.32464 0.378403
    43F
                       37.78400 0.224353 51.60123
                                                   1.083182
                       35.91077 0.242117 55.68693 0.686351
    43T
               641263
    46J
                       58.50556 0.316176 72.72050
                                                   1.430297
                950428 53.22399 0.376731 86.64817 1.379972 8.969822
```