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olis

MAKING BRILLIANT BREAKTHROUGHS HAPPEN. SINCE 1980

Software Tutorial for the *OLIS* RSM and RSM CD

Version I
5/18/94

On-Line Instrument Systems, Inc.

130 Conway Drive, Suites A & B
Bogart, Georgia 30622-1724

U.S. & Canada (800) 852-3504
Worldwide (706) 353-6547
Telefax (706) 353-1972

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Starting-up

LAMP

Whenever you sit down to use the RSM or RSM CD, always turn the lamp on first.

The xenon arc lamp supplied with your RSM or RSM CD generates a large RF pulse when it is turned on. This RF pulse can damage components in the computer and the electronics boxes.

Never fire the lamp on when the computer is on.

Do not use the automatic setting on the lamp starter. Always turn the lamp on manually. In the event of a power failure, the manual setting prevents the lamp from starting while the electronics are on.

Verify that the green ground wire is attached between the lamp and the RSM or RSM CD. This wire is attached during installation but can come loose if the equipment has been moved.

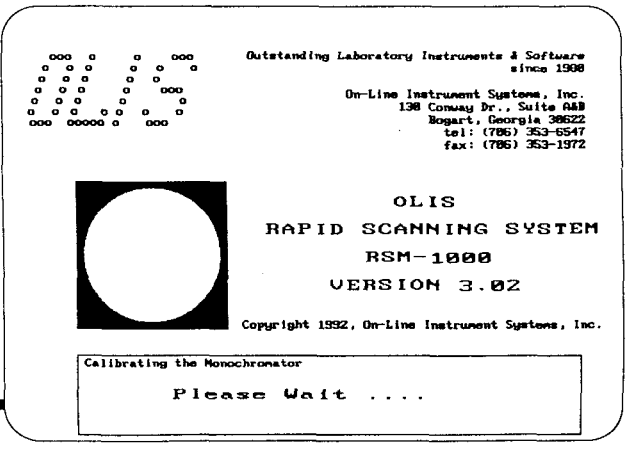
POWER SUPPLY

After the lamp is fired, use the power supply switch to turn on the computer and the supporting electronics.

When the computer prompts you, enter "RSM" or "RSM-CD" to run the appropriate program.

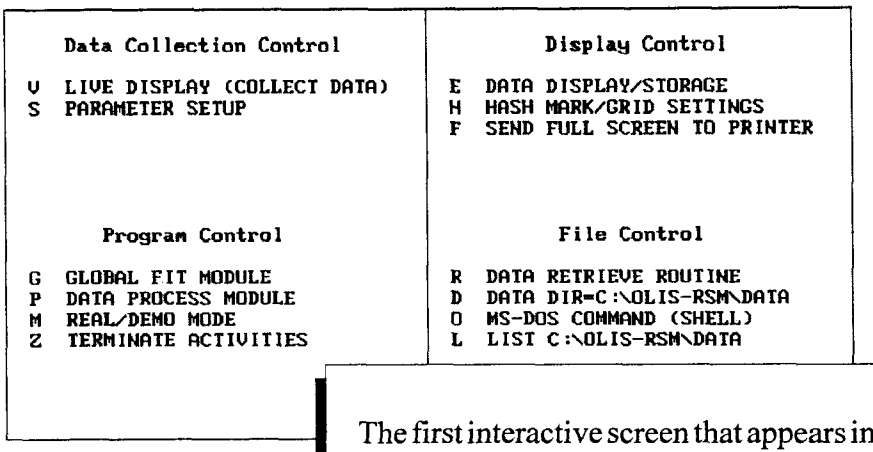
If you enter "RSM," the program displays the screen below while the monochromator is being calibrated.

If you enter "RSM-CD," the program proceeds directly to the Command Mode.



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Command Mode



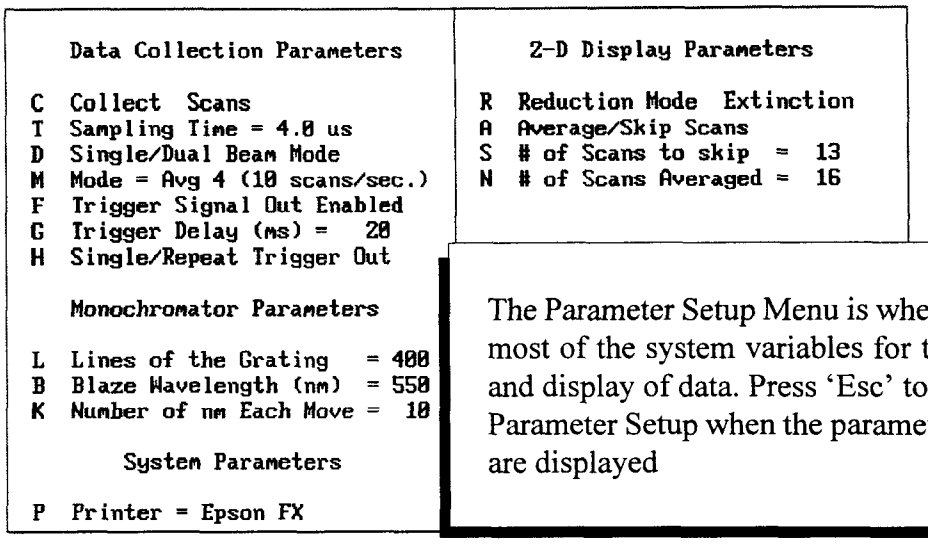
The first interactive screen that appears in both the *OLIS* programs is the Command Mode. The Command Mode contains commands listed under four headings. All commands are active.

Now you are ready to go to the Parameter Setup Menu!!!

Press 'S - Parameter Setup' from the Command Mode to enter the Parameter Setup Menu.

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RSM Parameter Setup



The Parameter Setup Menu is where you define most of the system variables for the collection and display of data. Press 'Esc' to exit the Parameter Setup when the parameters you want are displayed

First, select the type of data you plan to collect. Press 'C' to cycle through the available options:

Rapid-Scanning Data - This default data collection mode presumes the presence of a multiple slit ScanDisk which permits a scanning rate of 1000 scans/second. This top scanning speed can be affected by averaging during data collection.

Static Spectrum - Use this mode to collect 1000 scans/second from a non-changing sample. The RSM operates as a standard high quality UV-VIS instrument and averages the incoming data to produce a single spectrum.

Fixed Wavelength - This mode presumes the presence of a static ScanDisk and should be used for luminescence, fluorescence, and other data collection modes in which light intensity *from the sample* is measured and/or when you want to illuminate the sample with a minimum amount of light.

Dual Wavelength - Use this mode to minimize scatter effect by taking the difference of the signals of one wavelength at which the sample exhibits a signal (due to chemistry) and another wavelength which the sample does not absorb, but at which the effects of scatter are similar. The difference spectrum is the 'true absorbance' of the sample. To use this mode, your RSM must be fitted with an aperture which allows only two wavelengths to illuminate the sample.

Refer to the *OLIS* RSM Operating System User's Manual for additional information about these data collection modes.

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RSM Data Collection Parameters

BEAM

After you select the type of data you wish to collect, toggle 'B' to switch between the two beam modes.

If you choose the Single Beam mode, your sample and reference data are separated in time, as first one and then the other data set is collected.

If you want to read the signal from the sample and reference PMTs simultaneously, choose the Double Beam mode. *OLIS* recommends the Double Beam mode for all work.

MODE

Toggle 'M' to cycle through the modes available with the RSM system. The rate for each mode is displayed on the screen: NoAvg (1000 scans/sec), Avg 1 (62 scans/sec), Avg 2 (31 scans/sec), Avg 3 (21 scans/sec), Avg 4 (10 scans/sec), Avg 5 (5.2 scans/sec), Avg 6 (2 scans/sec), and Avg 7 (1 scan/sec). Choose a mode which produces time resolution appropriate for your experiment. Currently the Global Fit software can only fit up to 1000 raw scans or up to 4000 SVD condensed scans. A good rule of thumb is to choose a data collection rate which produces at least 100 time points (scans). For complex kinetics (2 or 3 exponentials) more scans help resolution of the multiple rates. Four or five hundred points should suffice for any reasonable situation.

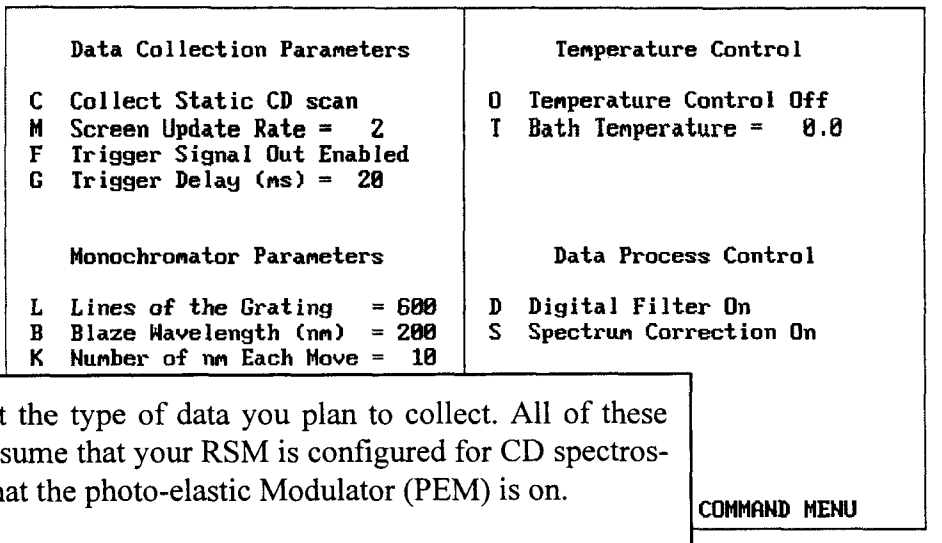
Note that data may be cut or averaged after data collection. Thus, if your reaction lasts one second, choose NoAvg; if the reaction lasts five seconds, choose Avg 1, etc.

TRIGGER

If you have a stopped-flow, or other external device which is to be triggered by the software, toggle 'F' to Enable the Trigger Signal Out or the stopped-flow will not fire.

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RSM CD Parameter Setup



First, select the type of data you plan to collect. All of these options presume that your RSM is configured for CD spectroscopy and that the photo-elastic Modulator (PEM) is on.

Static CD Spectrum - Use this mode to collect a non-kinetic CD spectrum. Real-time averaging allows you to presume that your RSM is configured for LD/CD spectroscopy and that the PEM is on.

Transient CD - Use this mode if you expect the CD data to change. Data is collected for M x 16 ms ('M - Screen Update Rate' is set in the Parameter Setup) and is stored as a 2D kinetic datum.

Ultrafast CD - Use this mode with a changing sample when you want to collect data continuously, waiting to perform the necessary computations until after collection. One second of data collection in this mode uses one megabyte of memory.

Refer to the *OLIS* RSM CD Operating System User's Manual for additional information about these data collection modes.

SCREEN UPDATE RATE

Toggle 'M' to set this value which is used in the RSM CD program

Used with static CD data collection, this value determines the number of 16 ms data that are accumulated before the screen is updated.

Used with transient CD data collection, this value determines the number of 16 ms data that are accumulated before the data is written as a kinetic trace.

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Monochromator Parameters

Monochromator Parameters

L Lines of the Grating
B Blaze Wavelength
K Number of nm Each Move

Change the monochromator parameters when you change the gratings.

To change the gratings, first loosen the thumbscrews on the top of the monochromator. The gratings are held in place by spring-locked clips. Remove tension from the clips by rotating the handle at the top of the grating 90° in either direction. Remove the gratings by grasping the sheet-metal "ears" on the top of each grating. After inserting the new gratings, return the spring-clip to its original position. There is an audible clip when the springs are set.

Do not touch or attempt to clean the surface of the gratings. Any dust may be removed with a gentle stream of dry air.

See hardware handbook for additional tips on changing gratings.

Now you are ready for data collection!!

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Live Display

Preparing for Data Collection

- Press 'V - Live Display' from the Command Mode to enter the Live Display Mode.

- If you notice an odd absorbance signal when you first enter the Live Display Mode, check that the light path is not obstructed, the cuvette is correctly positioned, and there are no bubbles in the observation cell.

- Make sure that the cuvette is securely positioned in the sample compartment.

- Wait enough time for the lamp to stabilize and for the ScanDisk to come up to speed. This takes one to two minutes from start-up, so the lamp and ScanDisk should be stable by the time you reach DVM; otherwise, wait until they are.

- If a "Scan Module Error" message appears on the screen, there may be a hardware problem. If this occurs, call *OLIS*.

- If you are using an RSM CD and receive a PEM error, first check that the PEM is on.

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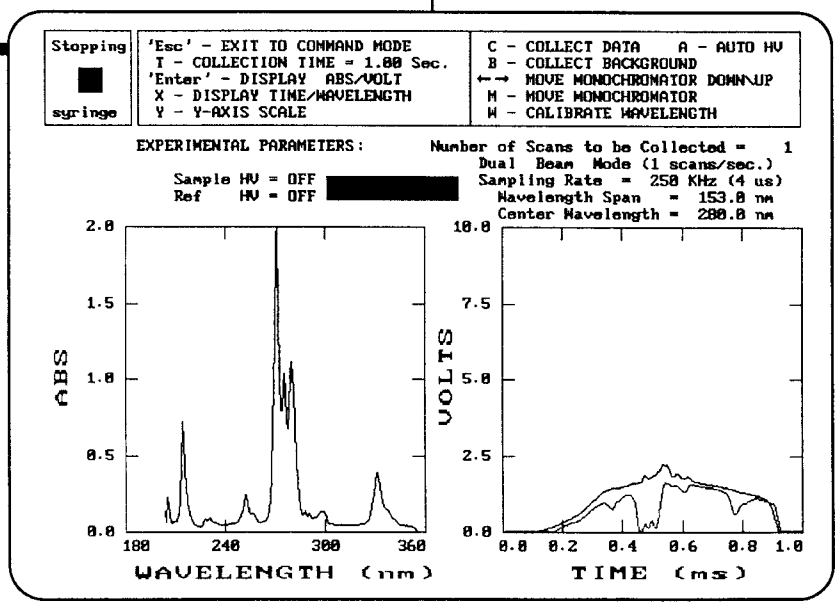
When you enter the Live Display Mode, you should see an absorbance and a voltage display such as the one below. If no signal appears on the screen, check:

1. the lamp; if the lamp is not on, turn the computer off and then start the lamp.

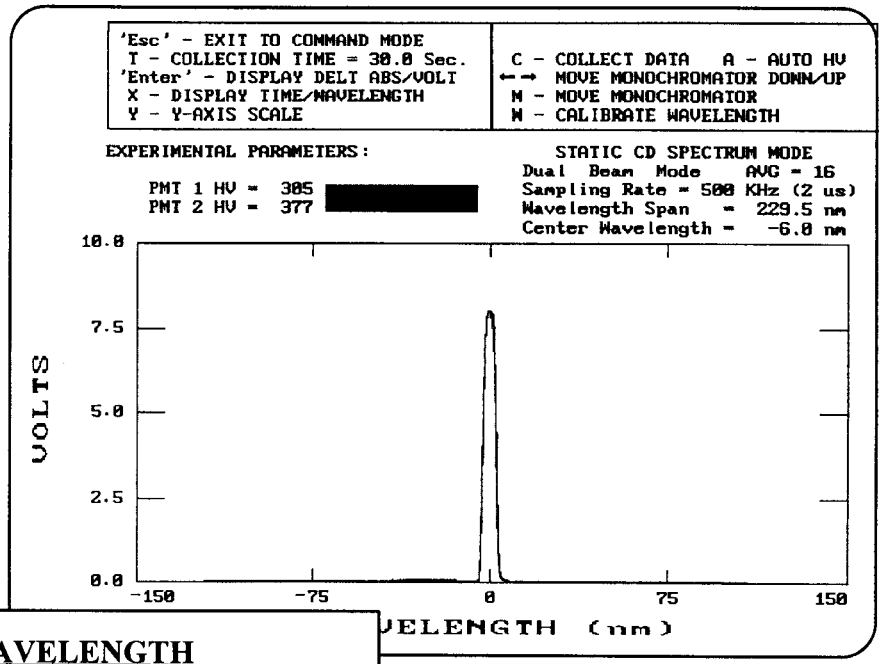
2. the entrance slit. Since the entrance slit should be pulled out slightly to block the light beam from the lamp to the monochromator when you are not collecting data, the previous user might have left the slit in this position.

3. the photomultiplier tube, in case it has been moved for a fluorescence experiment.

At the rate of 1000 scans/second, the program generates 1 MB of data per second. If you do not have enough room on your hard disk to accomodate the data you plan to collect, delete some of your files or you will get a "Disk Full Error" when you attempt to collect data.



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CALIBRATE WAVELENGTH

If your monochromator is not calibrated correctly, use 'W - Calibrate Wavelength' to calibrate. Use 'W,' not 'M - Move Monochromator,' to calibrate the monochromator. 'M' allows you to enter a new wavelength value while 'W' calibrates the wavelength.

After you press 'W,' the program displays a graph with a peak that represents the current calibration wavelength. You want this peak centered at zero. If the peak is not centered at zero, adjust the calibration wavelength according to the difference between the peak and zero. For example, if the peak is at 0.25 nm, input "-0.25" as the new calibration wavelength in order to center the peak.

If the peak is more than 10 nm from zero, the grating is probably not correctly installed. Open the trap door and confirm that the grating is securely seated.

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ADJUST HV

If the reference and sample voltages are very different, press 'A - Auto HV' to adjust the PMT HV to achieve a photocurrent which is approximately 75% of the full A/D range.

To adjust the voltages manually, toggle 'Tab' to highlight either "Sample HV" or "Ref HV" and use the up/down arrows keys to move the selected voltage in increments which you set by pressing 1-9 before the up or down arrow key.

COLLECT BACKGROUND

When you are using the RSM, an uncorrected baseline of a few tenths of the absorbance is not atypical. Pressing 'B - Collect Background' 'zeros' the absorbance and produces a flat baseline.

A baseline may also be recorded manually and stored for manual data processing.

CHOOSE TIME AND WAVELENGTH

From within the Live Display mode, press 'T' to input a data collection time.

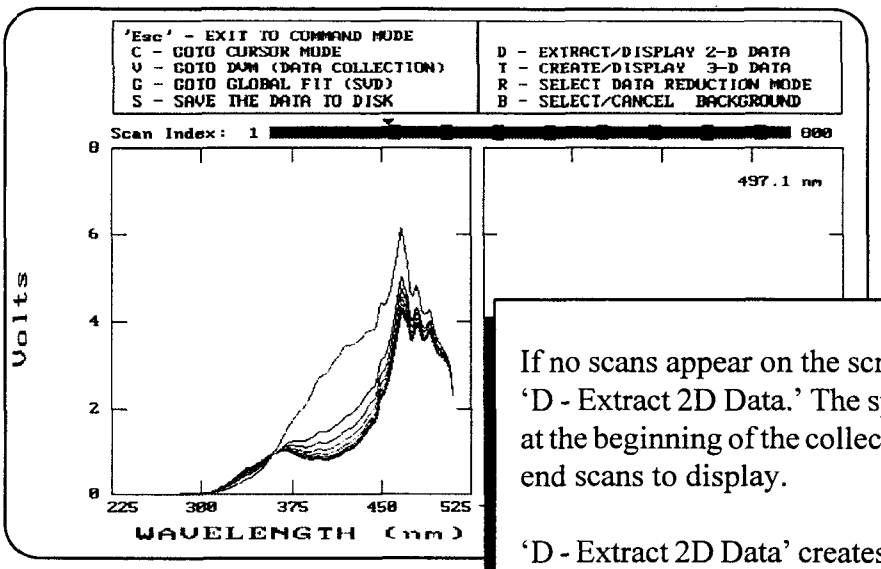
When choosing a collection time, remember that full speed collection time fills approximately one megabyte of RAM per second.

Select a data collection time in which approximately five half-lifes are collected. If the reaction occurs over several seconds, select one of the data averaging modes using 'M - Mode' in the Parameter Setup. The averaging modes allow you to collect the data with maximum time resolution and average it later.

When you are using the RSM with a stopped-flow, press 'F' to fire the stopped-flow; this allows you to observe spectral changes in real time. From this display, you can ascertain whether your reaction is fast or slow and whether you have selected the best center wavelength. The ability to monitor spectra helps you avoid the pitfalls of conventional, single wavelength systems in which you have no ability to view the entire reaction, thus restricting your ability to hone in on the wavelengths of interest.

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Data Display/Storage



If no scans appear on the screen after you collect data, press 'D - Extract 2D Data.' The spectra could be lumped together at the beginning of the collection time, etc. Input the start and end scans to display.

'D - Extract 2D Data' creates a display; it has no effect on the raw data. To alter the raw data, use 'T - Create/Display 3D Data' as explained on the next page.

If you have 1000 or less scans after data collection, you can proceed directly to Global Fitting. If the file contains more than 1000 scans, reduce the number first (see next section).

REDUCE DATA SETS

If you have less than 5000 scans after data collection, condense the data file by selecting 'S - Save the Data to Disk' and save the file as "SVD Condensed." Then, Escape to the Command Mode, select 'R - Data Retrieve Routine,' and reload the file. After you reload your file, you can proceed to Global Fitting.

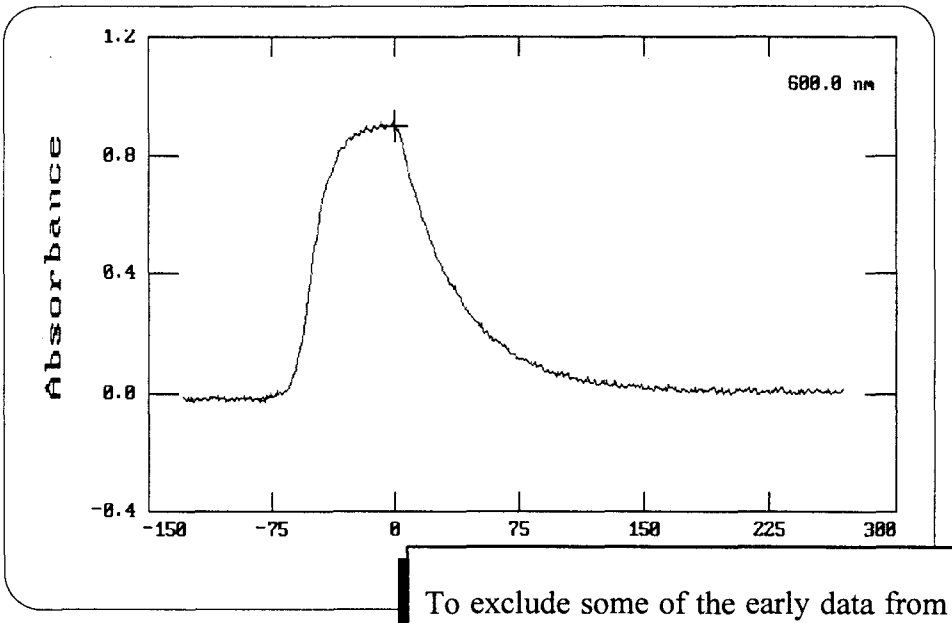
If you have more than 5000 scans after data collection, you must reduce your data by averaging or cutting before proceeding to Global Fitting.

Before reducing your data by either averaging or cutting, *always* save your raw data file. Once you reduce your data file, the raw data cannot be retrieved or restored.

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CUT DATA

Cut rather than average to reduce records when your data has large sections with no relevant information. To cut the record, press 'T - Create/Display 3D Data' while in the Data Display/Storage Mode. Then, specify which scans you wish to include in your 3D data record; select only the scans which are relevant to your experiment.

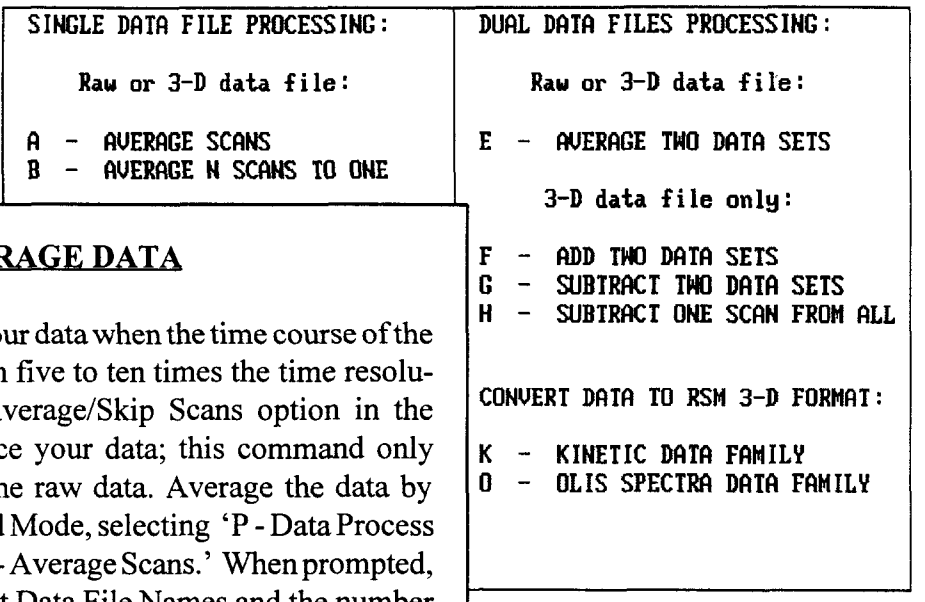


To exclude some of the early data from your 3D display, e.g., those that were captured before any interesting chemistry occurred, select a value at or after time 0. With the data above, you should cut data at the cursor position. In this example, you could also cut the data at 150 ms or later since the chemistry is over at this point.

After you create a 3D file, press 'Q' to exit the 3D Display, save the 3D file using 'S - Save the Data to Disk,' and then reload the file using 'R - Data Retrieve Routine.'

If you still have more than 5000 scans after cutting extraneous data from your data set, average your data using the method described on the next page.

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AVERAGE DATA

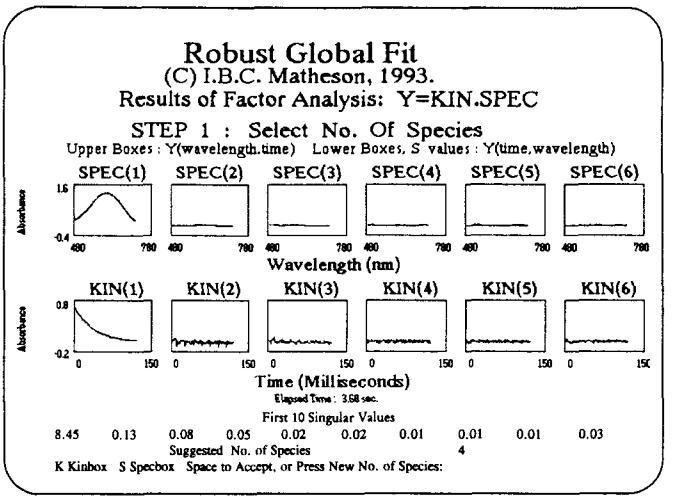
Average rather than cut your data when the time course of the experiment is greater than five to ten times the time resolution. Do not use the Average/Skip Scans option in the Parameter Setup to reduce your data; this command only effects the display, not the raw data. Average the data by Escaping to the Command Mode, selecting 'P - Data Process Module,' and pressing 'A - Average Scans.' When prompted, enter the Input and Output Data File Names and the number of scans to average. The averaging process can take a few seconds.

Always save your raw data before cutting or averaging your data.

If you forget to save your raw data, there is one chance to retrieve it. If you have not collected new data yet, your raw data is still available in the file "c:\olis-rsm\buffer\buffer.raw." You can retrieve this file using 'R - Data Retrieve Routine.' Immediately save the data under a new name after retrieving this file. Never tamper with or erase "c:\olis-rsm\buffer\buffer.raw" because the program might start performing erratically.

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Global Fitting



Once your data contains 1000 scans or less, press 'G' to proceed to Robust Global Fitting.

When you enter Robust Global Fitting, a screen similar to the one above appears. The first six wavelength factors are displayed in boxes labeled SPEC and the first six kinetic factors are displayed in boxes labeled KIN. The program displays likely species in color and likely noise contributions in gray. The program suggests the number of colored species necessary to describe the data set.

Estimate the number of species present by looking at the two sets of boxes and also by consulting the "First 10 Singular Values" listed at the bottom of the screen. Compare these numeric values to each other and to values for noise listed near the end, and from these numeric and graphic estimates, choose a number of species to fit.

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Kinetic Fit

One Species Options

1 Pure First Order Process
Fit Eqn. : Y = Ao.exp(-k.t)

2 Model Free Fit
Empirical Polynomial Fit

3 Pure Second Order Process
Fit Eqn. : Y = Ao/(1+kAo.t)

4 Pure First Order Rise
Fit Eqn. : Y = Ao.(1-exp(-kt))

5 Pure Zeroth Order Process
Fit Eqn. : Y = Ao - k.t

Press Selection 1 -- 5 :

Two Species Options

1 First Order with Background
Fit Eqn. : Y = Ao.exp(-k.t) + Bo

2 Second Order with Background
Fit Eqn. : Y = Ao.k/(1+k.Ao) + Bo

3 2 Concurrent First Orders
Fit Eqn. : Y = Ao.exp(-k1.t) + Co.exp(-k2.t)

4 Reversible First Order
Fit Eqn. : Y = Ao.exp(-(k1+k2).t) + Bo

Press Selection 1 -- 4 :

Three Species Options

1 2 Concurrent First Orders with Background
Fit Eqn. : Y = Ao.exp(-k1.t) + Co.exp(-k2.t) + Bo

2 3 Concurrent First Orders
Fit Eqn. : Y = Ao.exp(-k1.t) + Co.exp(-k2.t) + Eo.exp(-k3.t)

Press Selection 1 -- 2 :

Four Species Options

1 2 Concurrent 1st Orders with 2 Background
Fit Eqn. : Y = Ao.exp(-k1.t) + Co.exp(-k2.t) + Bo + Do

2 3 Concurrent First Orders with Background
Y= Ao.exp(-k1.t) + Co.exp(-k2.t) + Eo.exp(-k3.t) + Bo

Press Selection 1 -- 2 :

The next screen displays a set of kinetic fit models; select the process which you believe best defines your data. If you select a model which the program has trouble fitting to the data, it informs you that an error has been encountered at the successive integration level and that a good fit is unlikely. You have the option of forcing a fit (press 'P') or stopping the fit (press 'Esc').

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Spectral Reconstruction

1 First Order with Background

A -> B ;C const.

2 First Order Growing In :

A -> B

1 First Order with Background

A -> B ;C const.

2 First Order Growing In :

A -> B

1 Second Order with Background

A -> B ;C const.

2 Second Order Growing In :

A -> B

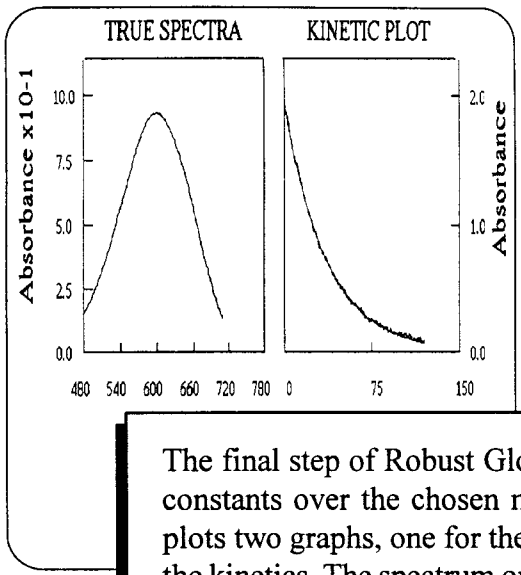
1 Two Species Background

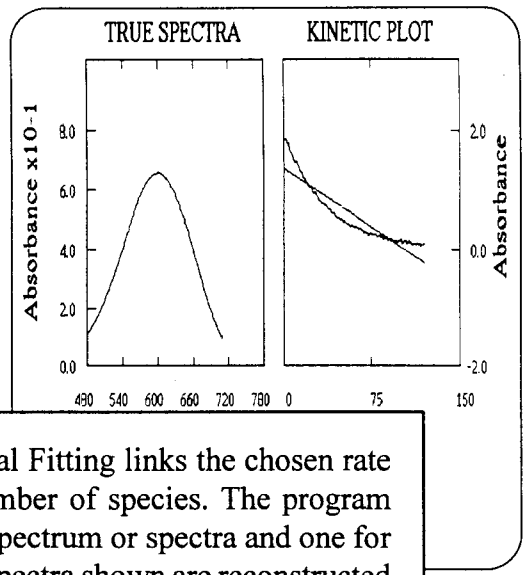
2 Sequential Reaction : A -> B -> C

3 A -> B + C ; B -> C

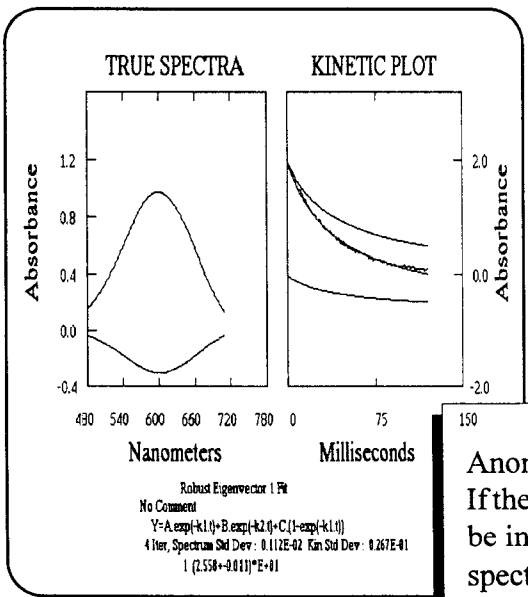
At fit completion, the program displays the spectral reconstruction options. Notice that the program uses color to represent colored species and gray tones to indicate a bleached or non-colored species.

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The final step of Robust Global Fitting links the chosen rate constants over the chosen number of species. The program plots two graphs, one for the spectrum or spectra and one for the kinetics. The spectrum or spectra shown are reconstructed based on the number of species changing and the chosen kinetic mechanism. On the kinetic plot, the red line represents the theoretical data while the yellow line represents the actual data. A kinetic fit is good if these two lines overlap each other as in the graph on the left. The graph on the right is an example of an unsuccessful fit; the theoretical and reduced data do not match since the wrong mechanism was chosen.



Anomolous spectra, such as negative ones, do not exist in nature. If the fit produces such a spectrum, the selected mechanism must be incorrect. You cannot be as absolute about realistic looking spectra; several kinetic and spectral models might result in one data set having multiple realistic answers. Further understanding of the chemistry is necessary to rule out possible options. And, recall the maxim: kinetics cannot tell you chemistry.

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After Global Fitting

Sometimes, the spectral and kinetic graphs returned by Robust Global Fitting are not on the same scale. The program normalizes the kinetic data to one.

If the display looks like some data was lost, it is probably just a matter of scaling since the kinetic data is normalized to an absorbance of one. To return to scaling which shows all the data, press 'Enter' from within the Cursor Mode for a full-screen display. The kinetic behavior at any wavelength is obtained by multiplying the absorbance at that wavelength by the kinetic shape.

The Global Fit data may be stored as ASCII records and manipulated or plotted from any spreadsheet or scientific graphics program.

When you exit Robust Global Fitting, the program returns to the RSM or RSM CD program and displays the fitted data you created using Robust Global Fitting. You can collect new data, reanalyze current data, or exit the program.

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Storing Data

DATA STORAGE DIRECTORY

Make sure that the subdirectory which appears under File Control in the Command Mode is the one in which you wish to save your data.

To change to another data directory, press 'D,' and then enter the name of the subdirectory you wish to use.

That the program follows DOS rules. Thus, the directory name you input becomes a subdirectory of the current directory, unless you enter "C:\" to create a directory with a path to the root directory.

File Control

R Data Retrieve Routine
D Data Dir = C:\OLIS-RSM\Buffer
O MS-DOS Command (Shell)
L List C:\OLIS-RSM\Buffer

DATA DISPLAY/STORAGE

To access the menu which contains data storage options press 'E - Data Display/Storage' in the Command Mode. From the Data Display/Storage Menu, press 'S - Save Data to Disk.'

Display Control

E Data Display/Storage
H Hash Mark/Grid Settings
F Full Screen to Printer

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Storage Options

When you press 'S - Save Data to Disk,' up to six storage options are presented. Only those options available are highlighted; all six are available only if all six types of files exist. That is, if you have not performed or global fit and/ or created 3D data, these storage options will not be available.

Data Storage Routine

A	Save the Raw Data	**D**	Save SVD Condensed Data
B	Save the 3D Data	**E**	Save as Grams Data File
C	Save the Gfit Data	**F**	Save in the Kinetic Family

Enter the letter which corresponds to the type of data you wish to save.

Raw Data - This option saves data as they were collected before any mathematical or graphical manipulations were performed.

3D Data - This option saves the data that are included in the 3D data file you created using the command 'T - Extract 3D Data.'

Gfit Data - These files contains the one, two, or three spectra and their associated kinetics returned at the completion of the global fit.

SVD Condensed - This option saves all the information necessary to restore the spectra and kinetics of an experimental session.

Grams Data - This option is an example of customized file formats which are available upon request.

Kinetic Family - This option stores the displayed kinetic trace. Multiple traces collected over an equal wavelength interval can be built into a kinetic family.

Refer to the RSM or RSM CD Operating System User's Manual for more information about these file formats.

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