Real-time Laboratory System (RLS)

Vol 1: User Guide

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CHAPTER 1

INTRODUCTION

The RLS system provides an English-like language to control a library of laboratory oriented programs. This system has been built with the following main objectives:

1. Provide an easy to use command language common to many applications.

2. Provide an easy interface for the inclusion of new application programs.

3. Provide mechanisms to interconnect different applications.

A user interacts with the central control program through a terminal using a high level English-like language. Each command entered invokes a program to perform the requested function. The executing program interacts with the user's input and output files and devices (and the user's terminal if necessary) to perform the required operations. After the executing program terminates the central control program returns to the user for more command instructions.

Sequences of commands can be composed with a standard text editor and then executed as a 'command program' to perform more complex problem-oriented analysis. In this mode control statements such as IF/THEN/ELSE and GOTO are available to permit a degree of end-user high level programming.

Several major application subsystems have been developed as part of RLS. These include real-time device control, chromatography processing, x-y plotting and some general mathematical routines.

RLS enables off-line development, or development of private systems, since no command definitions or programs or data files are required to reside within the main publicly accessible libraries.
This manual comes in two volumes. "Volume 1: User Guide" contains information on user commands and the use of the applications subsystems. "Volume 2: Programmer Guide" contains information on programming new commands and maintaining the system. In this volume, Chapter 2 describes general use of the RLS language and user interaction with the commands. Chapter 3 describes the creation and installation of RLS 'command programs'. Chapters 4 to 8 describe the main applications currently supported by RLS. Chapter 9 presents system information necessary for using and/or maintaining your version of RLS.
CHAPTER 2
USING RLS

This chapter describes the operation of the RLS system. General use of the RLS system requires familiarity with the following:

1. starting RLS
2. stopping RLS
3. general language syntax
4. showing commands
5. default values
6. PROMPT mode
7. setting default values
8. obtaining HELP

The following sections of this chapter provide detailed information on these items.

2.1 STARTING RLS

Run RLS by signing onto the computer and typing the following:

   RLS

The RLS control program will then write out its command prompt:

   RLS>

From this point you may begin to enter RLS commands as documented in this manual.
2.2 STOPPING RLS

To exit from the RLS system type one of EXIT, or STOP or <CONTROL-Z>.

2.3 GENERAL LANGUAGE SYNTAX

Commands are entered as a string of words and/or numbers. The blank character (space bar) is used as a separator between all words and symbols.

Commands are of the general form:

```
VERB OBJECT [KEYWORD VALUE KEYWORD VALUE ...]
```

The 'verb object' implies that an action is to be performed on a general object such as a device or data file.

**eg.**

```
START ANALOG
FIND PEAKS
PREPARE REPORT
etc.
```

The 'keyword value' pairs are optional and describe modifications to the operation. The 'keyword' names of the parameter to be changed and the 'value' gives the new value to be used.

**eg.**

```
START ANALOG CHANNEL 1
FIND PEAKS PEAK-FILE PEAK.DAT
PREPARE REPORT PEAK-FILE PEAK.DAT
etc.
```

The keywords vary from command to command but are presented in a consistent format. The modifiers are usually optional with some 'reasonable' default actions being performed when they are omitted. The set of 'keyword value' pairs do not have to be in any specific order.

Some modifiers, such as titles, are represented as an arbitrary string of characters with embedded blanks. Such sequences must be enclosed within double quote marks in order to keep the words together as one 'value'. This also prevents RLS from confusing the keyword value with as a keyword. For example:

```
PREPARE PLOT TITLE "Response Factor" FACTOR 2.0
```

will direct RLS to interpret the two uses of the word "factor" correctly. The quotes are used only on command
lines and are not necessary when RLS is prompting for a string of characters such as a title.

eg title '"" Response Factor

If all of the user modifiers cannot be contained on one line then the command can be continued on the next line by typing a dash, '−', character at the end of the line. The command is executed when the user enters a return with no preceding dash character. For example,

```
START ANALOG CHANNEL 1 −
FREQUENCY 10. −
DURATION 20
```

executes only after all three lines have been entered and is identical to the command:

```
START ANALOG CHANNEL 1 FREQ 10. DURATION 20
```

The words for the VERB, OBJECT and/or KEYWORDS can be abbreviated. For example:

```
START ANALOG CHANNEL 1
```

is equivalent to:

```
STA ANA CH 1
```

2.4 SHOWING COMMANDS

The SHOW command is used to provide a quick reference to commands and modifiers. You can obtain a list of all currently available commands by entering:

```
SHOW COMMANDS
```

RLS will print out the command identifier for each command that is currently available. The commands are printed in two sets, the first set gives the commands defined by the 'local' user and the second set gives the 'global' commands available to all users. For example,

```
RLS>SHOW COMMANDS
context command

general "analyze data"
general "print report"
```
device "start analog"
gc "find peaks"

RLS>

The above sequence shows that the user has 2 locally defined commands, "ANALYZE DATA" and "PRINT REPORT" and globally defined commands "START ANALOG" and "FIND PEAKS".

For each of the commands displayed the user can obtain more detailed information by entering:

SHOW identifier

where 'identifier' is the command identifier appearing in the SHOW COMMANDS list. This display will show all keywords accepted by the command, the current default value, and a brief description of the effect of the keyword. For example,

RLS>SHOW FIND PEAKS

<table>
<thead>
<tr>
<th>keyword</th>
<th>default</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>signal-file</td>
<td>ch7.dat</td>
<td>&quot;signal file name&quot;</td>
</tr>
<tr>
<td>peak-file</td>
<td>peak.dat</td>
<td>&quot;output peak file&quot;</td>
</tr>
<tr>
<td>gate</td>
<td>2</td>
<td>&quot;change counter&quot;</td>
</tr>
<tr>
<td>slope</td>
<td>.01</td>
<td>&quot;slope sensitivity&quot;</td>
</tr>
<tr>
<td>density</td>
<td>2</td>
<td>&quot;number of points&quot;</td>
</tr>
<tr>
<td>width</td>
<td>3.</td>
<td>&quot;peak width&quot;</td>
</tr>
<tr>
<td>frequency</td>
<td>1.</td>
<td>&quot;sampling frequency&quot;</td>
</tr>
</tbody>
</table>

RLS>

2.5 DEFAULT VALUES

Default values are defined for all command modifiers. When you invoke a command without keyword/value modifiers then these default values are used by RLS. Any modifier values you provide will override default values maintained for the command.

Global default values are generated when the command/program is written and installed in the system. They are stored in a central library that is accessible to all users. You can redefine the default values for commands by using the SET command described below. A redefined default does not affect the global defaults for other users.
If a default is given the value '?' then RLS will prompt for entry of a new value every time the command is invoked.

2.6 PROMPT MODE

You may find it convenient to have RLS prompt for command modifiers rather than try to remember them or look them up each time. A question mark character, '?', is used on a command line to instruct RLS to actively prompt for modifiers required by the target program. The question mark may appear anywhere on the command line and causes RLS to prompt for all keywords that have not already been entered. This allows the skipping of the prompt for any modifiers with which the user is already familiar.

When the question mark appears on a command line then RLS will print out the identifier of the command requesting the prompts. RLS will then print out each keyword, the current default value and then it will wait for you to enter the appropriate new value. The user selects a new value by entering the new value to the prompt. You can retain the current default value by typing a <return> to the prompt. For example:

RLS>START ANALOG CHANNEL 1 ?
"start analog"
frequency 1. : 
duration 30. :10
point -1 : 
signal-file iparda.dat :ch7.dat
subtitle "" : sample data
gain 0 : 
through 1 :

where the user updates the duration, output file and subtitle. Note that the 'CHANNEL' modifier was not requested since it was entered on the command line.

The user can obtain more information on the keyword being prompted for by entering another question mark as the 'value'. RLS will print out a brief description of the modifier being requested and then reprompt the user with the modifier keyword. For example,

START ANALOG CHANNEL 1 ?
frequency 1. :?
"sampling frequency in hz"
frequency 1. :5.
2.7 SETTING DEFAULT VALUES

Usually the predefined default values combined with the ability to override these values on a command line will provide sufficient flexibility. Occasionally though, you may plan on consistent use of a new command modifier value. The SET command enables you to define a new default value to be used for the modifier rather than enter the value every time the command is invoked.

The default value is changed by entering the following:

    SET IDENTIFIER KEYWORD VALUE KEYWORD VALUE ...

where 'identifier' is the command to be changed. This instructs RLS to change the default values for each keyword specified. The new value for the modifier will be used for all future uses of the command.

Note that the 'value' for logical variables can be expressed as any of TRUE, FALSE, YES, NO, ON, OFF.

2.8 OBTAINING HELP

Each command has a 'help' file which documents the function of the command for on-line users. The 'help' information is a duplicate of that contained in the 'COMMAND DEFINITION' section of the application description sections of this manual. This help is obtained for each command by entering:

    HELP identifier

where identifier is the string of words uniquely identifying the command.

2.9 COMMAND DEFINITIONS
/*
COMMAND
HELP 'identifier'
HELP 'identifier'

ACTION
This command displays the HELP information for the specified command.

EXAMPLE
HELP FIND PEAKS
*/
/*
COMMAND

SET 'identifier'

ACTION

This command changes the current default values for the command specified by the 'identifier'. The keyword and a new value are entered for each modifier to be changed.

EXAMPLE

SET SAMPLE ANALOG FREQUENCY 5. DURATION 20

The above command changes the frequency and duration for the 'SAMPLE ANALOG' command.
*/
COMMAND

SHOW COMMANDS

ACTION

This command displays the identifiers for all current RLS commands. The commands local to the user are displayed first and then the global commands are displayed.

EXAMPLE

SHOW COMMANDS

*/
COMMAND

SHOW 'identifier'

ACTION

This routine displays to a user the current default values for the modifiers of the command specified by the 'identifier'. For each modifier the keyword is listed, the default value, and a brief half line description is given.

EXAMPLE

SHOW SAMPLE ANALOG

*/
CHAPTER 3

WRITING COMMAND PROGRAMS

Sequences of commands can be entered into a data file and then executed as if they were in fact a single command. Some control statements, such as IF/THEN/ELSE and GOTO, are also available to execute the commands non-sequentially. This facility permits a user to put together fairly general 'programs' of commands.

Command programs are built using the standard text editor programs of the computer system. The commands should be entered exactly as they would appear if they were entered at a terminal directly. The programs are then added to the command catalog using the "ADD COMMAND" command.

Once a command program is installed in the system it is invoked in exactly the same manner as individual commands. Command modifiers for the command program are passed on to the individual commands, thus permitting unique modification of the individual commands at run time. For example, a chromatograph analysis can be placed into a data file as the following sequence:

```
START ANALOG CHANNEL 1 DURATION 5
WAIT ANALOG CHANNEL 1
FIND PEAKS
ZERO BASELINE
PREPARE REPORT
```

The text file can be installed with the identifier "DO CALIBRATION" and then when a user enters the command:

```
RLS>DO CALIBRATION
```

the sequence of commands in the program will be executed. Command modifiers entered by the user to the command program will be passed on to the individual commands. For instance, the command:

```
RLS>DO CALIBRATION FREQUENCY 5
```
would cause the sample analog command in the above sequence to use a frequency of 5 hz.

To facilitate the more complex analyses some control statements have been added such as appear in programming languages. The control statements include:

1. IF/THEN/ELSE
2. GOTO

These are described more fully below.

3.1 IF/THEN/ELSE

These statements allow certain sets of commands to be executed conditionally based on the results of some calculation. Each of these words must appear as the FIRST WORD in a command in front of the command identifier. For example, assume that a command called "NO STANDARD" has been written and installed in the chromatography applications which checks that the standard peak was found in the analysis and returns TRUE if it is and FALSE if it is not. Then the following sequence would conditionally inject the next compound:

```
IF NO STANDARD
  INJECT STANDARD
ELSE INJECT NEXT
```

3.2 GOTO

The goto statement enables a non-sequential execution of program statements. For example, assume that a chromatograph program command called "COLUMN OK" checks whether the results from the analyses indicate that the column is still operative. Then the following sequence would enable repeated injections unless the column was determined to be inoperative:

```
REPEAT: INJECT NEXT
  .
  .
  .
  do analysis
  .
  .
```
IF COLUMN OK
THEN GOTO REPEAT

Note that the target label of the goto command is terminated by a colon character and must have a space between it and the following command identifier.

3.3 COMMAND DEFINITIONS
/*
NAME

ADD COMMAND

ACTION

This command adds a new command to the RLS catalog file. The command places the following information into the RLS catalog file:

1. CONTEXT - the general command context
2. IDENTIFIER - the word or words entered by the user to invoke the command
3. PROGRAM-FILE - the file name of the target program
4. KEYWORD-FILE - the file name of a command definition
5. PROGRAM - YES if program is in C or FORTRAN
   NO if it is an RLS command program

KEYWORDS

CONTEXT     string     general command context
IDENTIFIER  string     command identifier
PROGRAM-FILE file name  name of target program
KEYWORD-FILE file name  name of a command definition
PROGRAM     logical     YES, for FORTRAN or C programs

EXAMPLE

ADD COMMAND ?
enter context   ?         :gc
enter identifier ?        :do gc analysis
enter program-file ?       :gc.dat
enter keyword-file x       :
enter program   no        :

The above sequence adds an RLS command program in file gc.dat. The user invokes the command with the identifier "DO GC ANALYSIS".

*/
/*

COMMAND

CREATE DEFINITION

ACTION

This command creates an RLS 'command definition' file. The user is prompted for the file name, and for each modifier:

1. **KEYWORD** - the keyword identifying the modifier
2. **TYPE** - the data type for the modifier, which is one of FLOAT, INT, OCTAL, LOGICAL, FILE, or STRING. If a type of 'FILE' is entered then the command asks for the stream number which is INPUTx or OUTPUTx where x is the stream number.
3. **HELP** - a brief half CRT line description of the modifier
4. **DEFAULT** - the value to be given to the modifier when it is not entered by the user.

The stream numbers are used to set up input and output files for the INPUT/OUTPUT REDIRECTION facility of RLS. These are set up to match the input and output streams of programs that will be sending data to, or receiving data from, the command being installed.

EXAMPLE

```
CREATE DEFINITION
enter file name : myprogram
enter keyword (or return to finish): name
enter type : file
enter stream : input0
enter help : name of input file
enter default : ?
enter keyword (or return to finish):
```

The above sequence creates a definition file for a program called 'myprogram' with one input parameter - a file name.

*/
/*
COMMAND

DELETE COMMAND

ACTION

This command deletes a command from the RLS catalog file. The CONTEXT and IDENTIFIER for the command to be removed are entered by the user.

KEYWORDS

CONTEXT string command context
IDENTIFIER string the command identifier

EXAMPLE

DELETE COMMAND CONTEXT GC IDENTIFIER "FIND PEAKS"
*/
CHAPTER 4

DEVICES

These commands are used to interface to and operate the laboratory instruments. Commands available include:

<table>
<thead>
<tr>
<th>VERB</th>
<th>OBJECT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>MONITOR</td>
<td>ANALOG</td>
<td>monitor analog start/stop switch</td>
</tr>
<tr>
<td>SHOW</td>
<td>ANALOG</td>
<td>show current analog sampling status</td>
</tr>
<tr>
<td>START</td>
<td>ANALOG</td>
<td>start an analog channel sampling</td>
</tr>
<tr>
<td>STOP</td>
<td>ANALOG</td>
<td>stop an analog channel sampling</td>
</tr>
<tr>
<td>WAIT</td>
<td>ANALOG</td>
<td>wait for analog sampling completion</td>
</tr>
<tr>
<td>WAIT</td>
<td>CLOCK</td>
<td>wait for a clock time or duration</td>
</tr>
<tr>
<td>PULSE</td>
<td>DIGITAL</td>
<td>pulse a digital output point</td>
</tr>
<tr>
<td>READ</td>
<td>DIGITAL</td>
<td>read a digital input point</td>
</tr>
<tr>
<td>WAIT</td>
<td>DIGITAL</td>
<td>wait for digital input</td>
</tr>
<tr>
<td>WRITE</td>
<td>DIGITAL</td>
<td>write a digital output point</td>
</tr>
<tr>
<td>READ</td>
<td>TERMINAL</td>
<td>read input from terminal operator</td>
</tr>
<tr>
<td>RING</td>
<td>TERMINAL</td>
<td>ring terminal bell</td>
</tr>
<tr>
<td>WAIT</td>
<td>TERMINAL</td>
<td>wait for terminal operator</td>
</tr>
<tr>
<td>WRITE</td>
<td>TERMINAL</td>
<td>write a message to the terminal</td>
</tr>
</tbody>
</table>

A typical layout for interfacing the computer to the laboratory instruments appears in the figure 4.1. Cables are run from a distribution panel in the computer room to distribution panels in the labs. The distribution panels contain connections for analog, digital and RS-232 (or 20-ma) terminal interfaces. Instruments are connected to the lab distribution panels using in-house designed and built electronic interface boxes.

For analog signals these interfaces convert voltage and current gains and offsets from the equipment to match those required by the LPA-ll device. Additional signal filtering may also be included as necessary although for most applications the filtering available from the instrument and the LPA-ll has been sufficient. The RLS software sets the
base sampling frequencies to be synchronous with the line frequency clock in order to obtain maximum noise rejection with respect to power line noise.

Digital input/outputs to control sampling and instruments are also connected to the computer through interface boxes, again to provide voltage/current signal conversion. On these boxes a manual start/stop switch and a three-way LED light are usually included. The switch is useful for manual instrument operation or testing. The LED light is used to indicate to the operator when the computer sampling is in progress (no light for power down, red for no sampling, green for sampling).

Digital signals to and from the instruments for automatic control of signal sampling are very dependent on the options provided by the manufacturer. Most instruments provide a digital output signal indicating when an injection and run is in progress, and a digital input signal that can be set to start or stop an injection. These signals can directly replace the manual switch/light signals described above or they can be electronically OR’ed with the manual signals to permit both automatic and manual control at an instrument.

Some instruments have further digital input/outputs to signal events to the computer or to allow the computer to open/close valves etc. These can be connected to the digital i/o ports of the computer and operated independently of the start/stop signals.

4.1 ANALOG SIGNALS

The analog sampling commands are used to collect signals from instruments. These commands cause the voltage levels at the computer a/d converter to be sampled and saved in data files on the computer.

The computers have 16 independent channels for collecting analog signals. These channels are normally set up to sample data at a maximum frequency of 60 hz, synchronous with line frequency to enhance noise rejection. The following commands control the collection of data from the analog-to-digital converters.

<table>
<thead>
<tr>
<th>VERB</th>
<th>OBJECT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>MONITOR</td>
<td>ANALOG</td>
<td>monitor analog start/stop switch</td>
</tr>
<tr>
<td>SHOW</td>
<td>ANALOG</td>
<td>show current analog sampling status</td>
</tr>
</tbody>
</table>
START ANALOG  
   start an analog channel sampling
STOP ANALOG  
   stop an analog channel sampling
WAIT ANALOG  
   wait for analog sampling completion

A typical command sequence to start and stop data collection on channel 1 at a frequency of 5 hz would be as follows:

RLS>START ANALOG CHANNEL 1 FREQUENCY 5
<pause while signal is collected>
RLS>STOP ANALOG CHANNEL 1

If a manual start/stop switch has been connected to the digital inputs of the computer then the signal collection can be started and stopped with the switch by using the following command:

RLS>MONITOR ANALOG CHANNEL 1 POINT 1

In this case sampling will begin when the switch is first set and terminated when the switch is reset.

Data processing can be synchronized with the collection of the signals using the "WAIT ANALOG" command. This command causes program execution to suspend until the sampling on the specified channel has completed. For example:

RLS>START ANALOG CHANNEL 7 DURATION 10 SIGNAL TEST.DAT
RLS>WAIT ANALOG CHANNEL 7
<pause while signal is collected>
RLS>PREPARE PLOT X-Y.NAME TEST.DAT
RLS>SEND PLOT DEVICE VT125

The above command sequence will start data collection on a channel for a time duration of 10 minutes. The "WAIT ANALOG" command will cause the program to go into a wait state until the data collection has completed. When data collection completes the signal data will be plotted on the user terminal. Figure 4.2 shows a sine wave signal that has been entered with this command sequence.

4.2 DIGITAL INPUT/OUTPUT

The computers have 16 bit digital input/output devices. The individual bits can be used as input to the computer to signal external events, such as the setting of a switch, and as output from the computer to control an external mechanism such as a valve. The following commands control input and output with the digital i/o devices.
Figure 4.2 Signal from Data Collection
<table>
<thead>
<tr>
<th>VERB</th>
<th>OBJECT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>PULSE</td>
<td>DIGITAL</td>
<td>pulse a digital output point</td>
</tr>
<tr>
<td>READ</td>
<td>DIGITAL</td>
<td>read a digital input point</td>
</tr>
<tr>
<td>WAIT</td>
<td>DIGITAL</td>
<td>wait for digital input</td>
</tr>
<tr>
<td>WRITE</td>
<td>DIGITAL</td>
<td>write a digital output point</td>
</tr>
</tbody>
</table>

A typical sequence to set a light on and then off would appear as:

```
RLS>WRITE DIGITAL POINT 5 VALUE 1
RLS>WRITE DIGITAL POINT 5 VALUE 0
```

The current value of a digital input can be displayed with the command "READ DIGITAL". The current status of the bit is displayed at the terminal as either a 0 or 1.

eg.
```
RLS>READ DIGITAL POINT 5
1
RLS>
```

### 4.3 EVENT CONTROL

An external event can trigger processing by using the "WAIT DIGITAL" command. For example:

```
RLS>WAIT DIGITAL POINT 5
```

which causes RLS to wait until the external event sets the digital input bit before continuing with further commands.

The various device handling commands can be used in an RLS command program to perform event control during data collection. For example, an RLS command program to collect signals from chromatograph auto-injection equipment would appear as follows:

```
LOOP: WAIT DIGITAL POINT 3
START ANALOG CHANNEL 3
WAIT CLOCK DURATION 00:00:60
WRITE DIGITAL POINT 4 VALUE 1
WAIT CLOCK DURATION 00:02:00
WRITE DIGITAL POINT 4 VALUE 0
WAIT DIGITAL POINT 3
STOP ANALOG CHANNEL 3
<process data here>
```
GOTO LOOP

The program waits for digital input 3 to be set by the instrument to indicate that an injection has been done. After an elapsed time of 60 seconds the program will set digital output point #4 to control an event at the instrument. After a further 2 minutes the program will clear the digital output point #4. The program will then wait for digital input #3 to clear signaling the completion of the injection. The program then stops its own sampling of the data and processes the data before repeating the sequence.

4.4 PRINTING FILES

Reports and listing files are sent to the printer using the commands of the host computer (RSX systems only). For example:

PRINT filename

where 'filename' is the name of the file to be printed.

4.5 COMMAND DEFINITIONS
/*
COMMAND

MONITOR ANALOG

ACTION

This command monitors a digital input POINT to signal start and stop times for sampling from an analog CHANNEL.

When the digital input point is set this command starts sampling data. The CHANNEL is sampled at a specified FREQUENCY and DURATION. Sampling is terminated when the digital input point is cleared. The digital output POINT will be set when sampling starts and cleared when sampling finishes.

The result sequence of sampled data is placed into a SIGNAL-FILE. A brief DESCRIPTION of the data can be given.

Sampling can be performed THROUGH several consecutive channels.

For the Chemistry Dept. computer an amplification GAIN of 1, 4, 16 or 64 can be applied (or auto-gaining will be performed if GAIN=0).

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>DATA TYPE</th>
<th>MEANING</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHANNEL</td>
<td>INTEGER</td>
<td>analog channel number</td>
</tr>
<tr>
<td>THROUGH</td>
<td>INTEGER</td>
<td>last channel number</td>
</tr>
<tr>
<td>FREQUENCY</td>
<td>REAL</td>
<td>sampling frequency per second</td>
</tr>
<tr>
<td>DURATION</td>
<td>REAL</td>
<td>sampling duration in minutes</td>
</tr>
<tr>
<td>POINT</td>
<td>INTEGER</td>
<td>digital point number</td>
</tr>
<tr>
<td>GAIN</td>
<td>INTEGER</td>
<td>amplification factor</td>
</tr>
<tr>
<td>SIGNAL-FILE</td>
<td>CHAR(40)</td>
<td>output file name</td>
</tr>
<tr>
<td>DESCRIPTION</td>
<td>CHAR(40)</td>
<td>user identification</td>
</tr>
</tbody>
</table>

EXAMPLE

MONITOR ANALOG CHANNEL 1 FREQ 10. DURATION 500
MONITOR ANALOG CHANNEL 3 DESCRIPTION "Test run" POINT 3

*/
/* COMMAND

SHOW ANALOG

ACTION

This command displays a listing of the current status of the analog sampling CHANNELs on the user's terminal. The listing is in the format:

channel # uic idle/active monitor switch start/stop

where 'uic' is the user identification, 'idle/active' indicates whether sampling is actually in progress and 'monitor switch start/stop' indicate the digital switch monitoring status.

KEYWORDS

CHANNEL integer channel number to display

EXAMPLE

RLS>SHOW ANALOG

channel 6 [300,246] idle monitor switch start
channel 7 [300,243] active monitor switch stop
channel 1 [300,243] active

RLS>

The above example would indicate that channel 6 is waiting for a switch start signal, channel 7 is active sampling and waiting for a switch stop signal and channel 1 is active and will terminate after the specified duration.

*/
COMMAND

START ANALOG

ACTION

This command starts sampling data from an analog channel. The CHANNEL is sampled at a specified FREQUENCY and DURATION. If a digital POINT is given then that output POINT will be set when sampling starts and cleared when sampling finishes.

The result sequence of sampled data is placed into a SIGNAL-FILE. A brief DESCRIPTION of the data can be given.

Sampling can be performed THROUGH several consecutive channels.

For the Chemistry Dept. computer an amplification GAIN of 1, 4, 16 or 64 can be applied (or auto-gaining will be performed if GAIN=0).

KEYWORDS

| CHANNEL   | INTEGER       | analog channel number |
| THROUGH   | INTEGER       | last channel number |
| FREQUENCY | REAL          | sampling frequency per second |
| DURATION  | REAL          | sampling duration in minutes |
| POINT     | INTEGER       | digital point number |
| GAIN      | INTEGER       | amplification factor |
| SIGNAL-FILE | CHAR(40)  | output file name |
| DESCRIPTION | CHAR(40) | user identification |

EXAMPLE

START ANALOG CHANNEL 1 FREQ 10. DURATION 500
START ANALOG CHANNEL 3 DESCRIPTION "Test run" POINT 3

*/
/*
COMMAND

STOP ANALOG

ACTION

This command stops the analog sampling currently in progress on a given CHANNEL.

KEYWORDS

CHANNEL integer channel number to stop

EXAMPLE

sample analog channel 1 frequency 5.
STOP ANALOG CHANNEL 1

*/
/*

COMMAND

WAIT ANALOG

ACTION

This command waits for an analog CHANNEL to complete sampling activity that has been started with either the "START ANALOG" or the "MONITOR ANALOG" command. This allows a command program to synchronize with real-time sampling activity for subsequent data processing.

KEYWORDS

CHANNEL INTEGER analog channel number

EXAMPLES

RLS>SAMPLE ANALOG CHANNEL 2 DURATION 10.
RLS>WAIT ANALOG CHANNEL 2
<wait for analog completion after 10 minutes>
RLS>
*/
/*
COMMAND

WAIT CLOCK

ACTION

This command waits for either a time DURATION to elapse or for a specific TIME of day. Both times are specified in the format:

hh:mm:ss

for hours, minutes and seconds respectively. Clock times are specified in 24 hour format.

KEYWORDS

| DURATION | CHAR     | duration time |
| TIME     | CHAR     | time of day   |

EXAMPLES

To wait for 10 seconds elapsed time:

RLS>WAIT CLOCK DURATION 00:00:10

To wait for 1:00 PM:

RLS>WAIT CLOCK TIME 00:13:00

*/
/*
COMMAND

PULSE DIGITAL

ACTION

This command pulses a digital POINT number for a specified DURATION. The duration is specified in seconds and may be a fractional part, eg:

RLS>PULSE DIGITAL POINT 1 DURATION .5

for a 1/2 second pulse on digital point 1. The actual duration will be to the nearest 1/60 second.

KEYWORDS

POINT INTEGER digital point number
DURATION REAL pulse width in seconds

EXAMPLE

RLS>PULSE DIGITAL POINT 5 DURATION 0.1
*/
DEVVICES

/*

COMMAND

READ DIGITAL

ACTION

This command reads the current value of a set of digital input POINTs. The digital input may have a field WIDTH greater than 1 indicating that several bits are to be read with POINT specifying the rightmost (least significant) bit. The current digital value is printed on the operator terminal.

KEYWORDS

POINT integer digital input point number
WIDTH integer number of digital bits

EXAMPLE

RLS>READ DIGITAL POINT 3
1
RLS>

*/
COMMAND

WAIT DIGITAL

ACTION

This command waits for a digital input POINT to be set (ON, HIGH, TRUE, whatever...) by an instrument or by a manual switch.

KEYWORDS

POINT integer digital switch number

EXAMPLES

RLS>WAIT DIGITAL POINT 2
<wait for event>
RLS>

*/
/*
COMMAND

WRITE DIGITAL

ACTION

This command writes a VALUE to a digital output POINT. The output field WIDTH may be greater than 1 indicating that several consecutive bits are to be updated with POINT specifying the rightmost (least significant bit).

KEYWORDS

POINT INTEGER digital output point number
WIDTH INTEGER field width for output
VALUE INTEGER new value for the output

EXAMPLE

RLS>WRITE DIGITAL POINT 3 VALUE 1

*/
/*

COMMAND

READ TERMINAL

ACTION

This command prompts the terminal operator and waits for a response. The command returns TRUE if the response is equal to REPLY and FALSE if the response does not equal REPLY. A DEFAULT value can be specified so that the operator only needs to enter a <return> key.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>PROMPT</td>
<td>string</td>
<td>prompt to terminal operator</td>
</tr>
<tr>
<td>REPLY</td>
<td>string</td>
<td>valid reply</td>
</tr>
<tr>
<td>DEFAULT</td>
<td>string</td>
<td>default value for the reply</td>
</tr>
</tbody>
</table>

EXAMPLE

RLS>IF READ TERMINAL PROMPT "Are you done ? " -
REPLY "yes" DEFAULT "no"
THEN GOTO EXIT
ELSE GOTO LOOP
*/
/*
COMMAND
RING TERMINAL

ACTION
This command rings the bell on the terminal. This provides a signalling mechanism to an operator.

KEYWORDS
none

EXAMPLE
RING TERMINAL
*/
/*
COMMAND

WAIT TERMINAL

ACTION

This command waits for an operator to push the <return> key at the terminal keyboard.

KEYWORDS

none

EXAMPLE

The following command segment will output a report at the user terminal and then wait for the operator to enter the <return> character before continuing with data processing.

RLS>PREPARE REPORT OUTPUT TI:
RLS>WAIT TERMINAL
PAUSE - enter a <return> to continue:
RLS>

*/
COMMAND

WRITE TERMINAL

ACTION

This command writes a MESSAGE to the user terminal.

KEYWORD

MESSAGE CHAR(132) message string to write

EXAMPLE

RLS>WRITE TERMINAL MESSAGE "Your report is on the line printer."
Your report is on the line printer.
RLS>

*/
CHAPTER 5

CHROMATOGRAPHY

This set of commands performs analysis for chromatography applications. The input to this analysis usually consists of a signal file collected using the analog sampling facilities of the device control commands. The output from this analysis is usually a report printed on either a terminal or line printer, and optionally an x-y plot on a hardcopy plotter using the device control commands. The following commands are described in this chapter:

<table>
<thead>
<tr>
<th>VERB</th>
<th>OBJECT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZERO</td>
<td>BASELINE</td>
<td>correct the peak baselines</td>
</tr>
<tr>
<td>FIND</td>
<td>CHN-PEAKS</td>
<td>find peaks in CHN signal file</td>
</tr>
<tr>
<td>ANALYZE</td>
<td>PEAKS</td>
<td>identify and normalize peaks</td>
</tr>
<tr>
<td>FIND</td>
<td>PEAKS</td>
<td>find peaks in a signal file</td>
</tr>
<tr>
<td>PREPARE</td>
<td>REPORT</td>
<td>prepare a chromatograph report</td>
</tr>
<tr>
<td>ADD</td>
<td>STANDARD</td>
<td>add a new calibration data set</td>
</tr>
<tr>
<td>CHANGE</td>
<td>STANDARD</td>
<td>change a calibration data set</td>
</tr>
<tr>
<td>DELETE</td>
<td>STANDARD</td>
<td>delete a calibration data set</td>
</tr>
<tr>
<td>ENTER</td>
<td>STANDARD</td>
<td>automatic entry of a new calibration data set</td>
</tr>
<tr>
<td>SHOW</td>
<td>STANDARDS</td>
<td>display calibration data set information</td>
</tr>
<tr>
<td>UPDATE</td>
<td>STANDARDS</td>
<td>automatic update of a calibration data set</td>
</tr>
<tr>
<td>ADD</td>
<td>TICS</td>
<td>add peak tic marks to a chromatograph plot</td>
</tr>
</tbody>
</table>
Figure 5.1 shows the usual processing sequence for chromatography data.

5.1 COLLECTING CHROMATOGRAPH SIGNALS

The chromatograph signals are collected using the device commands.

5.2 PLOTTING CHROMATOGRAPH SIGNALS

The chromatograph data is plotted on a graphics terminal or plotter using the "PREPARE PLOT" command. For example, if a chromatograph signal has been collected and stored in the file SIGNAL.DAT then the following command will send the plot to the plotter:

RLS> PREPARE PLOT X-Y.NAME SIGNAL

To add the typical tick marks to the chromatograph plot use the command "ADD TICS" to overlay the ticks on a previously created chromatograph plot. For example, if the peaks for the signal data in SIGNAL.DAT are contained in the peak file PEAK.DAT then the following sequence of commands will output a chromatograph with tick marks:

RLS> PREPARE PLOT X-Y.NAME SIGNAL
RLS> ADD TICS GRAPH.NAME SIGNAL
RLS> SEND PLOT

5.3 DETECTING AND INTEGRATING PEAKS

A signal file is collected using the "START ANALOG" device command. Chromatography peaks in the signal file are detected and integrated using the "FIND PEAKS" command. This command scans the signal file representing detector response and produces an output peak file containing information on peak retention time, peak area etc. The sensitivity of peak detection is controlled by command modifiers given by the user. These modifiers include:

1. DENSITY

The DENSITY modifier affects the signal smoothing by determining the number of data points to be averaged together to produce a single point for subsequent analysis. Higher values of DENSITY result in greater smoothing of the signal. This
convert units newx min
find peaks
zero baseline
analyze peaks method estd
prepare report format medium
pip peak.dat:*/pu

Figure 5.1 Normal Chromatography Processing Sequence
contributes significantly to noise elimination but also involves a loss of information in the signal. DENSITY=1 disables the averaging process. After averaging the signal is passed through a 7 point moving average filter for further noise reduction.

2. SLOPE

The SLOPE modifier determines the slope sensitivity of the peak detection to changes in the signal. Smaller values of SLOPE result in greater sensitivity to small (and/or noise) peaks in the signal. Any slope change below SLOPE is considered to be noise and any change above SLOPE is considered to be valid signal.

3. GATE

The GATE modifier also affects the sensitivity of the peak detection to changes in the signal. This modifier does not directly smooth the signal but specifies a count threshold for the number of persistent SLOPE changes which must be present to define an increasing or decreasing trend in the signal. Smaller values of GATE result in greater sensitivity to small peaks in the signal. Values of GATE of 3 to 5 are common.

4. WIDTH

The WIDTH modifier defines the earliest trailing point of a peak on which it can be terminated on baseline. A peak is only baseline terminated after (WIDTH x peak half width) beyond the peak crest. Since peak half width at half height corresponds roughly to the standard deviation of a normal curve then a WIDTH=3.0 should be adequate for most peak detection to recover the entire peak area.

The areas in a peak file produced by the "FIND PEAKS" command are calculated to a 0 reference. For most chromatography analysis the offset from the 0 reference to the signal baseline must be removed using the "ZERO BASELINE" command.
5.4 GENERATING REPORTS

The command "PREPARE REPORT" generates an output report file suitable for listing on a printer. The input data to this command is a peak information file as produced by any of the "FIND PEAKS", "ZERO BASELINE" or "ANALYZE PEAKS" commands. The type of report is selected with the command modifier FORMAT as one of SHORT, MEDIUM, LONG, or EXTENDED. Each report format is a subset of the next larger format. Figure 5.2 gives an example of a chromatograph report.

5.5 USING CALIBRATIONS

Calibration data sets can be defined for the chromatograph runs for the following purposes:

1. to identify (and name) the peaks that are expected to appear in the run
2. to scale the amounts reported for the components to standard units
3. to compensate amounts reported for changing detector responses

A user can maintain many calibration data sets with each being identified by a specific name. In analyzing individual chromatograph runs the user names the calibration data to be used for the identifications and normalizations.

5.5.1 Calibration Data Definition

The information in the calibrations is maintained in 3 major record definitions:

1. calibration method information
2. component information
3. component curve information

The data elements in each of these records is defined as follows:

1. calibration method

   1. NAME

      Any user defined character string of alphabetic
| CHANNEL | 7 |
| METHOD  | zero |
| INJECTED AT | 07-FEB-83 09:18:18 |

| GATE | 4 |
| SLOPE | 1.000e-01 |
| DENSITY | 1 |
| WIDTH | 3.000e+00 |
| SCALE | 0.000e+00 |
| FREQUENCY | 6.000e+01 |

| REF-RTW | 0.000e+00 |
| ID-LVL | 0.000e+00 |
| %RTW | 0.000e+00 |
| RF-UNK | 0.000e+00 |
| DVT | 0.000e+00 |
| DIL-FTR | 0.000e+00 |

<table>
<thead>
<tr>
<th>RT</th>
<th>%</th>
<th>AREA</th>
<th>HEIGHT</th>
<th>ITM</th>
<th>FACTOR</th>
<th>NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.700e+00</td>
<td>0.000e+00</td>
<td>7.638e-01</td>
<td>2.558e+00</td>
<td>bb</td>
<td>0.000e+00</td>
<td></td>
</tr>
<tr>
<td>3.300e+00</td>
<td>0.000e+00</td>
<td>2.183e-01</td>
<td>9.012e-01</td>
<td>bb</td>
<td>0.000e+00</td>
<td></td>
</tr>
<tr>
<td>4.083e+00</td>
<td>0.000e+00</td>
<td>1.985e-02</td>
<td>5.878e-02</td>
<td>bb</td>
<td>0.000e+00</td>
<td></td>
</tr>
<tr>
<td>7.767e+00</td>
<td>0.000e+00</td>
<td>3.431e-02</td>
<td>6.925e-02</td>
<td>bv</td>
<td>0.000e+00</td>
<td></td>
</tr>
</tbody>
</table>

| TOTALS | 0.000e+00 | 1.036e+00 | 3.587e+00 |

Figure 5.2 Chromatography Report Example
and special characters that will be used to identify the data set.

2. METHOD

An abbreviation for the chromatograph amount normalization method to be used, which must be one of zero (ZERO), area percent (APCT), normalize (NORM), external standard (ESTD) and internal standard (ISTD).

3. USING

This variable instructs the analysis commands to use either areas (AREAS) or heights (HEIGHTS) in determining the concentrations. For example gas chromatography will normally use areas and ion chromatography will normally use heights.

4. UNITS

This variable specifies the units with which the amount data is to be reported. This can be any character string such as "%", "ppm", "gram/liter", etc.

5. DESCRIPTION

This is any user defined comment sentence which provides a brief description of the calibration data set. For example the data set may be identified as "oil sands standard #1", etc.

2. component information

1. NAME

Any character string identifying the name of the component.

2. TYPE

The component type instructs the analysis commands on how to use the peak in identification and normalization in the chromatograph run. The peak type is one of:

1. NORMAL

A 'normal' peak that is not to be used as a
reference or standard is indicated by just entering a <return> character as a type.

2. REFERENCE

Enter "#" for peaks to be used as retention time references for scaling the time axis in order to identify all peaks.

3. STANDARD

Enter "z" for a peak to be used as an internal standard for amount normalization.

4. REFERENCE AND STANDARD

Enter "s" for a peak that is both a reference peak and a standard peak.

3. RET.TIME

This is the retention time of the peak.

4. POLY.ORDER

This is the order of the polynomial curve to be fit to the data points defining the peak. The order is from 1 to 3 (i.e. a linear to a cubic curve). The number of data points placed in the calibration set for the peak must be at least 1 greater than POLY.ORDER. Linear calibrations through the point (0,0) are the only exception. For these the command will accept a single point definition and assume the first point to be (0,0).

5. X**3

This is the coefficient of the cubic term in the polynomial equation.

6. X**2

This is the coefficient of the quadratic term in the polynomial equation.

7. X**1

This is the coefficient of the linear curve in the polynomial equation.

8. X**0

This is the coefficient of the constant term in
the polynomial equation.

3. component curve information

1. AMOUNT

The amount of the component injected for this point, reported in the units identified above.

2. AREA/HEIGHT

The area or height of the peak which resulted from the injection of this amount, in whatever units should appear in the report listings (eg. volt-minutes, volts, etc.).

5.5.2 Maintaining Calibration Data

Several commands have been implemented to permit users to manipulate the information in the calibration data sets as defined above. You identify the records to be manipulated with each command by using the keywords NAME, PEAK and AMOUNT. If the command line includes only NAME then the commands will work with the calibration method information. For example,

ADD STANDARDS CALIB LABSTD

DELETE STANDARD CALIB LABSTD

If the PEAK is also present then the commands will operate on the component records. For example,

ADD STANDARD CALIB LABSTD PEAK CHLORIDE

And finally if the AMOUNT keyword is present then the commands will operate on the component curve information. For example,

CHANGE STANDARD CALIB LABSTD PEAK CHLORIDE AMOUNT 100.

The commands will prompt for the information to be placed in the other data fields of the records.
5.5.2.1 SHOW STANDARDS -

You can request a list of all calibrations currently stored with the command:

SHOW STANDARDS

This produces a 'directory' style listing of each calibration giving its name, method, etc. A complete listing of any individual calibration data set can be obtained with a command such as:

SHOW STANDARD CALIB LABSTD

Figure 5.3 gives an example of a calibration listing.

5.5.2.2 ADD STANDARD -

New calibrations can be defined with the command "ADD STANDARD". You enter the name of the calibration or the component or the amount to be added and the command will prompt for the rest of the information for the data set. For example, to add a new calibration the following sequence might be followed:

ADD CALIBRATION CALIB LABSTD

METHOD       apct : estd
USING         areas :
UNITS         % : ppm
DESCRIPTION   "" : lab calibration for chloride
ris>
ADD CALIBRATION CALIB LABSTD PEAK CHLORIDE
TYPE         :
RET.TIME     0. : 3.9
POLY.ORDER   1 : 2
X**3         0. :
X**2         0. :
X**1         0. :
X**0         0. :

5.5.2.3 DELETE STANDARD -

Information can be removed from the calibration data set with the "DELETE STANDARD" command. An entire calibration can be deleted using the command:

DELETE STANDARD CALIB LABSTD

This will remove the calibration, all components defined for
**Figure 5.3 Example of Calibration Listing**

<table>
<thead>
<tr>
<th>Line</th>
<th>Calibration Method</th>
<th>Using</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>standards3 estd</td>
<td>heights ppm</td>
<td>&quot;calibration curves for f, cl, po4, no3, so4 at 3 umhos&quot;</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Line</th>
<th>Peak</th>
<th>Ret.</th>
<th>Poly.</th>
<th>X**3</th>
<th>X**2</th>
<th>X**1</th>
<th>X**0</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>fluoride</td>
<td>2.3</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.562e-01</td>
<td>1.81e-02</td>
</tr>
<tr>
<td>2</td>
<td>chloride</td>
<td>3.4e+00</td>
<td>1.0e+00</td>
<td>0.0e+00</td>
<td>3.01e-01</td>
<td>-5.93e-02</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>nitrate</td>
<td>7.967e+00</td>
<td>1.0e+00</td>
<td>0.0e+00</td>
<td>1.319e+00</td>
<td>-1.335e-01</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>sulfate</td>
<td>1.047e+01</td>
<td>1.0e+00</td>
<td>0.0e+00</td>
<td>1.091e+00</td>
<td>1.231e-02</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Line</th>
<th>Peak</th>
<th>Amount</th>
<th>Size</th>
<th>Est. Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>chloride</td>
<td>0.1</td>
<td>5.955e-01</td>
<td>1.679e-01</td>
</tr>
<tr>
<td>2</td>
<td>chloride</td>
<td>1.5</td>
<td>5.430e+00</td>
<td>2.762e-01</td>
</tr>
<tr>
<td>3</td>
<td>chloride</td>
<td>1.5</td>
<td>1.583e+00</td>
<td>3.155e-01</td>
</tr>
<tr>
<td>4</td>
<td>chloride</td>
<td>1</td>
<td>3.760e+00</td>
<td>2.660e-01</td>
</tr>
<tr>
<td>5</td>
<td>chloride</td>
<td>2</td>
<td>6.551e+00</td>
<td>3.053e-01</td>
</tr>
<tr>
<td>6</td>
<td>fluoride</td>
<td>1</td>
<td>4.832e-01</td>
<td>2.070e-01</td>
</tr>
<tr>
<td>7</td>
<td>fluoride</td>
<td>0.7</td>
<td>4.037e+00</td>
<td>1.734e-01</td>
</tr>
<tr>
<td>8</td>
<td>fluoride</td>
<td>1.2</td>
<td>7.512e+00</td>
<td>1.597e-01</td>
</tr>
<tr>
<td>9</td>
<td>fluoride</td>
<td>0.5</td>
<td>3.405e+00</td>
<td>1.468e-01</td>
</tr>
<tr>
<td>10</td>
<td>fluoride</td>
<td>1</td>
<td>6.391e+00</td>
<td>1.565e-01</td>
</tr>
<tr>
<td>11</td>
<td>nitrate</td>
<td>0.5</td>
<td>5.327e-01</td>
<td>9.386e-01</td>
</tr>
<tr>
<td>12</td>
<td>nitrate</td>
<td>1</td>
<td>8.330e-01</td>
<td>1.199e+00</td>
</tr>
<tr>
<td>13</td>
<td>nitrate</td>
<td>2</td>
<td>1.668e+00</td>
<td>1.199e+00</td>
</tr>
<tr>
<td>14</td>
<td>nitrate</td>
<td>5</td>
<td>4.119e+00</td>
<td>1.214e+00</td>
</tr>
<tr>
<td>15</td>
<td>nitrate</td>
<td>7</td>
<td>5.315e+00</td>
<td>1.317e+00</td>
</tr>
<tr>
<td>16</td>
<td>sulfate</td>
<td>0.5</td>
<td>3.856e-01</td>
<td>1.297e+00</td>
</tr>
<tr>
<td>17</td>
<td>sulfate</td>
<td>1</td>
<td>9.766e-01</td>
<td>1.024e+00</td>
</tr>
<tr>
<td>18</td>
<td>sulfate</td>
<td>2</td>
<td>1.321e+00</td>
<td>1.098e+00</td>
</tr>
<tr>
<td>19</td>
<td>sulfate</td>
<td>5</td>
<td>4.562e+00</td>
<td>1.096e+00</td>
</tr>
</tbody>
</table>
the calibration and all points defining the calibration curves. A specific component can be removed from a calibration with the command:

DELETE STANDARD CALIB LABSTD PEAK CHLORIDE

which will leave the rest of the calibration definition while removing all information on chloride. Specific points defining a component calibration curve can be removed with the command:

DELETE STANDARD CALIB LABSTD PEAK CHLORIDE AMOUNT 100.

5.5.2.4 CHANGE STANDARD -

This command enables a user to modify any information in the calibration data set without having to delete and reenter information that is not being changed. You identifies the record level to be modified and then the command will display the keyword, the current data value and read in the new value. To leave a value as it is simply enter <return>. For instance, the following command sequence show a change of the METHOD of a calibration from ISTD to ESTD:

```
CHANGE STANDARD CALIB LABSTD
METHOD istd : estd
USING heights :
UNITS ppm :
DESCRIPTION "lab.test" :
```

A word of caution on the use of this command; the command permits a change of the 'calibration name' or a 'peak name' for which it will update all the subsidiary information in the data files. However the subsidiary information is not resorted during this change so that subsequent "ADD STANDARD" and "CHANGE STANDARD" commands which do sort the records properly may not place them in the proper order for retention time processing. Therefore, changes to calibration and peak names should be limited to minor spelling errors only and not to major changes which will affect the alphabetical ordering of the records.
5.5.3.3 Automatic Update Of Peak Information

Some of the calibration information can be updated automatically. Peak retention times, amounts and areas/heights can be corrected by the command "UPDATE STANDARD" from information in a peak data file. For example, to update the points from a peak file named 'PEAK.DAT':

```
UPDATE STANDARD CALIB LABSTD FILE PEAK.DAT
```

For each identified peak in the file the peak retention time and the amount and area/height will be replaced with those in the peak file. The calibration curve coefficients will then be calculated for the new point. The new values can be
averaged in, instead of doing a complete replacement, by specifying two weights, RT-FTR and SIZE-FTR, to be given to the new retention time and new peak size respectively.

The command operates in either automatic or manual mode. In automatic mode the calibration curve point to be updated is identified entirely by information contained in the peak file. The curve point updated is that which is within a specified per cent window of the amount given in the peak data file. If no curve point is found to be within this window the command prints out an error message. In manual mode, the name, retention time and calculated amount are printed at the terminal for each peak and the user is requested to enter the exact amount of the component as it will be found in the calibration file. Furthermore, if the new size differs from the old peak size by more than a per cent window then the command will print the percent variation out on the terminal and ask the user to confirm whether the update should be done.

5.5.3.4 Plotting The Calibration Curve -

To plot the calibration curve, first 'extract' the points from the calibration data set into an x-y data file using the "EXTRACT STANDARD" command. A formatted graph can then be produced from this x-y data using the RLS X-Y PLOTTING application system. For example,

RLS>EXTRACT STANDARD CALIB LABSTD PEAK CHLORIDE -  
   X-Y.NAME CHLOR
RLS>PREPARE PLOT X-Y.NAME CHLOR
RLS>SEND PLOT

Figure 5.4 gives an example of a calibration curve plot.

5.5.3.5 Curve Fits To Calibration Curves -

It may be necessary to experiment with various orders of polynomials in order to find the best for the calibration points being used. To do this extract the points into an x-y data file using the "EXTRACT STANDARD" command and then use the RLS MATH routines "FIT CURVE" and "GENERATE CURVE". For example,

RLS>EXTRACT STANDARDS CALIB LABSTD PEAK CHLORIDE X-Y.NAME CHLOR
RLS>FIT CURVE X-Y.NAME CHLOR FORM 2-POLY
RLS>GENERATE CURVE COEFF CHLOR FIT.NAME CURVE -  
   XMIN 10. XMAX 200. NPOINTS 100
RLS>PREPARE PLOT X-Y.NAME CURVE
RLS>SEND PLOT GRAPH.NAME CURVE
Figure 5.4 Plot of Calibration Curve
where the above sequence:

1. puts the calibration points in X-Y data set CHLOR
2. calculates the best fit 2nd order polynomial coefficients
3. generates a curve for the polynomial at 100 points from amount=10. to amount=200.
4. plots the graph of the evaluated polynomial points.

Figure 5.5 gives an example of a curve fit to a calibration curve.

5.6 IDENTIFYING PEAKS AND NORMALIZING AMOUNTS

Peaks are identified and/or normalized using the "ANALYZE PEAKS" command. This command refers to the calibration data set named by the operator in order to identify the components in a run and normalize the weights. The input data to the command is a peak information file as produced by the "FIND PEAKS" and/or "ZERO BASELINE" command. The output data of the command is another peak information file in exactly the same format. This command performs any of the methods zero (ZERO), area percent (APCT), normalization (NORM), external standard (ESTD) and internal standard (ISTD).

Peaks are identified by referring to the retention times specified in the calibration data. The peak input file is first scanned for any peaks in the calibration time windows specified for reference peaks. If there are several peaks in the reference peak time window then the biggest peak is selected as the actual reference peak. At least one reference peak must be defined in the calibration data. The actual retention times for any reference peaks found are then used to linearly rescale the identification times for the rest of the peaks. A second scan of the peak file is done to match the peaks according to the rescaled identification times. If there are several peaks in a normal peak reference time window then the peak closest to the center of an identification time window is selected as the peak to be used for identification and normalization.

For METHODS NORM, ESTD and ISTD the peak concentrations are normalized by referring to the calibration curves defined in the calibration data. For each peak in the
Figure 5.5 Calibration Curve Fit
calibration a set of coefficients are maintained which are the polynomial coefficients for a least squares fit to the calibration curve points. The "ANALYZE PEAKS" command calculates the actual amount by using the peak size (area/height) as the independent variable for the polynomial equation as follows:

\[ \text{AMOUNT} = c3 \times (\text{size}^2) + c2 \times (\text{size}^2) + c1 \times \text{size} + c0 \]

This amount is then reported in one of several formats as specified by the METHOD modifier:

1. ZERO and APCT
   
   a straight percentage of the total area (no reference to calibration curve):
   
   \[ C = \text{SIZE} \times \text{DIL-FTR} \times 100. / \text{TOTAL-SIZE} \]

2. NORM
   
   a percentage of the total area normalized using the calibration curve coefficients:
   
   \[ C = \text{AMOUNT} \times \text{DIL-FTR} \times 100. / \text{TOTAL-AMOUNT} \]

3. ESTD
   
   the concentration is reported in the units defined in the calibration data:
   
   \[ C = \text{AMOUNT} \times \text{DIL-FTR} \]

4. ISTD
   
   the concentration is corrected by an internal standard and reported as:
   
   \[ C = \text{AMOUNT} \times (\text{STD-AMT} / \text{CALC-STD}) \times \text{DIL-FTR} / \text{SMP-AMT} \]

   where  
   
   \[ \text{STD-AMT} = \text{amount of standard injected} \]  
   \[ \text{CALC-STD} = \text{calculated amount of the standard} \]  
   \[ \text{SMP-AMT} = \text{AMOUNT of sample injected} \]  

   If SMP-AMT=1. then the concentration will be in the units of the calibration data (as for ESTD). If SMP-AMT=(total amount injected) and DIL-FTR=100.0 then the concentration will be in percentage.
NOTE

SMP-AMT should exclude the amount in STD-AMT.

The dilution factor (DIL-FTR) applied to all of the above equations is a command modifier entered by the user and is normally set at 1.

Figure 5.6 gives an example of a chromatograph report with identified peaks and normalized amounts.

5.7 COMMAND DEFINITIONS
**Figure 5.6 Chromatograph Report with Identified Peaks and Normalized Amounts**

<table>
<thead>
<tr>
<th>RT</th>
<th>pHn</th>
<th>AREA</th>
<th>HEIGHT</th>
<th>INT</th>
<th>FACTOR</th>
<th>NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.350e+00</td>
<td>4.118e-02</td>
<td>4.352e-02</td>
<td>1.477e-01</td>
<td>bb</td>
<td>2.350e+00</td>
<td>2.788e-01 # fluoride</td>
</tr>
<tr>
<td>3.267e+00</td>
<td>2.925e+00</td>
<td>4.567e+00</td>
<td>9.912e+00</td>
<td>bb</td>
<td>3.474e+00</td>
<td>2.951e-01 chloride</td>
</tr>
<tr>
<td>7.400e+00</td>
<td>6.433e+00</td>
<td>4.095e+00</td>
<td>5.020e+00</td>
<td>bv</td>
<td>3.140e+00</td>
<td>1.281e+00 nitrate</td>
</tr>
<tr>
<td>9.433e+00</td>
<td>5.125e+00</td>
<td>4.325e+00</td>
<td>5.125e+00</td>
<td>vb</td>
<td>1.000e+00</td>
<td></td>
</tr>
</tbody>
</table>

| TOTALS | 1.452e+01 | 1.303e+01 | 2.020e+01 |
**COMMAND**

**ZERO BASELINE**

**ACTION**

This command corrects the areas in a chromatograph peak information file by subtracting from each peak area the portion of the peak area contributed by the baseline offset from zero reference. The area subtracted is that defined by the leading and trailing point of the peak, or for groups of peaks, that area defined by the lead point of the first peak and the trail point of the last peak.

**KEYWORDS**

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEAK-FILE</td>
<td>CHAR(40)</td>
<td>peak information file name</td>
</tr>
</tbody>
</table>

**EXAMPLE**

```
ZERO BASELINE PEAK-FILE PEAK.DAT
```
FIND CHN-PEAKS

ACTION

This command finds the appropriate heights for the peaks in the CHN signal files. The two CHN files produced by the instrument and identified as SIGNAL-FILE are scanned for the heights of the levels identifying NITROGEN, CARBON, and HYDROGEN. An output PEAK-FILE is produced which is suitable for processing by the chromatograph analysis commands.

NOTE voltage level times in seconds are assumed to be:

NITROGEN  CARBON  HYDROGEN

BLANK  23   22   25
SAMPLE 31   33   35

with a 2 to 3 second settling time.

KEYWORDS

SIGNAL-FILE  CHAR  CHN signal file name
PEAK-FILE    CHAR  peak file name
STEP SIZE     REAL  sample point interval

EXAMPLE

An RLS program to repeatedly sample and analyze data from the CHN instrument:

MONITOR ANALOG CH 10
LOOP:
  WAIT ANALOG CH 10
  FIND CHN-PEAKS
  ANALYZE PEAKS
  PREPARE REPORT
  GOTO LOOP
*/
/* COMMAND

ANALYZE PEAKS

ACTION

This program processes an input peak information file as obtained from a chromatograph peak finding program and identifies the peaks and normalizes the concentrations as defined in a previously generated CALIBRATION.NAME.

Reference peaks are identified as the largest peak found within a time window of + or - REF-RTW minutes around their expected retention times. These provide a time framework for locating all other peaks. The expected retention time of all peaks are then scaled linearly with the nearest reference peaks. The peaks are then identified as the largest within a time window of + or - %RTW around their own expected retention times.

Only peaks having an area/height greater than ID-LVL volt-min. and a retention time after DVT minutes are identified by name.

Concentrations for unidentified peaks use RF-UNK as a response factor. The amount of the standard, STD-AMT, and the amount of the sample, SMP-AMT, must be entered for the ISTD method. A dilution factor (DIL-FTR) (normally 1.) is applied to all peak concentrations.

KEYWORDS

| PEAK-FILE  | CHAR(40) | input peak information file name |
| CALIBRATION.NAME  | CHAR(20) | calibration name |
| SMP-AMT  | REAL | amount of sample injected |
| STD-AMT  | REAL | amount of standard injected |
| REF-RTW  | REAL | reference peak retention window |
| ID-LVL  | REAL | identification level |
| %RTW  | REAL | % normal peak retention window |
| RF-UNK  | REAL | response factor for unknowns |
| DVT  | REAL | dead volume time |
| DIL-FTR  | REAL | dilution factor |

EXAMPLE

ANALYZE PEAKS SMP-AMT 10. STD-AMT 200.
ANALYZE PEAKS DIL-FTR 2. %RTW 5

*/
**COMMAND**

**FIND PEAKS**

**ACTION**

This command scans a signal file for the presence of chromatograph peaks. Results are output to a peak information file containing information such as retention times, peak area, etc. The signal is assumed to be represented as equidistant y values as obtained from a sampling program at a specific FREQUENCY. The signal data is smoothed using piecewise averaging of DENSITY number of points. Peaks are detected by a signal change greater than a specified SLOPE.

The slope must persistently exceed this slope by more than GATE threshold number of sampling points. Peaks are ended on baseline at a distance of at least (WIDTH * half width) past the peak crest. For gaussian peaks half width at half height is roughly equivalent to the standard deviation so this WIDTH would normally be 3.0 in order to capture 99.7% of the area. FREQUENCY is normally set by the analog sampling program.

**KEYWORDS**

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIGNAL-FILE</td>
<td>CHAR(40)</td>
<td>input signal data file</td>
</tr>
<tr>
<td>PEAK-FILE</td>
<td>CHAR(40)</td>
<td>output peak information file</td>
</tr>
<tr>
<td>GATE</td>
<td>INTEGER</td>
<td>persistent change threshold</td>
</tr>
<tr>
<td>SLOPE</td>
<td>REAL</td>
<td>slope sensitivity</td>
</tr>
<tr>
<td>DENSITY</td>
<td>INTEGER</td>
<td>number of points to average</td>
</tr>
<tr>
<td>WIDTH</td>
<td>REAL</td>
<td>peak termination width</td>
</tr>
<tr>
<td>FREQUENCY</td>
<td>REAL</td>
<td>sampling frequency of the signal</td>
</tr>
</tbody>
</table>

**EXAMPLES**

FIND PEAKS SIGNAL-FILE CH10.DAT
FIND PEAKS SLOPE .01 DENSITY 4
/*
COMMAND

PREPARE REPORT

ACTION

This command produces a summary report of a chromatograph
analysis in an OUTPUT-FILE. The input file is a peak
information file as produced by any of the "find peaks",
"correct baseline" or "analyze peaks" commands.

The report FORMAT can be one of SHORT,
MEDIUM, LONG or EXTENDED. The SHORT report provides the
retention times, amounts and names for each peak. The
MEDIUM report adds peak areas, heights and separation codes.
The LONG report also adds identification times, and the
EXTENDED report also adds response factor estimates.
The response factor estimate is the peak amount divided
by the peak size (area or height) and gives an indication
of the factor that would be used for a linear calibration
through the point (0,0).

Unidentified peaks can be suppressed from the report
by specifying SUP-UNK equal to the concentration threshold
below which peaks should not be reported.

The rest of the modifiers are usually picked up from the
processed data file.

KEYWORDS

PEAK-FILE CHAR(40) input peak information file name
OUTPUT-FILE CHAR(40) output report file name
FORMAT CHAR(10) SHORT, MEDIUM, LONG or EXTENDED
METHOD string concentration calculation method
TITLE string title line
SUBTITLE string subtitle line
UNITS string units for the 'amount' column
SUP-UNK logical suppress unknowns threshold
TIME string injection time
STD-AMT float amount of standard injected
SAMP-AMT float amount of sample injected
misc... ...... several parameters set by computer

EXAMPLE

PREPARE REPORT FORMAT MEDIUM
PREPARE REPORT TITLE "bitumen analysis"

*/
CHROMATOGRAPHY

/*
NAME

ADD STANDARD

ACTION

This command adds new information to the calibration data currently stored. There are three major variations on the command:

1. ADD STANDARD CALIBRATION.NAME xxxx
2. ADD STANDARD CALIBRATION.NAME xxxx PEAK yyy
3. ADD STANDARD CALIBRATION.NAME xxxx PEAK yyy AMOUNT zzzz

Entering the first form indicates that you want to add a new calibration to the current set, the second form indicates that you want to add a new peak to CALIBRATION.NAME xxxx, and the third form indicates that you want to add a new data point to PEAK yyy in CALIBRATION.NAME xxxx.

You will be prompted for all further information to be entered into the calibration data. The prompt line presents the keyword identifier for the data item and the default value if any. Enter a <return> to accept the default value.

KEYWORDS

<table>
<thead>
<tr>
<th>CALIBRATION.NAME</th>
<th>CHAR(20)</th>
<th>calibration name</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEAK</td>
<td>CHAR(20)</td>
<td>peak name</td>
</tr>
<tr>
<td>AMOUNT</td>
<td>REAL</td>
<td></td>
</tr>
</tbody>
</table>

EXAMPLE

To define a new calibration with one peak named fluoride, and one calibration point at 100 ppm:

RLS>ADD CALIBRATION.NAME LABSTD
method norm : estd
using areas :
units % : ppm
description : lab standard #1
RLS>ADD CALIBRATION.NAME LABSTD PEAK FLUORIDE
peak type #:
retention time 0.:
poly.order 1 : 
**3 0 : 
**2 0 :
**1 0 :
**0 0 :
RLS>ADD CALIBRATION.NAME LABSTD PEAK FLUORIDE AMOUNT 100
area 0 : 1241
*/
/*
NAME

CHANGE STANDARD

ACTION

This command is used to change information on calibrations that is already contained in the data set. This allows you to change some items without having to delete and reenter a lot of information. The three major forms of the command are:

1. CHANGE STANDARD CALIBRATION.NAME xxxx
2. CHANGE STANDARD CALIBRATION.NAME xxxx PEAK yyyy
3. CHANGE STANDARD CALIBRATION.NAME xxxx PEAK yyyy AMOUNT zzzz

which allow you to change respectively the overall calibration information, any peak item information, and any calibration curve information. The command will prompt you to enter information on all data fields that can be changed. For each data field the command will print out the identifying keyword, the current value and then will wait for your response. To accept the current value simply type a <return> character.

KEYWORDS

CALIBRATION.NAME CHAR(20) calibration name
PEAK CHAR(20) peak name
AMOUNT REAL calibration curve amount

EXAMPLE

To change calibration name LABSTANDARD peak CHLORIDE

POLY.ORDER:

CHANGE STANDARD CALIB NAME LABSTANDARD PEAK CHLORIDE
enter name chloride :
enter type # :
enter ret.time 5.2 :
enter poly.order 1 :2
enter x**3 0. :
enter x**2 0. :
enter x**1 0. :
enter x**0 0. :
*/
/*
NAME
DELETE STANDARD

ACTION

This command deletes information from the calibration data. The command deletes all information for a specified CALIBRATION.NAME, or just information on a specific peak (CALIBRATION.NAME & PEAK) or just specific calibration curve points (CALIBRATION.NAME & PEAK & AMOUNT). The three forms of the command to accomplish these deletes are:

1. DELETE STANDARD CALIBRATION.NAME xxxx
2. DELETE STANDARD CALIBRATION.NAME xxxx PEAK yyy
3. DELETE STANDARD CALIBRATION.NAME xxxx PEAK yyy AMOUNT zzzz

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>CALIBRATION.NAME</td>
<td>CHAR(20)</td>
<td>calibration name</td>
</tr>
<tr>
<td>PEAK</td>
<td>CHAR(20)</td>
<td>peak name</td>
</tr>
<tr>
<td>AMOUNT</td>
<td>REAL</td>
<td>peak amount</td>
</tr>
</tbody>
</table>

EXAMPLE

To delete all information related to the calibration named LABSTANDARD:

RLS>DELETE STANDARD CALIBRATION LABSTANDARD

To delete only the fluoride peak in LABSTANDARD:

RLS>DELETE STANDARD CALIBRATION LABSTANDARD PEAK FLUORIDE
*/
/*
NAME

ENTER STANDARD

ACTION

This command enters new calibration curve points from a peak data file and updates the response coefficients. The calibration name and file are identified by the user. The retention times in the calibration file are replaced with the new retention times and the calibration points (amounts and area/heights) are inserted into the calibration. Note that the peak name etc. must have been defined previously but the peak amounts and areas should not be defined first. Identified peaks in the data file are ignored (ie. it is assumed that you are adding a new peak from a processed peak file.

The command will print out the peak number, peak retention time and peak area or height and request that you enter the peak name and amount.

KEYWORDS

CALIBRATION.NAME CHAR(20) calibration name to be updated
PEAK-FILE CHAR(40) peak file containing curve points

EXAMPLE

To add peaks from the file peak.dat:

RLS> ENTER CALIBRATION.NAME LABSTANDARD PEAK-FILE PEAK.DAT

PEAK # 1 RETENTION TIME = 0.2300e+01 HEIGHT = 0.4321e+04 peak amount :chloride :10.
PEAK # 2 RETENTION TIME = 0.5900e+01 HEIGHT = 0.3212e+04 name amount :fluoride :120.

RLS>
*/
EXTRACT STANDARD

ACTION

This command extracts the points defining a particular calibration curve from a standard. The peak sizes (areas or heights) and amounts are placed into an X-Y data set as x and y data values respectively. That is, amounts are given as a function of the sizes. The points can then be tested with various curve fits before finalizing the production versions.

If there is only one point in the calibration then this command also inserts the point (0,0) into the x-y data file.

KEYWORDS

X-Y.NAME
CALIBRATION.NAME
PEAK

CHAR(20)  x-y data set
CHAR(20)  calibration name
CHAR(20)  peak name

EXAMPLE

The following command places data points into the data set named LAB:

EXTRACT STANDARD CALIBRATION LAB PEAK FLUORIDE

*/
NAME

SHOW STANDARDS

ACTION

This command produces a listing of the current calibrations either on the user's terminal or into a named file. A 'directory' listing of all calibrations stored or a full listing of a specific CALIBRATION.NAME can be produced. The full listing contains the information for each peak in the sample followed by the data points defining the calibration curves (if any). For each point in the calibration curve an 'estimated response factor' is calculated and displayed. This is the amount divided by the peak area and estimates the factor for a single point calibration through (0,0).

The two major variations on the command are therefore:

1. SHOW STANDARDS
2. SHOW STANDARD CALIBRATION.NAME xxxxx

KEYWORDS

OUTPUT-FILE CHAR(40) output file name
CALIBRATION.NAME CHAR(20) specific calibration name

EXAMPLE

RLS>SHOW STANDARDS

<table>
<thead>
<tr>
<th>LINE</th>
<th>CALIBRATION</th>
<th>METHOD</th>
<th>USING</th>
<th>UNITS</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>oil.sands</td>
<td>estd</td>
<td>heights</td>
<td>%</td>
<td>&quot;bitumen sample&quot;</td>
</tr>
<tr>
<td>2</td>
<td>lab_sample#1</td>
<td>norm</td>
<td>areas</td>
<td>ppm</td>
<td>&quot;standard lab sample&quot;</td>
</tr>
</tbody>
</table>

RLS>SHOW STANDARD CALIBRATION.NAME lab_sample#1

<table>
<thead>
<tr>
<th>LINE</th>
<th>CALIBRATION</th>
<th>METHOD</th>
<th>USING</th>
<th>UNITS</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>lab_sample#1</td>
<td>norm</td>
<td>areas</td>
<td>ppm</td>
<td>&quot;standard lab sample&quot;</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LINE</th>
<th>PEAK</th>
<th>TYPE</th>
<th>RET-TIME</th>
<th>POLY.ORDER</th>
<th>X**3</th>
<th>X**2</th>
<th>X**1</th>
<th>X**0</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>fluoride #</td>
<td>5.4</td>
<td>2</td>
<td>0.0</td>
<td>2.3</td>
<td>1.4</td>
<td>4.2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>chloride #</td>
<td>8.9</td>
<td>1</td>
<td>0.0</td>
<td>0.0</td>
<td>2.0</td>
<td>3.0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LINE</th>
<th>PEAK</th>
<th>AMOUNT</th>
<th>SIZE</th>
<th>EST-RF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>chloride</td>
<td>10.</td>
<td>3921</td>
<td>.034</td>
</tr>
<tr>
<td>2</td>
<td>chloride</td>
<td>100.</td>
<td>4023</td>
<td>.526</td>
</tr>
<tr>
<td>3</td>
<td>fluoride</td>
<td>200.</td>
<td>2401</td>
<td>.193</td>
</tr>
<tr>
<td>4</td>
<td>fluoride</td>
<td>220.</td>
<td>2491</td>
<td>.345</td>
</tr>
<tr>
<td></td>
<td>fluoride</td>
<td>230.</td>
<td>3421</td>
<td>.391</td>
</tr>
<tr>
<td>---</td>
<td>---------</td>
<td>------</td>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>6</td>
<td>fluoride</td>
<td>240.</td>
<td>4092</td>
<td>.419</td>
</tr>
</tbody>
</table>

RLS> */
UPDATE STANDARD

ACTION

This command updates calibration curve points and response
coefficients. The CALIBRATION.NAME specified is updated from the
PEAK-FILE identified by the user. The retention
times and peak area/heights are changed and then the
the response coefficients are recalculated. The stored
values for retention time and peak area/height are weighted towards
the new values by specifying the retention time weight
(RT-FTR) and the peak area/height weight (SIZE-FTR).
The stored values are entirely replaced if RT-FTR=1.0 and
SIZE-FTR=1.0. The calculation is:

STORED = NEWVALUE * FTR + OLDVALUE * (1.0 - FTR)

The command operates in two major modes, automatic and manual.
In automatic mode the calibration curve point to be updated
is identified entirely by information contained in the peak
file. The curve point updated is that which is within plus
or minus %WINDOW of the amount given in the peak data file.
If no curve point is found to be within this window then
the command prints out an error message.

In manual mode the name, retention time and calculated
amount are printed at the terminal for each peak and the
user is requested to enter the exact amount of the component
as it will be found in the calibration file. Furthermore,
if the new size differs from the old peak size by more
than plus or minus %WINDOW then the command will print the
percent variation out on the terminal and ask the user to
confirm whether the the update should be done.

Unidentified peaks in the peak data file are ignored.

KEYWORDS

| CALIBRATION.NAME    | CHAR(20) | calibration name to be updated |
| PEAK-FILE           | CHAR(40) | peak file containing curve points |
| %WINDOW             | REAL     | update window in % |
| RT-FTR              | REAL     | retention time factor |
| SIZE-FTR            | REAL     | peak size factor |

EXAMPLE

RLS>START ANALOG CH 10 DURATION 5. SIGNAL-FILE CH10.DAT
RLS>FIND PEAKS SIGNAL-FILE CH10.DAT PEAK-FILE PEAK.DAT
RLS>UPDATE STANDARD CALIBRATION.NAME LABSTD PEAK-FILE PEAK.DAT

*/
COMMAND

ADD TICS

ACTION

This command adds the tick marks to a chromatograph plot to indicate the integration points. The input data is a peak information file as produced by one of the commands "FIND PEAKS", "CORRECT BASELINE" or "ANALYZE PEAKS", etc. The output is to a graph dat set which must previously have been created for a chromatograph signal with the "PREPARE GRAPH" command.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEAK-FILE</td>
<td>CHAR(40)</td>
<td>peak information file name</td>
</tr>
<tr>
<td>GRAPH.NAME</td>
<td>CHAR(20)</td>
<td>plot descriptor file name</td>
</tr>
</tbody>
</table>

EXAMPLES

To prepare and plot an x-y plot of a chromatograph signal with integration tick marks:

RLS>START ANALOG CH 10 DURATION 5. SIGNAL-FILE SIGNAL RLS>FIND PEAKS SIGNAL-FILE SIGNAL PEAK-FILE PEAK.DAT RLS>PREPARE GRAPH PEAK-FILE PEAK.DAT GRAPH.NAME PICTURE RLS>ADD TICS PEAK-FILE PEAK.DAT GRAPH.NAME PICTURE RLS>SEND PLOT GRAPH.NAME PICTURE
CHAPTER 6

X-Y PLOTTING

These commands format and display x-y data in graphical form. Sets of x-y data are produced by other sub-systems including manual data entry, analog signal sampling, chromatograph calibration curves, etc. These data sets must be converted into intermediate forms which are the graph data sets that may be subsequently displayed on various graphics devices (Figure 6.1). The commands in this section create, manipulate and display the graph data sets.

```
-------------------
| x-y data set     |
-------------------
|                   |
-------------------
| graph data set    |
-------------------
|                   |
-------------------
| display device    |
-------------------
```

Figure 6.1

The output devices that are supported for the x-y plots include:

1. Benson 1312 drum plotter
2. Calcomp 566 drum plotter
3. DEC LXY printer/plotter
4. DEC VT125 graphics terminal
5. Tektronix 4006 graphics terminal
6. Tektronix 4014 graphics terminal
7. Tektronix 4662 flatbed plotter

The following commands are available for the creation and maintenance of the graph data sets:
<table>
<thead>
<tr>
<th>VERB</th>
<th>OBJECT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>DELETE</td>
<td>PLOT</td>
<td>delete a graph</td>
</tr>
<tr>
<td>PREPARE</td>
<td>PLOT</td>
<td>format a graph</td>
</tr>
<tr>
<td>SEND</td>
<td>PLOT</td>
<td>display an x-y graph on a terminal or send it to a plotter</td>
</tr>
<tr>
<td>SHOW</td>
<td>PLOTS</td>
<td>display information on graphs</td>
</tr>
</tbody>
</table>

### 6.1 MAINTAINING GRAPHS

The commands "SHOW PLOTS" and "DELETE PLOT" are used to maintain the current set of graphs. The name of each graph created is stored in a list of current graphs. The list can be displayed by entering the "SHOW PLOTS" command as in the following sequence:

**RLS>SHOW PLOTS**

<table>
<thead>
<tr>
<th>LINE</th>
<th>GRAPH.NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>picture1</td>
<td>&quot;figure 1 - calibration curve&quot;</td>
</tr>
<tr>
<td>2</td>
<td>signal</td>
<td>&quot;figure 2 - chromatograph signal&quot;</td>
</tr>
</tbody>
</table>

**RLS>**

The DESCRIPTION that appears in this list is taken from the TITLE line that appears at the bottom of the x-y plots. More detailed information on a graph in the list can be obtained by entering the command "SHOW PLOT GRAPH.NAME x". For example:

**RLS>SHOW PLOT GRAPH.NAME PICTURE1**

<table>
<thead>
<tr>
<th>LINE</th>
<th>GRAPH.NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>picture1</td>
<td>&quot;figure 1 - calibration curve&quot;</td>
</tr>
</tbody>
</table>

```
<table>
<thead>
<tr>
<th>#</th>
<th>XMIN</th>
<th>XMAX</th>
<th>YMIN</th>
<th>YMAX</th>
<th>LEGEND</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10.0</td>
<td>100.0</td>
<td>-30.0</td>
<td>200.</td>
<td>2</td>
</tr>
</tbody>
</table>
```

**RLS>**

This more detailed information contains the minimum and maximum values for both axes for scaling overlays and the legend number for the next overlay.
A graph that appears in the list can be deleted by entering the command "DELETE PLOT GRAPH.NAME x". For example:

RLS>DELETE PLOT GRAPH.NAME PICTURE1

would delete the graph named picture1.plt from the above list and cause the following display on the next "SHOW PLOTS" command:

RLS>SHOW PLOTS

<table>
<thead>
<tr>
<th>LINE</th>
<th>GRAPH.NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>signal</td>
<td>&quot;figure 2 - chromatograph signal&quot;</td>
</tr>
</tbody>
</table>

RLS>

The graph information can be placed into an output file for printing by using the keyword OUTPUT-FILE and specifying the output file name as follows:

RLS>SHOW PLOTS OUTPUT-FILE GRAPH.LST
RLS>SHOW PLOT GRAPH.NAME SIGNAL OUTPUT-FILE GRAPH.LST
RLS>

6.2 FORMATTING A GRAPH

The "PREPARE PLOT" command is used to format a set of x-y data that can be subsequently displayed on a graphics device. The command accepts an x-y data set as input and prepares a graph containing a series of plotting commands for the graphics devices. The graphs are formatted into a standard x-y data plot with axes, axes labelling, titles and legends, which can be controlled by the various keywords for the command.

Every graph is given a name to identify it. The output graph name is normally the same name as your input data set name. A plot descriptor file is created in your disk area for each graph created, with the file name taken from the NAME of the graph. Therefore this graph name must also be a valid file name.

In the most basic variation of this command, an x-y data set named MYDATA may be formatted and plotted with the following commands:

RLS>PREPARE PLOT X-Y.NAME MYDATA
RLS>SEND PLOT GRAPH.NAME MYDATA

In this form the graph will appear as in Figure 6.2.
Figure 6.2 Formatted Graph
The axes scales will be automatically scaled to contain all data points within the graph. Axes will be drawn with appropriate annotation as to the length and scale of the axis.

Further annotation is displayed by defining the keywords XLABEL, YLABEL, TITLE and DESCRIPTION. This can be done beforehand in the x-y data set information or they may be supplied as keywords to the "PREPARE PLOT" command. If an XLABEL or YLABEL is defined then these will appear as annotation on the appropriate axes. If a TITLE is defined then this will appear centered at the bottom of the plot. If a DESCRIPTION is defined then a legend will appear at the top of the graph with the plotting symbol along side the description line. The following variation of the command will add these items to the graph and produce the plot of Figure 6.3 for the same data set as described above:

RLS>PREPARE PLOT X-Y,NAME MYDATA -
   XLABEL "Time in Minutes" -
   YLABEL "Sensitivity in Volts" -
   DESCRIPTION "Test Data" -
   TITLE "Fig. 3 - Annotated Plot"
RLS>SEND PLOT GRAPH,NAME MYDATA

Note that all axes and annotations can be ommitted by giving "AXIS NO" on the command line. For example:

RLS>PREPARE PLOT X-Y,NAME MYDATA AXIS NO
RLS>SEND PLOT GRAPH,NAME MYDATA

will produce the plot of Figure 6.4 (untitled) for the same data as above.

The command automatically scans the x-y data to find the minimum and maximum values contained in the data. These values are determine the boundaries of the graph axes. This automatic scaling of the data can be suppressed by entering values for the minimum and maximum values with the keywords XMIN, XMAX, YMIN, YMAX. The values may be entered singly or in any combination. The command will still scan the data to find the minimums or maximums for any data that have not been entered manually. For example, a portion of the data set above may be magnified by setting the minimums and maximums to a subset of the data (Figure 6.5):

RLS>PREPARE PLOT X-Y,NAME MYDATA -
   XMIN 2 XMAX 5 YMIN 160 YMAX 220 -
   TITLE "Fig. 6 - Magnified Data Set"
RLS>SEND PLOT GRAPH,NAME MYDATA

Furthermore the axis boundaries are rounded up so that the
Test Data

Fig. 3 - Annotated Plot

Figure 6.3 Graph with Annotation
Figure 6.4 Graph without Axis
**Fig. 6 - Magnified Data Set**

Figure 6.5 Magnified Graph Segment
tick marks will appear at 'nice' intervals. This rounding can be omitted, with the data scaled so that the extreme data points lie exactly on the axis boundaries by giving "AUTO NO" on the command line as follows:

RLS>PREPARE PLOT X-Y.NAME MYDATA AUTO NO -
   TITLE "Fig. 5 - Exact Axis Scaling"
RLS>SEND PLOT GRAPH.NAME MYDATA

which produces the plot of Figure 6.6.

By default a data set that is plotted is normally connected by lines with no symbols at the data points. The color of the line drawn can be controlled by using the PEN keyword for any plotters which support automatic pen changes (eg. BENSON 1312 plotter). (The pen is identified by entering a number which is very device dependent.) In addition to the line plots a symbol may be drawn at the location of each point in the data plot. This is done by using the SYMBOL keyword on the "PREPARE PLOT" command and specifying one of the symbol numbers as given in Figure 6.7. The first 14 symbols in this figure are 'centered' symbols which are normally used for marking the data points. If a symbol plot only is required, with no lines interconnecting the data points, then give "POINTS YES" in the command. For example, to plot the data set MYDATA using symbol #1 and no connecting lines, use the following commands which will produce the graph of Figure 6.8:

RLS>PREPARE PLOT X-Y.NAME MYDATA -
   SYMBOL 1 POINTS YES -
   TITLE "Fig. 8 - Symbols Only"
RLS>SEND PLOT GRAPH.NAME MYDATA

6.3 PLOTTING THE GRAPH

The "SEND PLOT" command is used to display a graph on an output device such as a graphics terminal or plotter. A formatted graph as produced by the "PREPARE PLOT" command is displayed with the command "SEND PLOT GRAPH.NAME x", where 'x' is the name of the graph data set to be plotted. The output device to be used can be specified with the DEVICE keyword and a device name from the following list:
Fig. 5 - Exact Axis Scaling

Figure 6.6 Graph with Exact Axis Scaling
Fig. 8 - Symbols Only

Figure 6.8 Graph with Symbols Only
NAME                DESCRIPTION
BENSON              Benson 1312 drum plotter
CALCOMP             Calcomp 566 drum plotter
LXY                 DEC LXY printer/plotter
PLOTTER             Tektronix 4662 flatbed plotter
TEK4006             Tektronix 4006 graphics terminal
TEK4014             Tektronix 4014 graphics terminal
VT125               DEC VT125 graphics terminal

For example the commands:

RLS>SEND PLOT GRAPH.NAME PICTURE1 DEVICE PLOTTER
RLS>SEND PLOT GRAPH.NAME PICTURE1 DEVICE TEK4014

will send the same graph PICTURE1 to the Tektronix 4662 hard copy plotters and the Tektronix 4014 graphics terminal respectively.

NOTE

When the Tektronix terminals are specified as output devices the command assumes the terminal to be used is the one from which the command is issued.

6.4 OVERLAYING GRAPHS

The plots for several x-y data sets can be overlaid on a single graph. For example, a curve fitted to the data points of the file MYDATA (in the previous examples) can be placed on top of the set of data points with the following commands (Figure 6.9):

RLS>PREPARE PLOT X-Y.NAME MYDATA POINTS YES SYMBOL 4 -
       TITLE "Fig. 9 - Data and Curve Overlay"
RLS>PREPARE PLOT X-Y.NAME CURVE GRAPH.NAME MYDATA
RLS>SEND PLOT GRAPH.NAME MYDATA
Fig. 9 - Data and Curve Fitting Overlay

Figure 6.9 Overlaid Plots
The first data set placed into the graph overlay will determine the axis scaling, axis notations and titles that will be placed on the graph. Subsequent data sets will be scaled to the maximum and minimum values as determined by the first data set and will be placed into the graph with no further axis and title notation. If a DESCRIPTION is specified for each overlaid data set then a legend will be produced for each that will display the symbol that it was plotted with alongside the DESCRIPTION.

6.5 COMMAND DEFINITIONS
/*
NAME

DELETE PLOT

ACTION

This command deletes graphs created by the "PREPARE PLOT" command. All information on GRAPH.NAME is removed.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRAPH.NAME</td>
<td>CHAR(20)</td>
<td>graph name</td>
</tr>
</tbody>
</table>

EXAMPLE

To delete a plot:

RLS>SHOW PLOTS

<table>
<thead>
<tr>
<th>LINE</th>
<th>GRAPH.NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>picture1</td>
<td>&quot;figure 1 - lab data&quot;</td>
</tr>
<tr>
<td>2</td>
<td>picture2</td>
<td>&quot;bitumen sample&quot;</td>
</tr>
<tr>
<td>3</td>
<td>test</td>
<td>&quot;curve fit data&quot;</td>
</tr>
</tbody>
</table>

RLS>DELETE PLOT GRAPH.NAME PICTURE2
RLS>SHOW PLOTS

<table>
<thead>
<tr>
<th>LINE</th>
<th>GRAPH.NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>picture1</td>
<td>&quot;figure 1 - lab data&quot;</td>
</tr>
<tr>
<td>3</td>
<td>test</td>
<td>&quot;curve fit data&quot;</td>
</tr>
</tbody>
</table>

RLS>
*/
/* COMMAND

PREPARE PLOT

ACTION

This command prepares a formatted graph of an x-y data set which can be displayed on a plotter or graphics terminal. The command accepts an input x-y data file and prepares an output GRAPH.NAME. As graphs are created they are placed into a list which can be displayed with the "SHOW PLOTS" command. A graph that has been prepared can be displayed on an output device with the "SEND PLOT" command.

Several x-y data plots can be overlaid on a graph by using the same output GRAPH.NAME. The first data set placed into the plot determines the axis boundaries, scaling and labelling. Subsequent data plots are assumed to be overlays on the first data set.

A TITLE, DESCRIPTION, XLABEL and YLABEL can be given for the graph. These can be suppressed from the graph (along with the axes) by specifying "AXIS NO". The axes can be placed on the top and right hand sides of the graph by specifying "UP YES".

The graph boundaries can be specified using the keywords XMIN, XMAX, YMIN and YMAX. If any of these are not specified in the "PREPARE PLOT" command then the command will scan the x-y data file to find the appropriate minimums and maximums. The graph boundaries will normally be rounded up to some 'nice' values for placement of the axis tick marks, but this rounding may be suppressed with "AUTO NO".

Logarithmic graphs can be done by specifying X-TRANSFORM and/or Y-TRANSFORM of ln(x), log(x), ln(y) or log(y).

The data points are normally connected by lines. A SYMBOL may also be plotted at each data point by specifying the character number from the standard CALCOMP set. The symbols with no connecting lines will be drawn if the keyword "POINT YES" is present. The PEN number can be specified to select from various colours available on the plot devices.

The graph size defaults to a 21.3 cm x 27.6 cm page (8.5 x 11 in) but this can be scaled up or down by specifying an arbitrary scale FACTOR.

KEYWORDS
**X-Y PLOTTING**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-Y.NAME</td>
<td>CHAR(20)</td>
<td>x-y data set name</td>
</tr>
<tr>
<td>GRAPH.NAME</td>
<td>CHAR(20)</td>
<td>graph data set name</td>
</tr>
<tr>
<td>AXIS</td>
<td>LOGICAL</td>
<td>yes for axes and titles</td>
</tr>
<tr>
<td>TITLE</td>
<td>CHAR(80)</td>
<td>main title for the graph</td>
</tr>
<tr>
<td>DESCRIPTION</td>
<td>CHAR(80)</td>
<td>description for the x-y data</td>
</tr>
<tr>
<td>XLABEL</td>
<td>CHAR(80)</td>
<td>a label for the x axis</td>
</tr>
<tr>
<td>YLABEL</td>
<td>CHAR(80)</td>
<td>a label for the y axis</td>
</tr>
<tr>
<td>UP</td>
<td>LOGICAL</td>
<td>yes for axes on top and right</td>
</tr>
<tr>
<td>AUTO</td>
<td>LOGICAL</td>
<td>yes to round tic marks</td>
</tr>
<tr>
<td>XMIN</td>
<td>REAL</td>
<td>minimum x value</td>
</tr>
<tr>
<td>XMAX</td>
<td>REAL</td>
<td>maximum x value</td>
</tr>
<tr>
<td>YMIN</td>
<td>REAL</td>
<td>minimum y value</td>
</tr>
<tr>
<td>YMAX</td>
<td>REAL</td>
<td>maximum y value</td>
</tr>
<tr>
<td>POINTS</td>
<td>LOGICAL</td>
<td>yes for point plot only</td>
</tr>
<tr>
<td>SYMBOL</td>
<td>INTEGER</td>
<td>CALCOMP symbol number</td>
</tr>
<tr>
<td>PEN</td>
<td>INTEGER</td>
<td>plotter pen number</td>
</tr>
<tr>
<td>FACTOR</td>
<td>REAL</td>
<td>scaling factor for the graph</td>
</tr>
<tr>
<td>STEPSIZE</td>
<td>REAL</td>
<td>equidistant data interval</td>
</tr>
<tr>
<td>X-TRANSFORM</td>
<td>CHAR(10)</td>
<td>ln(x), log(x)</td>
</tr>
<tr>
<td>Y-TRANSFORM</td>
<td>CHAR(10)</td>
<td>ln(y), log(y)</td>
</tr>
</tbody>
</table>

**EXAMPLES**

If two sets of data are available, MYDATA containing some data points and CURVE containing a fitted curve, then these can be plotted using:

RLS>PREPARE PLOT X-Y.NAME MYDATA POINTS YES SYMBOL 5
RLS>PREPARE PLOT X-Y.NAME CURVE GRAPH MYDATA
RLS>SEND PLOT

*/
/*
NAME

SEND PLOT

ACTION

This command causes a graph created by the "PREPARE PLOT" or "PREPARE TEXT" commands to be plotted on one of several output devices. The output DEVICE can be specified as one of the following:

<table>
<thead>
<tr>
<th>NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>BENSON</td>
<td>BENSON 1312 drum plotter</td>
</tr>
<tr>
<td>CALCOMP</td>
<td>CALCOMP 566 drum plotter</td>
</tr>
<tr>
<td>LXY</td>
<td>DEC LXY printer-plotter</td>
</tr>
<tr>
<td>PLOTTER</td>
<td>Tektronix 4662 flatbed plotter</td>
</tr>
<tr>
<td>TEK4006</td>
<td>Tektronix 4006 graphics terminal</td>
</tr>
<tr>
<td>TEK4014</td>
<td>Tektronix 4014 graphics terminal</td>
</tr>
<tr>
<td>VT125</td>
<td>DEC VT125 graphics terminal</td>
</tr>
</tbody>
</table>

When the output device is a graphics terminal then the plot output is directed towards the terminal from which the command is issued.

The plot can be scaled in size by an arbitrary FACTOR. If the plot is too big for the output device then it is automatically rescaled to fit the display surface.

KEYWORDS

<table>
<thead>
<tr>
<th>GRAPH.NAME</th>
<th>CHAR(20)</th>
<th>graph data set name</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEVICE</td>
<td>CHAR(10)</td>
<td>output device name</td>
</tr>
<tr>
<td>FACTOR</td>
<td>REAL</td>
<td>scaling factor</td>
</tr>
</tbody>
</table>

EXAMPLE

To plot the file PICTURE1 on the Tektronix terminal while enlarging it by a factor of 2.0:

RLS>SEND PLOT GRAPH.NAME PICTURE1 -
DEVICE TEK4014 FACTOR 2.0

To send the same file to the plotter:

RLS>SEND PLOT GRAPH.NAME PICTURE1 DEVICE PLOTTER

*/
SHOW PLOTS

This command produces a listing of the current graphs. The listing is written to an output device or file which is usually the terminal from which the command is issued.

The command "SHOW PLOTS" with no qualifying keywords will produce a 'directory' style listing of the graphs. If a GRAPH.NAME is specified as in:

RLS>SHOW PLOT GRAPH.NAME PICTURE1

then specific information on the named graph will be displayed. This information includes the graph boundaries (minimum and maximum x and y values) and the legend number.

KEYWORDS

GRAPH.NAME CHAR(20) graph data set name
OUTPUT-FILE CHAR(40) output file name

EXAMPLE

RLS>SHOW PLOTS

<table>
<thead>
<tr>
<th>LINE</th>
<th>GRAPH.NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>picture1</td>
<td>&quot;figure 1 - lab data #1&quot;</td>
</tr>
<tr>
<td>2</td>
<td>picture2</td>
<td>&quot;figure 9 - bitumen sample&quot;</td>
</tr>
</tbody>
</table>

RLS>SHOW PLOTS GRAPH.NAME PICTURE1

<table>
<thead>
<tr>
<th>LINE</th>
<th>GRAPH.NAME</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>picture1</td>
<td>&quot;figure 1 - lab data #1&quot;</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LINE</th>
<th>XMIN</th>
<th>XMAX</th>
<th>YMIN</th>
<th>YMAX</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000e+00</td>
<td>1.000e+01</td>
<td>0.000e+00</td>
<td>2.000e+03</td>
</tr>
</tbody>
</table>
/*
COMMAND

PREPARE TEXT

ACTION

This command prepares text for output to a graphics device. The INPUT-FILE containing text characters is converted to a plot descriptor file in GRAPH.NAME. As 'text' graphs are created they are placed into a list that can be displayed with the "SHOW PLOTS" command. The graphs can be displayed on an output device with the "SEND PLOT" command.

The character HEIGHT can be adjusted and the PEN color can be selected.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>INPUT-FILE</td>
<td>CHAR(40)</td>
<td>input file name</td>
</tr>
<tr>
<td>GRAPH.NAME</td>
<td>CHAR(20)</td>
<td>plot descriptor name</td>
</tr>
<tr>
<td>HEIGHT</td>
<td>REAL</td>
<td>character height in cm</td>
</tr>
<tr>
<td>PEN</td>
<td>INTEGER</td>
<td>pen number</td>
</tr>
</tbody>
</table>

EXAMPLE

To plot a text file on the plotter:

RLS> PREPARE TEXT INPUT-FILE MYDATA
RLS> SEND PLOT GRAPH.NAME MYDATA DEVICE PLOTTER
RLS>

*/
CHAPTER 7

MATH Routines

These commands perform various mathematical manipulations on data files. The main applications included in this section are:

1. curve fitting
2. unit conversion

The following commands are currently available:

<table>
<thead>
<tr>
<th>VERB</th>
<th>OBJECT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIT</td>
<td>CURVE</td>
<td>fit a function to data using the least squares criteria</td>
</tr>
<tr>
<td>GENERATE</td>
<td>CURVE</td>
<td>evaluate a function over some range</td>
</tr>
<tr>
<td>BUNCH</td>
<td>DATA</td>
<td>smooth and reduce signal data</td>
</tr>
<tr>
<td>ADD</td>
<td>FUNCTION</td>
<td>add a new function</td>
</tr>
<tr>
<td>DELETE</td>
<td>FUNCTION</td>
<td>delete a function</td>
</tr>
<tr>
<td>SHOW</td>
<td>FUNCTIONS</td>
<td>show function data</td>
</tr>
<tr>
<td>GENERATE</td>
<td>RESIDUALS</td>
<td>place residuals into x-y data set</td>
</tr>
<tr>
<td>SHOW</td>
<td>STATISTICS</td>
<td>show estimates on goodness of fit between functions and data sets</td>
</tr>
<tr>
<td>CONVERT</td>
<td>UNITS</td>
<td>convert data units</td>
</tr>
</tbody>
</table>
7.1 MAINTAINING FUNCTION INFORMATION

The commands "ADD FUNCTION", "DELETE FUNCTION" and "SHOW FUNCTION" are used to maintain function information. The function information is primarily the coefficients of some equation.

The current list of functions can be displayed with the "SHOW FUNCTIONS" command as in the following sequence:

RLS>SHOW FUNCTIONS

<table>
<thead>
<tr>
<th>LINE</th>
<th>NAME</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>fnl</td>
<td>y=a+b*x</td>
<td>&quot;linear fit&quot;</td>
</tr>
<tr>
<td>2</td>
<td>fnl</td>
<td>y=a+b/x</td>
<td>&quot;non-linear fit&quot;</td>
</tr>
<tr>
<td>3</td>
<td>calib</td>
<td>y=a<em>b</em>x</td>
<td>&quot;calibration curve fit&quot;</td>
</tr>
</tbody>
</table>

RLS>

Note that the function name is usually derived from the name of the x-y data set to which the function is being fit. Therefore, there may be multiple occurrences of the same function name for which the various forms of the function will be identified by the FORM field. More detailed information on a function can be displayed by entering the command "SHOW FUNCTION COEFFICIENTS x" as in the following sequence:

RLS>SHOW FUNCTION COEFFICIENTS FN1

<table>
<thead>
<tr>
<th>LINE</th>
<th>NAME</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>fnl</td>
<td>y=a+b/x</td>
<td>&quot;non-linear fit&quot;</td>
</tr>
</tbody>
</table>

LINE COEFFICIENT

1 1.3
2 2.3

RLS>

A function that appears in the above list can be deleted by entering the command "DELETE FUNCTION COEFFICIENTS x" as follows:

RLS>DELETE FUNCTION COEFFICIENTS FN1 FORM Y=A+B/X

after which the next "SHOW FUNCTIONS" command would produce the following:

RLS>SHOW FUNCTIONS

<table>
<thead>
<tr>
<th>LINE</th>
<th>NAME</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
</table>
fnl y=a+b*x "linear fit"

calib y=a*x^b "calibration curve fit"

The coefficients of a function can be entered manually with the "ADD FUNCTION" command. After entering the command you will be prompted for the following information:

DESCRIPTION
This is a brief description of the function for your own information.

FORM
This is the specific form of the function which is taken from the following table:

<table>
<thead>
<tr>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-POLYNOMIAL</td>
<td>General polynomial of order N</td>
</tr>
<tr>
<td>Y=A*X</td>
<td>Straight line through (0,0)</td>
</tr>
<tr>
<td>Y=A+B*X</td>
<td>Straight line</td>
</tr>
<tr>
<td>Y=A<em>EXP(B</em>X)</td>
<td>Exponential curve</td>
</tr>
<tr>
<td>Y=1/(A+B*X)</td>
<td></td>
</tr>
<tr>
<td>Y=A+B/X</td>
<td></td>
</tr>
<tr>
<td>Y=A+B*LOG(X)</td>
<td>Log base 10 curve</td>
</tr>
<tr>
<td>Y=A*X^B</td>
<td>Power curve</td>
</tr>
<tr>
<td>Y=X/(A+B*X)</td>
<td></td>
</tr>
<tr>
<td>Y=A+B*LN(X)</td>
<td>Natural logarithm</td>
</tr>
<tr>
<td>Y=A*B^X</td>
<td>Power curve</td>
</tr>
</tbody>
</table>

COEFFICIENTS
These are the coefficients of the function in increasing order of significance. Where the function form is denoted with the letters A and B then A will be the first coefficient in the list and B the second.

For example, to add the function name FN1 as above:

RLS>ADD FUNCTION COEFFICIENTS FN1

description "" :non-linear fit
form y=a+b*x :y=a+b/x
coefficient #1 0. :1. 
coefficient #2 0. :2.3

RLS>
7.2 FITTING A CURVE TO DATA

The command "FIT CURVE" is used to fit a curve to an X-Y data set using the conventional least squares criteria. After performing this command a new function will be created and added to the current function list. The function coefficients can be displayed with the "SHOW FUNCTION" command. The goodness of fit estimates can be displayed with the "SHOW STATISTICS" command. The function can be evaluated over a range of points with the "GENERATE CURVE" command and then the resulting curve can be plotted on a graph over the original data points. This section will outline the above operations using an example from Page 35 of:

Applied Linear Statistical Models, J.Neter and W.Wasserman. which appears as follows with the "SHOW X-Y" command:

RLS>SHOW X-Y X-Y.NAME WESTWOOD

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>WESTWOOD</td>
<td>&quot;Westwood Company&quot;</td>
</tr>
<tr>
<td>LINE</td>
<td>&quot;Lot Size&quot;</td>
<td>&quot;Labour&quot;</td>
</tr>
<tr>
<td>&quot;units&quot;</td>
<td></td>
<td>&quot;man-hours&quot;</td>
</tr>
<tr>
<td>1</td>
<td>30</td>
<td>73</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>50</td>
</tr>
<tr>
<td>3</td>
<td>60</td>
<td>128</td>
</tr>
<tr>
<td>4</td>
<td>80</td>
<td>170</td>
</tr>
<tr>
<td>5</td>
<td>40</td>
<td>87</td>
</tr>
<tr>
<td>6</td>
<td>50</td>
<td>108</td>
</tr>
<tr>
<td>7</td>
<td>60</td>
<td>135</td>
</tr>
<tr>
<td>8</td>
<td>30</td>
<td>69</td>
</tr>
<tr>
<td>9</td>
<td>70</td>
<td>148</td>
</tr>
<tr>
<td>10</td>
<td>60</td>
<td>132</td>
</tr>
</tbody>
</table>

RLS>

Fit a 1st order polynomial curve to the data set by specifying the data set name WESTWOOD and the FORM of the equation as N-POLYNOMIAL as follows:

RLS>FIT CURVE X-Y.NAME WESTWOOD FORM 1-POLY

RLS>

Please note that a function FORM of * can also be used in which case the command will fit all forms that follow the 'Y=' format (ie. everything except the general polynomials). Display the new function coefficients:

RLS>SHOW FUNCTION COEFFICIENTS WESTWOOD
LINE NAME FORM DESCRIPTION
1 WESTWOOD 1-POLYNOMIAL "Westwood Company"

LINE COEFFICIENTS
1 1.000000e+01
2 2.000000e+00

RLS>

The coefficients in the above list are displayed in the order of increasing significance. For the function forms that are specified in the format ‘Y=’ the A coefficient is listed first and the B coefficient is second. i.e. The 1st order polynomial function is:

Y=10+2*X

The goodness of fit estimates now be displayed with the command:

RLS>SHOW FITS

LINE DATA FUNCTION FORM R-SQUARE F-VALUE DF-REGR DF-RES
1 DATA1 FN1 1-POLYNOMIAL 9.95610e-01 1.81333e+03 1 8

RLS>

In the above listing the R-SQUARE value is the ‘Coefficient of Multiple Determination’. The F-VALUE and the two degrees of freedom printed out can be used to estimate the confidence level of the fit as discussed below. In order to generate a curve to plot over the data points the function must be evaluated over a range:

RLS>GENERATE CURVE COEFFICIENTS WESTWOOD FORM 1-POLY FIT.NAME CURVE XMIN 20 XMAX 80 NPOINTS 7

RLS>

Prepare and plot a graph using the X-Y Plotting commands. "PREPARE PLOT" and "SEND PLOT":

RLS>PREPARE PLOT X-Y.NAME WESTWOOD SYMBOL 4 POINTS YES
RLS>PREPARE PLOT X-Y.NAME CURVE
RLS>SEND PLOT GRAPH.NAME WESTWOOD

The graph for the above set of data points and fitted line are shown in Figure 7.1.
Figure 7.1 Data with Fitted Curve
7.3 ESTIMATING THE GOODNESS OF FIT

The brief form of the command "SHOW STATISTICS" produces the following listing:

RLS>SHOW STATISTICS

LINE DATA   FUNCTION   FORM  R-SQUARE  F-VALUE  DF-REGR  DF-RES
           DATA1          FN1  1-POLYNOMIAL  9.95610e-01  1.81333e+03  1     8

RLS>

The value labelled R-SQUARE is what is known as the 'Coefficient of Multiple Determination'. This value is:

R-SQUARE = SSR / (SSE + SSR)

where SSE is the sum of squares of deviations of the data points about the fitted points and SSR is the sum of squares of the deviations of the fitted points about the mean value. R-SQUARE is always between 0.0 and 1.0 where values closer to 1.0 indicate a better fit. The F-VALUE is defined as:

F-VALUE = MSR / MSE

where MSE is the mean value of SSE and MSR is the mean value of SSR. Since both MSE and MSR follow a CHI-SQUARE probability distribution, this statistic will follow an F probability distribution with DF.REGR and DF.RES degrees of freedom. DF.REGR is shown in the listing and is the degrees of freedom used in calculating MSR from the regression function and DF.RES is the degrees of freedom used in calculating MSE from the original data. This value of F can be used for a test of whether or not there exists a relationship between the dependent and independent variables (please refer to the references). Briefly, the hypothesis to be formed is:

C1: all coefficients are zero
C2: not all coefficients are zero

At a confidence level of ALPH A the F-VALUE should be compared to the F statistic from a table such that if:

F-VALUE < F(ALPHA;DF.REGR,DF.RES) then conclude C1
F-VALUE > F(ALPHA;DF.REGR,DF.RES) then conclude C2

For the Westwood example given above the F-VALUE is 1813.33. At a confidence level of 95% the critical value for the F statistic will be found from a probability table to be:
F-CRITICAL = F(.05;1,8) = 5.32 Since the F-VALUE for the Westwood example is greater than 5.32 we can conclude that there is a relationship between the two variables.

A more complete display of goodness of fit parameters can be obtained by using the keyword FULL on the command line as follows:

RLS>SHOW STATISTICS FULL YES

This version of the command produces a listing as shown in Figure 7.2.
This listing follows a form given in the Neter and Wasserman text on page 247. For a detailed discussion please refer to the text. Briefly the elements are:

1. The columns of information under the heading VARIABLES gives the mean and standard deviations of the X and Y data sets.

2. The CORRELATION MATRIX is for the X and Y variables and is based on the following equations:

   \[ r(i,j) = \frac{\text{cov}(i,j)}{\text{sqrt}(\text{var}(i)\times\text{var}(j))} \]

3. The columns under COEFFICIENTS present the coefficients in both the original and linearized forms, and the standard deviations. The T-VALUE is calculated as:

   \[ T-\text{VALUE} = \frac{\text{COEFFICIENT}(i)}{\text{std.dev.}(i)} \]

   and can be used to test the hypothesis that a particular coefficient is 0 as follows:

   C1: coefficient is 0.
   C2: coefficient is not 0.

   At a confidence level of ALPHA the T-VALUE should be compared to the T statistic from a table such that if:

   \[ \text{ABS}(T-\text{VALUE}) < T(1-\text{ALPHA}/2;\text{DF.RES}) \] then conclude C1
   \[ \text{ABS}(T-\text{VALUE}) > T(1-\text{ALPHA}/2;\text{DF.RES}) \] then conclude C2

4. The ANALYSIS OF VARIANCE table presents information on the SUM and MEAN OF SQUARES of the regression and the SUM and MEAN OF SQUARES of the residuals.

5. The COVARIANCE MATRIX presents the estimates of the variances of the coefficients.
NOTE

All of the goodness of fit calculations for non-linear function forms are made on the linearized form of the original data.

A plot of the residuals can be obtained by using the command "GENERATE RESIDUALS" to place the residuals into an x-y data set. The data set of residuals can then be plotted using the usual graph commands.

7.4 A NON-LINEAR EXAMPLE

The following figures present output from a fitting of non-linear curves to a set of non-linear data from Neter and Wasserman page 125. The form of the equation is $Y = A \times BX$ with $A = 31.71$ and $B = 1.363$.

7.5 MATHEMATICS OF THE CURVE FIT

The method used in the solution of the least squares curve fits follows a matrix formulation. Please refer to the following texts:


A set of basis functions is developed for the particular form of the equation being used. The inner products of vectors formed from the basis functions build a system of linear equations called the 'normal' equations. The coefficients are then found by solving the system of equations.

All of the non-linear equations currently handled are such that the data can be transformed into a form that is linear in two parameters, A and B, such that $Y = A + BX$. A straight line is then fit to the transformed data using the method of least squares for a polynomial as described above. The transformations used are as follows:
LINE DATA
SET # FUNCTION NAME FUNCTION FORM
1 westwood westwood 1-polynomial

VARIABLES

VARIABLE MEAN VARIANCE ST.DEV
X 5.00000e+01 3.40000e+03 5.33095e+01
Y 1.10000e+02 1.36600e+04 1.16876e+02

CORRELATION MATRIX

1.00000e+00 9.97801e-01
9.97801e-01 1.00000e+00

COEFFICIENTS

NO. ORIGINAL LINEARIZED ST.ERROR T-VALUE
COEFF.

1 1.00000e+01 1.00000e+01 2.50294e+00 3.99530e+00
2 2.00000e+00 2.00000e+00 4.69688e-02 4.25832e+01

ANALYSIS OF VARIANCE

SOURCE SS DF MS
REGRESSION 1.36000e+04 1 1.36000e+04
RESIDUAL 6.00000e+01 8 7.50000e+00
TOTAL 1.36600e+04 9

F-VALUE 1.81333e+03
S.E. OF ESTIMATE 2.73861e+00
R-SQUARE 9.95606e-01

COVARIANCE MATRIX

-2.6471e+00 -1.10294e-01
-1.10294e-01 2.20588e-03

RESIDUALS

NO. OBSERVED ESTIMATED RESIDUAL
1 7.30000e+01 7.00000e+01 3.00000e+00
2 5.00000e+01 5.00000e+01 0.00000e+00
3 1.28000e+02 1.30000e+02 -2.00000e+00
4 1.70000e+02 1.70000e+02 0.00000e+00
5 3.70000e+01 9.00000e+01 -3.00000e+00
6 1.05000e+02 1.10000e+02 -2.00000e+00
7 1.35000e+02 1.30000e+02 5.00000e+00
8 6.90000e+01 7.00000e+01 -1.00000e+00
9 1.48000e+02 1.50000e+02 -2.00000e+00
10 1.32000e+02 1.30000e+02 2.00000e+00

MAX DEVIATION 5.00000e-
\[ Y = A \times X \]  
no transformation

\[ Y = A + B \times X \]  
no transformation

\[ Y = A \times \exp(B \times X) \]  
take the natural logarithm of both sides of the equation:  
\[ \ln(Y) = \ln(A) + B \times X, \quad Y > 0 \]  
\[ Y' = A' + B \times X \]  
\[ A = \exp(A') \]

\[ Y = \frac{1}{A + B \times X} \]  
take the inverse of \( Y \)  
\[ \frac{1}{Y} = A + B \times X, \quad Y > 0 \]  
\[ Y' = A + B \times X' \]

\[ Y = A + B \div X \]  
take the inverse of \( X \)  
\[ Y = A + B \times (\frac{1}{X}), \quad X > 0 \]  
\[ Y = A + B \times X' \]

\[ Y = A + B \times \log_{10}(X) \]  
take the logarithm base 10 of \( X \)  
\[ Y = A + B \times \log_{10}(X), \quad X > 0 \]  
\[ Y = A + B \times X' \]

\[ Y = A + X \times B \]  
take the natural logarithm of both sides of the equation  
\[ \ln(Y) = \ln(A) + B \times \ln(X), \quad X, Y > 0 \]  
\[ \ln(Y) = A' + B \times \ln(X) \]  
\[ A = \exp(A') \]

\[ Y = \frac{X}{A + B \times X} \]  
take inverse of \( X \) and \( Y \)  
\[ \frac{1}{Y} = A \div X + B, \quad X, Y > 0 \]

\[ Y = A + B \times \ln(X) \]  
take the natural logarithm of \( X \)  
\[ Y = A + B \times \ln(X), \quad X > 0 \]  
\[ Y = A + B \times X' \]

\[ Y = A \times B \times X \]  
take the natural logarithm of both sides of the equation  
\[ \ln(Y) = \ln(A) + \ln(B) \times X \]  
\[ Y' = A' + B' \times X \]  
\[ A = \exp(A') \]  
\[ B = \exp(B') \]

7.6 UNIT CONVERSION

The "CONVERT UNITS" command is used to convert the units of an x-y data file. Unit conversion is used primarily to convert the time units in the signal files from the "START ANALOG" command from seconds to minutes. For example, if an analog signal file is collected in the file
SIGNAL.DAT which has the x axis in units of SECONDS, then the data units can be converted to MINUTES with the following sequence:

RLS> CONVERT UNITS SIGNAL SIGNAL.DAT NEWX MINUTES

7.7 COMMAND DEFINITIONS
/*
COMMAND

ADD FUNCTION

ACTION

This command adds a new set of function coefficients

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>COEFFICIENT.NAME</td>
<td>CHAR(20)</td>
<td>function name</td>
</tr>
</tbody>
</table>

EXAMPLE

RLS>ADD FUNCTION COEFFICIENT FN1
   enter FORM y=a+b*x
   enter description "" : y=a*exp(b*x)
   enter coefficient #1 0. : exponential fit
   enter coefficient #2 0. : 1.
   RLS>SHOW FUNCTION COEFFICIENT FN1

<table>
<thead>
<tr>
<th>LINE</th>
<th>FUNCTION</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FN1</td>
<td>y=a<em>exp(b</em>x)</td>
<td>exponential fit</td>
</tr>
</tbody>
</table>

LINE COEFFICIENT

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.</td>
</tr>
<tr>
<td>2</td>
<td>2.3</td>
</tr>
</tbody>
</table>

RLS>
*/
NAME

CONVERT UNITS

ACTION

This command converts the units in an x-y data file from one form to another. The conversions that are currently supported include:

<table>
<thead>
<tr>
<th>FROM</th>
<th>TO</th>
</tr>
</thead>
<tbody>
<tr>
<td>lpa-11 a/d counts</td>
<td>volts</td>
</tr>
<tr>
<td>lps-11 a/d counts</td>
<td>volts</td>
</tr>
<tr>
<td>minutes</td>
<td>seconds</td>
</tr>
<tr>
<td>seconds</td>
<td>minutes</td>
</tr>
<tr>
<td>microvolts</td>
<td>volts</td>
</tr>
<tr>
<td>millivolts</td>
<td>volts</td>
</tr>
<tr>
<td>volts</td>
<td>lpa-11 a/d counts</td>
</tr>
<tr>
<td>volts</td>
<td>lps-11 a/d counts</td>
</tr>
<tr>
<td>volts</td>
<td>microvolts</td>
</tr>
<tr>
<td>volts</td>
<td>millivolts</td>
</tr>
</tbody>
</table>

Either of the data axes (x or y) or both can be converted. The units are identified with one of the following keywords:

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>LPA-11</td>
<td>lpa-11 a/d counts</td>
</tr>
<tr>
<td>LPS-11</td>
<td>lps-11 a/d counts</td>
</tr>
<tr>
<td>MICROVOLTS</td>
<td>microvolts</td>
</tr>
<tr>
<td>MILLIVOLTS</td>
<td>millivolts</td>
</tr>
<tr>
<td>MINUTES</td>
<td>time in minutes</td>
</tr>
<tr>
<td>SECONDS</td>
<td>time in seconds</td>
</tr>
<tr>
<td>VOLTS</td>
<td>voltage</td>
</tr>
</tbody>
</table>

KEYWORDS

<table>
<thead>
<tr>
<th>SIGNAL-FILE</th>
<th>x-y data file name</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEWX</td>
<td>new units for x data</td>
</tr>
<tr>
<td>NEWY</td>
<td>new units for y data</td>
</tr>
<tr>
<td>XUNITS</td>
<td>current units for x data</td>
</tr>
<tr>
<td>YUNITS</td>
<td>current units for y data</td>
</tr>
<tr>
<td>STEPSIZE</td>
<td>float stepsize for equidistant x-y data</td>
</tr>
</tbody>
</table>

EXAMPLE

If a signal file has been collected from the "SAMPLE ANALOG" command with the x axis in units of SECONDS then the following command will convert the X units to MINUTES:

CONVERT -TS SIGNAL-FILE SIGNAL.DAT NEWX MINUTES
/* 
NAME

DELETE FUNCTION

ACTION

This command deletes a specified function from the function list. Since one function name may be included in the list with several forms, the FORM of the function to be deleted can also be specified.

KEYWORDS

COEFFICIENT.NAME :R(20) . function name
FORM :CHAR(15) . function form

EXAMPLE

To delete a function:

RLS>SHOW FUNCTIONS

<table>
<thead>
<tr>
<th>LINE</th>
<th>FUNCTION</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FN1</td>
<td>y=a*x</td>
<td>&quot;test function&quot;</td>
</tr>
<tr>
<td>2</td>
<td>FN1</td>
<td>y=a+b/x</td>
<td>&quot;non-linear fit&quot;</td>
</tr>
<tr>
<td>3</td>
<td>FN2</td>
<td>y=a+b*x</td>
<td>&quot;linear fit&quot;</td>
</tr>
</tbody>
</table>

RLS>DELETE FUNCTION COEFFICIENT FN1 FORM Y=A+B/X

RLS>SHOW FUNCTIONS

<table>
<thead>
<tr>
<th>LINE</th>
<th>FUNCTION</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FN1</td>
<td>y=a*x</td>
<td>&quot;test function&quot;</td>
</tr>
<tr>
<td>2</td>
<td>FN2</td>
<td>y=a+b*x</td>
<td>&quot;linear fit&quot;</td>
</tr>
</tbody>
</table>

RLS>
*/
COMMAND

GENERATE CURVE

ACTION

This command evaluates function coefficients of specified FORM over a range placing the results into an X-Y data set. The range of the function evaluation is specified from a starting point (XMIN) to a final point (XMAX) and NPOINTS number resulting points will be produced at equidistant intervals over the range.

KEYWORDS

<table>
<thead>
<tr>
<th>COEFFICIENT.NAME</th>
<th>CHAR(20)</th>
<th>function name</th>
</tr>
</thead>
<tbody>
<tr>
<td>FORM</td>
<td>CHAR(15)</td>
<td>function form</td>
</tr>
<tr>
<td>X-Y.NAME</td>
<td>CHAR(20)</td>
<td>name of resulting x-y data set</td>
</tr>
<tr>
<td>XMIN</td>
<td>REAL</td>
<td>starting x value</td>
</tr>
<tr>
<td>XMAX</td>
<td>REAL</td>
<td>ending x value</td>
</tr>
<tr>
<td>NPOINTS</td>
<td>INTEGER</td>
<td>number of points to evaluate</td>
</tr>
</tbody>
</table>

EXAMPLE

RLS> GENERATE CURVE COEFFICIENT FN1 FORM Y=A+B/X - XMIN 12. XMAX 20. NPOINTS 30

*/
COMMAND

GENERATE RESIDUALS

ACTION

This command places the residuals between a set of data points and a set of fitted points as calculated by a function into an x-y data set.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>DATA TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>COEFFICIENT.NAME</td>
<td>CHAR(20)</td>
<td>function name</td>
</tr>
<tr>
<td>FORM</td>
<td>CHAR(15)</td>
<td>function form</td>
</tr>
<tr>
<td>X-Y.NAME</td>
<td>CHAR(20)</td>
<td>data set name</td>
</tr>
<tr>
<td>RESIDUAL.NAME</td>
<td>CHAR(20)</td>
<td>new X-Y data set</td>
</tr>
<tr>
<td>VERSUS</td>
<td>CHAR</td>
<td>X or Y</td>
</tr>
</tbody>
</table>

EXAMPLE

RLS>GENERATE RESIDUALS COEFFICIENT FNL X-Y.NAME XY1 - RESIDUAL.NAME RES1

*/
/*
COMMAND

FIT CURVE

ACTION

This command finds the coefficients for a function to fit a set of X-Y data using the least-squares criteria. The function coefficients and FORM and data set name are entered as parameters. The function information is placed into the current function list.

The function form may be any one of the following:

<table>
<thead>
<tr>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-POLYNOMIAL</td>
<td>general polynomial y=a0+a1<em>x+a2</em>x^2+...+aN*x^N</td>
</tr>
<tr>
<td>Y=A*X</td>
<td>straight line through point (0,.0.)</td>
</tr>
<tr>
<td>Y=A+B*X</td>
<td>straight line</td>
</tr>
<tr>
<td>Y=A<em>EXP(B</em>X)</td>
<td>exponential curve</td>
</tr>
<tr>
<td>Y=1/(A+B*X)</td>
<td></td>
</tr>
<tr>
<td>Y=A+B/X</td>
<td>log base 10 curve</td>
</tr>
<tr>
<td>Y=A+B*LOG(X)</td>
<td></td>
</tr>
<tr>
<td>Y=A*X^B</td>
<td>power curve</td>
</tr>
<tr>
<td>Y=X/(A+B*X)</td>
<td></td>
</tr>
<tr>
<td>Y=A+B*LN(X)</td>
<td>natural logarithm curve</td>
</tr>
<tr>
<td>Y=A*B^X</td>
<td></td>
</tr>
</tbody>
</table>

The resulting function coefficients can be displayed with the "SHOW FUNCTION" command. After calculating the coefficients, goodness of fit estimates are also calculated and can be displayed with the "SHOW FUNCTION" command.

KEYWORDS

| NEXT | CHAR(20) | X-Y data set name |
| COEFFICIENTS-NAME | CHAR(20) | function name |
| FORM | CHAR(15) | function form |

EXAMPLE

RLS>FIT CURVE COEFFICIENT X-Y.NAME FN2 FORM Y=A*X^B

*/
/*
COMMAND

SHOW STATISTICS

ACTION

This command estimates the goodness of fit for a function with respect to an X-Y data set. The function name and FORM are specified and the data set name is specified.

KEYWORDS

COEFFICIENT_NAME CHAR(20) function name
FORM CHAR(15) function form
X-Y_NAME CHAR(20) X-Y data set name
OUTPUT-FILE CHAR(20) output file name
FULL LOGICAL yes for full listing

EXAMPLE

RLS>SHOW STATISTICS COEFFICIENT FN1 FORM Y=1(A+B*X)

*/
SHOW FUNCTIONS

ACTION

This command produces a listing of the current functions. The listing is written to an output device or file which is usually the terminal from which the command is issued.

The command "SHOW FUNCTIONS" with no qualifying keywords will produce a 'directory' style listing of the functions. If a function name is specified as in:

RLS>SHOW FUNCTION COEFFICIENT FN1

then specific information on the named function will be displayed. This detailed information includes all of the function coefficients. Since a function may have several forms, the FORM may also specified to limit the listing to a single version.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>DATA TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>COEFFICIENT.NAME</td>
<td>CHAR(20)</td>
<td>function name</td>
</tr>
<tr>
<td>FORM</td>
<td>CHAR(15)</td>
<td>function form</td>
</tr>
<tr>
<td>OUTPUT-FILE</td>
<td>CHAR(40)</td>
<td>output file name</td>
</tr>
</tbody>
</table>

EXAMPLE

RLS>SHOW FUNCTIONS

<table>
<thead>
<tr>
<th>LINE</th>
<th>FUNCTION</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FN1</td>
<td>y=a*x</td>
<td>&quot;test line&quot;</td>
</tr>
<tr>
<td>2</td>
<td>FN2</td>
<td>y=a+b/x</td>
<td>&quot;non-linear fit&quot;</td>
</tr>
<tr>
<td>3</td>
<td>CURVE</td>
<td>y=a<em>exp(b</em>x)</td>
<td>&quot;exponential curve&quot;</td>
</tr>
</tbody>
</table>

RLS>SHOW FUNCTION COEFFICIENT FN2

<table>
<thead>
<tr>
<th>LINE</th>
<th>FUNCTION</th>
<th>FORM</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FN2</td>
<td>y=a+b/x</td>
<td>&quot;non-linear fit&quot;</td>
</tr>
</tbody>
</table>

LINE                        COEFFICIENT

<table>
<thead>
<tr>
<th>LINE</th>
<th>COEFFICIENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>2.3</td>
</tr>
</tbody>
</table>

*/
CHAPTER 8
DATA ENTRY

These commands handle the manual entry and the maintenance of x-y data sets. The following commands are available:

<table>
<thead>
<tr>
<th>VERB</th>
<th>OBJECT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADD</td>
<td>DATASET</td>
<td>enter an x-y data set</td>
</tr>
<tr>
<td>CHANGE</td>
<td>DATASET</td>
<td>change an x-y data set</td>
</tr>
<tr>
<td>DELETE</td>
<td>DATASET</td>
<td>delete an x-y data set</td>
</tr>
<tr>
<td>SHOW</td>
<td>DATASET</td>
<td>display an x-y data set</td>
</tr>
</tbody>
</table>

8.1 DISPLAYING X-Y DATA SETS

The current collection of x-y data sets is displayed with the "SHOW DATASET" commands as follows:

RLS>SHOW DATASET

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>lab1</td>
<td>&quot;lab set #1&quot;</td>
</tr>
<tr>
<td>2</td>
<td>lab2</td>
<td>&quot;lab set #2&quot;</td>
</tr>
<tr>
<td>3</td>
<td>xytest</td>
<td>&quot;xy test data&quot;</td>
</tr>
</tbody>
</table>

RLS>

Detailed information on a specific data set can be obtained by using the keyword DATA on the "SHOW" command:

RLS>SHOW DATASET X-Y.NAME XYTEST

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
</table>

8.2 DELETING X-Y DATA SETS

An X-Y data set that appears in the current list can be deleted with the "DELETE DATASET" command. For example:

RLS>SHOW DATASET

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>lab1</td>
<td>&quot;lab set #1&quot;</td>
</tr>
<tr>
<td>2</td>
<td>lab2</td>
<td>&quot;lab set #2&quot;</td>
</tr>
<tr>
<td>3</td>
<td>xytest</td>
<td>&quot;xy test data&quot;</td>
</tr>
</tbody>
</table>

RLS>DELETE DATASET X-Y.NAME LAB2
RLS>SHOW DATASET

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>lab1</td>
<td>&quot;lab set #1&quot;</td>
</tr>
<tr>
<td>2</td>
<td>xytest</td>
<td>&quot;xy test data&quot;</td>
</tr>
</tbody>
</table>

8.3 ENTERING A NEW X-Y DATA SET

A new X-Y data set can be entered with the command "ADD DATASET". You will be prompted for information related to the data and for all of the X-Y points. Enter a <return> character with no data to terminate the x-y data entry. For example:

RLS>ADD DATASET X-Y.NAME STD1
description "" :sample standard
The above sequence appears with the "SHOW DATASET" command as:

```
RLS> SHOW DATASET X-Y.NAME STD1

LINE  DATA  DESCRIPTION
1    STD1  "sample standard"

LINE  NROWS  NCOLS
1      4      2

LINE  "amount injected"  "detector response"
     "volts"        "ppm"
1     10         2.453e-01
2     20         5.321e-01
3     40         1.921e+00
```

8.4 CHANGING AN X-Y DATA SET

An existing data set can be modified by using the "CHANGE DATASET" command. The command will prompt for a new value for each of the fields in the data set. For each value it will print out the current value which will be retained if you enter simply a <return> to the prompt. If you want to change the current value then enter the value followed by a <return>. For example, to change the units in the above example and to change the "amount injected" for item # 2 to 30 ppm:

```
RLS> CHANGE DATASET X-Y.NAME STD1

name     std1 : 
description  "sample standard" : 
```
8.5 COMMAND DEFINITIONS
/*
COMAND

ADD DATASET

ACTION

This routine interacts with a user to build an x-y data set. The command will
prompt for a DESCRIPTION, XLABEL, XUNITS, YLABEL
and YUNITS for the data. The values of X and Y
will then be prompted for in sequence. The data
entry is terminated by entering a <return> to
an X prompt.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-Y.NAME</td>
<td>CHAR(20)</td>
<td>x-y data set name</td>
</tr>
</tbody>
</table>

EXAMPLE

RLS>ADD DATASET X-Y.NAME TEST
  enter description       "" : test data
  enter xlabel            "" : 
  enter xunits            "" : 
  enter ylabel            "" : 
  enter yunits            "" : 
  enter x(1)              : 1.
  enter y(1)              : 3.4
  enter x(2)              : 2.
  enter y(2)              : 5.2
  enter x(3)              :

*/
/*
COMMAND

CHANGE DATASET

ACTION

This routine interacts with a user to change an x-y data set. The command will prompt for a DESCRIPTION, XLABEL, XUNITS, YLABEL and YUNITS for the data. The values of X and Y will then be prompted for in sequence. The data entry is terminated by entering a <return> to an X prompt.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-Y.NAME</td>
<td>CHAR(20)</td>
<td>x-y data set name</td>
</tr>
</tbody>
</table>

EXAMPLE

```
RLS> CHANGE DATASET X-Y.NAME WESTWOOD
enter description "" : 
enter xlabel "" : 
enter xunits "" : 
enter ylabel "" : 
enter yunits "" : 
enter x(1) 1. : 
enter y(1) 3.4 : 
enter x(2) 2. : 
enter y(2) 5.2 : 
enter x(3) : 
```
/*
NAME

DELETE DATASET

ACTION

This command deletes X-Y data sets from the current list.
All information on data set XY-NAME is removed.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-Y.NAME</td>
<td>CHAR(20)</td>
<td>X-Y data set name</td>
</tr>
</tbody>
</table>

EXAMPLE

To delete an x-y data set:

RLS>SHOW DATASET

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>test</td>
<td>&quot;lab data&quot;</td>
</tr>
<tr>
<td>2</td>
<td>xydata</td>
<td>&quot;bitumen sample&quot;</td>
</tr>
</tbody>
</table>

RLS>DELETE DATASET X-Y.NAME TEST
RLS>SHOW DATASET

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>xydata</td>
<td>&quot;bitumen sample&quot;</td>
</tr>
</tbody>
</table>

*/
SHOW DATASET

ACTION

This command produces a listing of the current X-Y data sets. The listing is written to an output device or file which is usually the terminal from which the command is issued.

The command "SHOW X-Y" with no qualifying keywords will produce a 'directory' style listing of the data sets. If the keyword X-Y.NAME is specified as in:

RLS>SHOW DATASET X-Y.NAME XY1

then specific information on the named data set will be displayed.

KEYWORDS

<table>
<thead>
<tr>
<th>KEYWORD</th>
<th>TYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-Y.NAME</td>
<td>CHAR(20)</td>
<td>X-Y data set name</td>
</tr>
<tr>
<td>OUTPUT-FILE</td>
<td>CHAR(40)</td>
<td>output file name</td>
</tr>
</tbody>
</table>

EXAMPLE

To obtain the directory listing of data sets:

RLS>SHOW DATASET

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>test1</td>
<td>&quot;lab data #1&quot;</td>
</tr>
<tr>
<td>2</td>
<td>test2</td>
<td>&quot;bitumen sample&quot;</td>
</tr>
</tbody>
</table>

RLS>SHOW DATASET X-Y.NAME TEST2

<table>
<thead>
<tr>
<th>LINE</th>
<th>DATA</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>test2</td>
<td>&quot;lab data #1&quot;</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LINE</th>
<th>X</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>3.5</td>
</tr>
<tr>
<td>2</td>
<td>2.0</td>
<td>7.9</td>
</tr>
<tr>
<td>3</td>
<td>3.0</td>
<td>5.2</td>
</tr>
<tr>
<td>4</td>
<td>4.0</td>
<td>9.2</td>
</tr>
</tbody>
</table>

*/
CHAPTER 9
SYSTEM NOTES

This chapter presents system information necessary for using and/or maintaining the RLS system.

9.1 ADDING A NEW USER

9.1.1 VAX/VMS

The login file, LOGIN.COM, should contain the following symbol definition:

RLS:==@USERS:[RLS]RLS

9.1.2 PDP-11/RSX

No special operations are required — the program is installed by system operations staff.

9.2 FILES

As you use the RLS system data files will be entered into your disk area to maintain RLS information. It is important that you not delete files with the names *.PLT and *.RLS since these are used by the system to maintain your data.

9.3 SYSTEM DIFFERENCES
9.3.1 Host Computer Commands

On RSX systems if RLS does not recognize a command then it will pass the command through to the host computer command interpreter (MCR). This feature is not currently implemented in the VMS version of RLS.