Real-time Laboratory System (RLS)

Vol 1:   User Guide

Lorne Bechtel*

Chemistry Department
Alberta Research Council
11315-87 Ave.
Edmonton, Alberta
T6G 2C2

July, 1984

Alberta Research Council Open File Report

* Current Address:
3200 NW 179 Ave.
Portland, OR
USA, 97229

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 developm t, or development of private systems, since no command de inirions 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

```
keyword         default         description

signal-file     ch7.dat         "signal file name"
peak-file       peak.dat        "output peak file"
gate            2               "change counter"
slope           .01             "slope sensitivity"
density         2               "number of points"
width           3.              "peak width"
frequency       1.              "sampling frequency"
```

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             lparda.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'                                    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   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'   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. example, a chromatograph analysis can be placed into a 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                                    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   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   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:

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

    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-11 device. Additional signal filtering
may also be included as necessary although for most
applications the filtering available from the instrument and
the LPA-11 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.

VERB	OBJECT	DESCRIPTION
MONITOR	ANALOG	monitor analog start/stop switch
SHOW	ANALOG	show current analog sampling status

```
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.
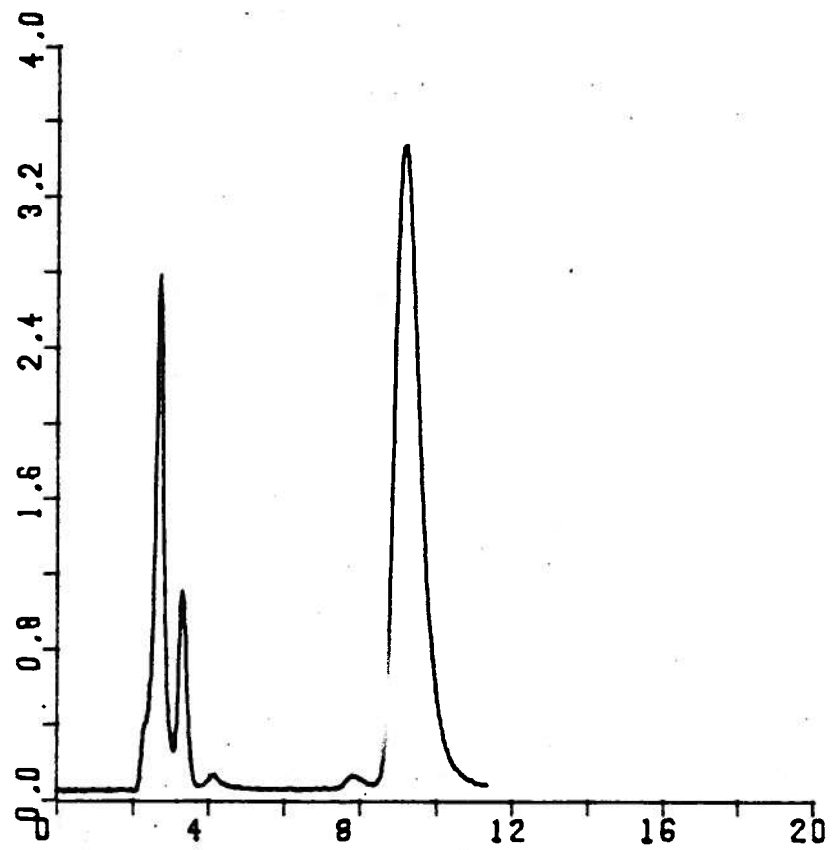
Figure 4.2 Signal from Data Collection

VERB	OBJECT	DESCRIPTION
PULSE	DIGITAL	pulse a digital output point
READ	DIGITAL	read a digital input point
WAIT	DIGITAL	wait for digital input
WRITE	DIGITAL	write a digital output point

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
>   FRQUENCY 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

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

>   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
       FRQUENCY 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   r format.

KEYWORDS

    DURATION   CHAR   du ation 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
*/

/*
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

KEYWORD	TYPE	DESCRIPTION
PROMPT	string	prompt to terminal operator
REPLY	string	valid reply
DEFAULT	string	default value for the reply

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
```

```
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:

VERB	OBJECT	DESCRIPTION
ZERO	BASELINE	correct the peak baselines
FIND	CHN-PEAKS	find peaks in CHN signal file
ANALYZE	PEAKS	identify and normalize peaks
FIND	PEAKS	find peaks in a signal file
PREPARE	REPORT	prepare a chromatograph report
ADD	STANDARD ,	add a new calibration data set
CHANGE	STANDARD	change a calibration data set
DELETE	STANDARD	delete a calibration data set
ENTER	STANDARD	automatic entry of a new calibration data set
SHOW	STANDARDS	display calibration data set information
UPDATE	STANDARDS	automatic update of a calibration data set
ADD	TICS	add peak tic marks to a chromatograph plot

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
```

RT	%	AREA	HEIGHT	ITM	FACTOR	NAME
2.700e+00	0.000e+00	7.638e-01	2.558e+00	bb	0.000e+00	
3.300e+00	0.000e+00	2.183e-01	9.012e-01	bb	0.000e+00	
4.083e+00	0.000e+00	1.985e-02	5.878e-02	bb	0.000e+00	
7.767e+00	0.000e+00	3.431e-02	6.925e-02	bv	0.000e+00	
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 "%" for a peak to be used as an
internal standard for amount normalization.

4. RE ENCE AND STANDARD

En   "&" for a peak that is both a
re   ence 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 (ie. 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
ca ibrations through the point (0.,0.) are the
on y exception. For these the command will
accept a sinle 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 it's 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
propmt 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
        rls>
        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

LINE #	CALIBRATION NAME	METHOD	USING	UNITS	DESCRIPTION
1	standards3	estd	heights	ppm	"calibration curves for f,cl,po4,no3,so4 at 3 umhos"

LINE #	PEAK NAME	RET. TIME	POLY. ORDER	X**3	X**2	X**1	X**0
1	fluoride	# 2.3	1	0.	0.	1.562e-01	1.811e-02
2	chloride	3.4e+00	1	0.000e+00	0.000e+00	3.011e-01	-5.934e-02
3	nitrate	7.967e+00	1	0.000e+00	0.000e+00	1.319e+00	-1.335e-01
4	sulfate	1.047e+01	1	0.000e+00	0.000e+00	1.091e+00	1.231e-02

LINE #	PEAK NAME	AMOUNT	SIZE	EST. FACTOR
1	chloride	.1	5.955e-01	1.679e-01
2	chloride	1.5	5.430e+00	2.762e-01
3	chloride	.5	1.585e+00	3.155e-01
4	chloride	1	3.760e+00	2.660e-01
5	chloride	2	6.551e+00	3.053e-01
6	fluoride	1	4.832e-01	2.070e-01
7	fluoride	.7	4.037e+00	1.734e-01
8	fluoride	1.2	7.512e+00	1.597e-01
9	fluoride	.5	3.405e+00	1.468e-01
10	fluoride	1	6.391e+00	1.565e-01
11	nitrate	.5	5.327e-01	9.386e-01
12	nitrate	1	8.333e-01	1.199e+00
13	nitrate	2	1.668e+00	1.199e+00
14	nitrate	5	4.119e+00	1.214e+00
15	nitrate	7	5.315e+00	1.317e+00
16	sulfate	.5	3.856e-01	1.297e+00
17	sulfate	1	9.766e-01	1.024e+00
18	sulfate	2	1.321e+00	1.098e+00
19	sulfate	5	4.562e+00	1.096e+00

Figure 5.3 Example of Calibration Listing

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 Maintaining Calibration Curves

5.5.3.1 Automatic Calculation Of Coefficients -

The coefficients for the polynomial curves fitting the calibration points can be entered manually using the commands described above. However, there is a command available for automatic calculation of the coefficients. By entering the command:

UPDATE STANDARD CALIB x

you will invoke a program that will find the coefficients for the polynomial best approximating the calibration curve points using the method of least squares. Any current coefficients maintained in the calibration data will be replaced with the new coefficients.

5.5.3.2 Automatic Entry Of Peak Information -

Some of the calibration information can be entered (semi)automatically. Exact peak retention times, amounts and areas/heights can be entered by the command "ENTER STANDARD" after defining the calibration method and each peak in the file. For example, to enter the points from a peak file named 'PEAK.DAT':

ENTER STANDARD CALIB LABSTD PEAK-FILE PEAK.DAT

For each unidentified peak in the file you will be prompted to enter the name of the peak and the amount injected. The peak retention time will be replaced with that in the peak file and the amount and area/height will be inserted into the calibration data set. The calibration curve coefficients will then be calculated for the new point.

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 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
```
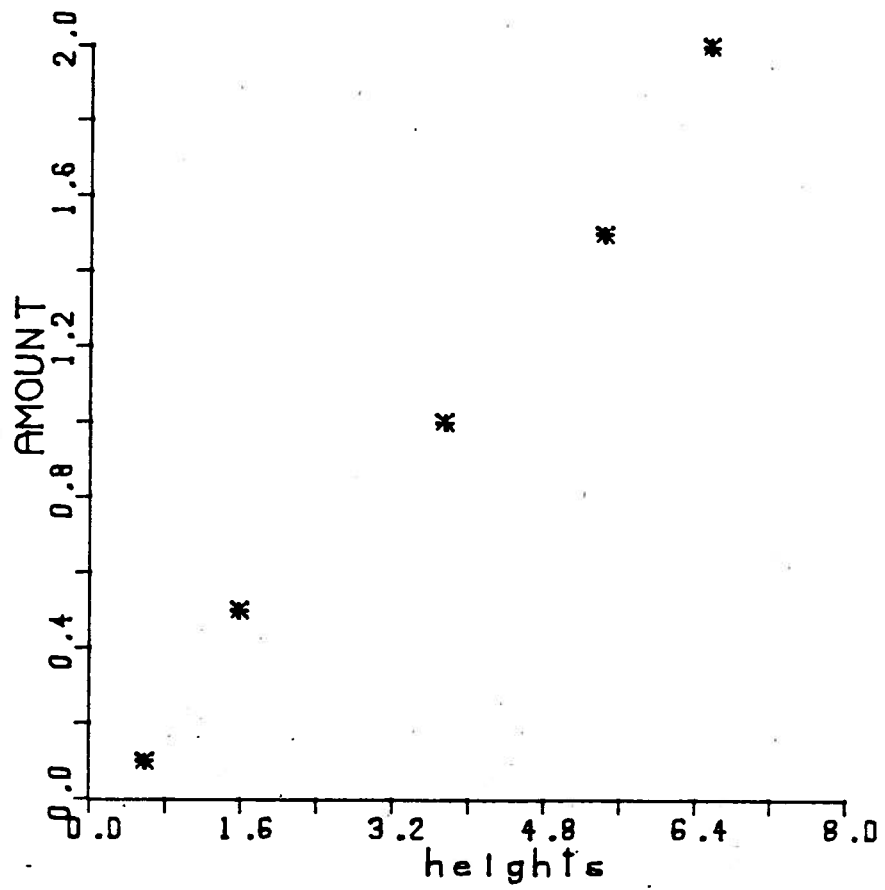
Figure 5.4 Plot of Calibration Curve

where the above sequence:

    1. puts the calibration points in X-Y data
       set CHLOR

    2. calculates the best fit 2nd order
       polynomial coefficents

    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
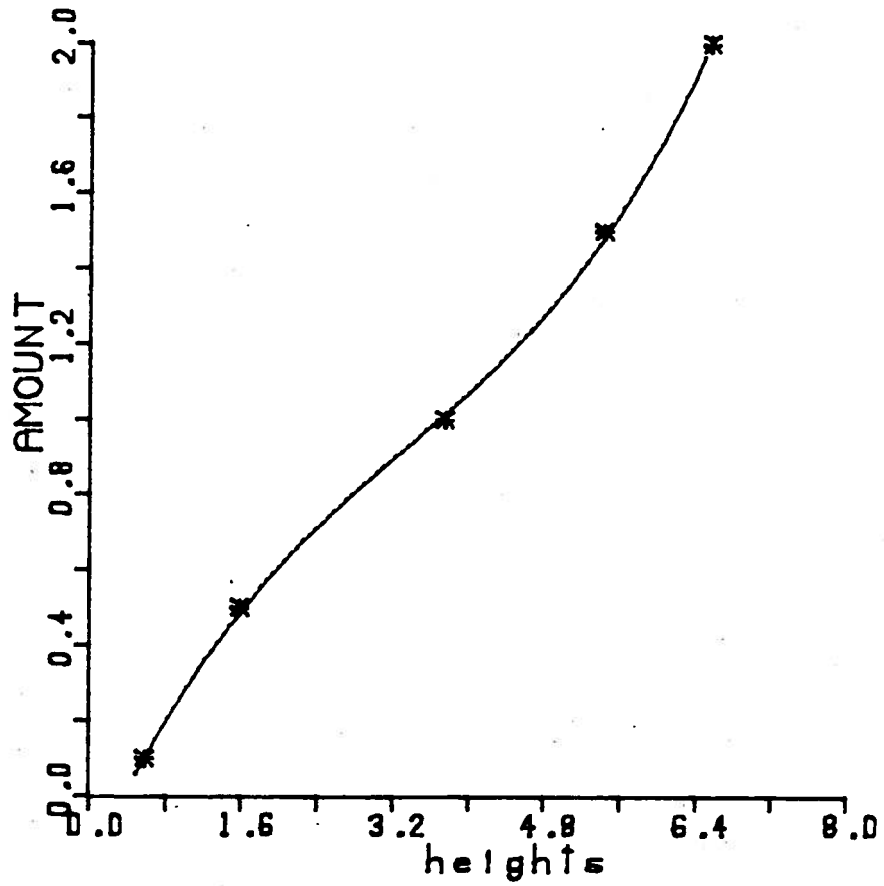
Figure 5.5 Calibration Curve Fit

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:

$$AMOUNT = c_3 * (size^{**}3) + c_2 * (size^{**}2) + c_1 * size + c_0$$

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):

   $$C = SIZE \times DIL\text{-}FTR \times 100. / TOTAL\text{-}SIZE$$

2. NORM

   a percentage of the total area normalized using the calibration curve coefficients:

   $$C = AMOUNT \times DIL\text{-}FTR \times 100. / TOTAL\text{-}AMOUNT$$

3. ESTD

   the concentration is reported in the units defined in the calibration data:

   $$C = AMOUNT \times DIL\text{-}FTR$$

4. ISTD

   the concentration is corrected by an internal standard and reported as:

   $$C = AMOUNT \times (STD\text{-}AMT / CALC\text{-}STD) \times DIL\text{-}FTR / SMP\text{-}AMT$$

   where STD-AMT = amount of standard injected
          CALC-STD = calculated amount of the standard
          SMP-AMT = 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

```
CHANNEL              7
METHOD               estd
INJECTED AT          22-MAR-83 09:51:58

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

REF-RTW              5.000e-01
ID-LVL               0.000e+00
%RTW                 1.000e+01
RF-UNK               1.000e+00
DVT                  0.000e+00
DIL-FTR              1.000e+00
```

RT	ppm	AREA	HEIGHT		ITH	FACTOR	NAME
2.350e+00	4.118e-02	4.352e-02	1.477e-01	bb	2.350e+00	2.788e-01	# fluoride
3.567e+00	2.925e+00	4.567e+00	9.912e+00	bb	3.474e+00	2.951e-01	chloride
7.400e+00	6.433e+00	4.095e+00	5.020e+00	bv	8.140e+00	1.231e+00	nitrate
9.433e+00	5.125e+00	4.325e+00	5.125e+00	vb		1.000e+00	

```
              ----------  ----------  ----------
TOTALS        1.452e+01   1.303e+01   2.020e+01
```

Figure 5.6   Chromatograph Report with Identified Peaks and Normalized Amounts

```
c  COMMAND
c
c          ZERO BASELINE
c
c  ACTION
c
c          This command corrects the areas in a chromatograph
c          peak information file by subtracting from each peak area the
c          portion of the peak area contributed by the baseline offset
c          from zero reference. The area subtracted is that defined
c          by the leading and trailing point of the peak, or for groups
c          of peaks, that area defined by the lead point of the first
c          peak and the trail point of the last peak.
c
c  KEYWORDS
c
c          KEYWORD          TYPE              DESCRIPTION
c
c          PEAK-FILE        CHAR(40)          peak information file name
c
c  EXAMPLE
c
c          ZERO BASELINE PEAK-FILE PEAK.DAT
```

```
/*
COMMAND

        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
STEPSIZE	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 prevously 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 unkowns
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

*/

```
c COMMAND
c
c        FIND PEAKS
C
c ACTION
c
c        This command scans a signal file for the presence of
c        chromatograph peaks. Results are output to a peak information
c        file containing information such as retention times, peak area,
c        etc. The signal is assumed to be represented as equidistant
c        y values as obtained from a sampling program at a specific
c        FREQUENCY. The signal data is smoothed using piecewise
c        averaging of DENSITY number of points. Peaks are detected
c        by a signal change greater than a specified SLOPE.
c        The slope must persistently exceed this slope by more than
c        GATE threshold number of sampling points. Peaks are ended
c        on baseline at a distance of at least (WIDTH * half width)
c        past the peak crest. For gaussian peaks half width at half
c        height is roughly equivalent to the standard deviation so this
c        WIDTH would normally be 3.0 in order to capture 99.7% of the area.
c        FREQUENCY is normally set by the analog sampling program.
c
c KEYWORDS
c
c        SIGNAL-FILE     CHAR(40)        input signal data file
c        PEAK-FILE       CHAR(40)        output peak information file
c        GATE            INTEGER         persistent change threshold
c        SLOPE           REAL            slope sensitivity
c        DENSITY         INTEGER         number of points to average
c        WIDTH           REAL            peak termination width
c        FREQUENCY       REAL            sampling frequency of the signal
c
c EXAMPLES
c
c        FIND PEAKS SIGNAL-FILE CH10.DAT
c        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
SMP-AMT	float	amount of sample injected
misc...	.....	several parameters set by computer

EXAMPLE

> PREPARE REPORT FORMAT MEDIUM
> PREPARE REPORT TITLE "bitumen analysis"

```
*/
```

```
/*
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 yyyy
        3. ADD STANDARD CALIBRATION.NAME xxxx PEAK yyyy 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 yyyy 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

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

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               :
x**3                    0               :
x**2                    0               :
x**1                    0               :
x**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 yyyy
        3. DELETE STANDARD CALIBRATION.NAME xxxx PEAK yyyy AMOUNT zzzz

KEYWORDS

KEYWORD	TYPE	DESCRIPTION
CALIBRATION.NAME	CHAR(20)	calibration name
PEAK	CHAR(20)	peak name
AMOUNT	REAL	peak amount

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   :chloride
      amount   0.   :10.
      PEAK # 2 RETENTION TIME = 0.5900e+01 HEIGHT = 0.3212E+04
      name   :fluoride
      amount   0.   :120.

      RLS>
*/

```
/*
```
NAME

      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   CHAR(20)   x-y data set
      CALIBRATION.NAME   CHAR(20)   calibration name
      PEAK   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

LINE	CALIBRATION	METHOD	USING	UNITS	DESCRIPTION
1	oil.sands	estd	heights	%	"bitumen sample"
2	lab_sample#1	norm	areas	ppm	"standard lab sample"

      RLS>SHOW STANDARD CALIBRATION.NAME LAB_SAMPLE#1

LINE	CALIBRATION	METHOD	USING	UNITS	DESCRIPTION
1	lab_sample#1	norm	areas	ppm	"standard lab sample"

LINE	PEAK	TYPE	RET-TIME	POLY.ORDER	X**3	X**2	X**1	X**0
1	fluoride	#	5.4	2	0.0	2.3	1.4	4.2
2	chloride	#	8.9	1	0.0	0.0	2.0	3.0

LINE	PEAK	AMOUNT	SIZE	EST-RF
1	chloride	10.	3921	.034
2	chloride	100.	4023	.526
3	fluoride	200.	2401	.193
4	fluoride	220.	2491	.345

```
       5        fluoride        230.    3421    .391
       6        fluoride        240.    4092    .419

       RLS>
*/
```

```
/*
NAME
```

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
an 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

        KEYWORD   TYPE   DESCRIPTION

        PEAK-FILE   CHAR(40)   peak information file name
        GRAPH.NAME   CHAR(20)   plot descriptor file name

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

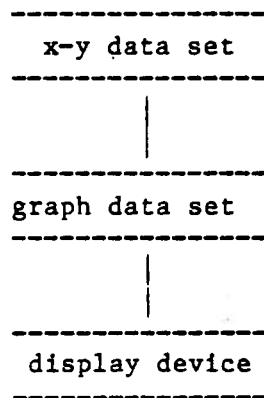The output devices that are supported for the x-y plots include:

    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:

VERB	OJBECT	DESCRIPTION
DELETE	PLOT	delete a graph
PREPARE	PLOT	format a graph
SEND	PLOT	display an x-y graph on a terminal or send it to a plotter
SHOW	PLOTS	display information on graphs

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

LINE	GRAPH.NAME	DESCRIPTION
1	picture1	"figure 1 - calibration curve"
2	signal	"figure 2 - chromatograph signal"

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

LINE	GRAPH.NAME	DESCRIPTION
1	picture1	"figure 1 - calibration curve"

LINE #	XMIN	XMAX	YMIN	YMAX	LEGEND
1	10.0	100.0	-30.0	200.	2

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

LINE   GRAPH.NAME   DESCRIPTION

 1   signal   "figure 2 — chromatograph signal"

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

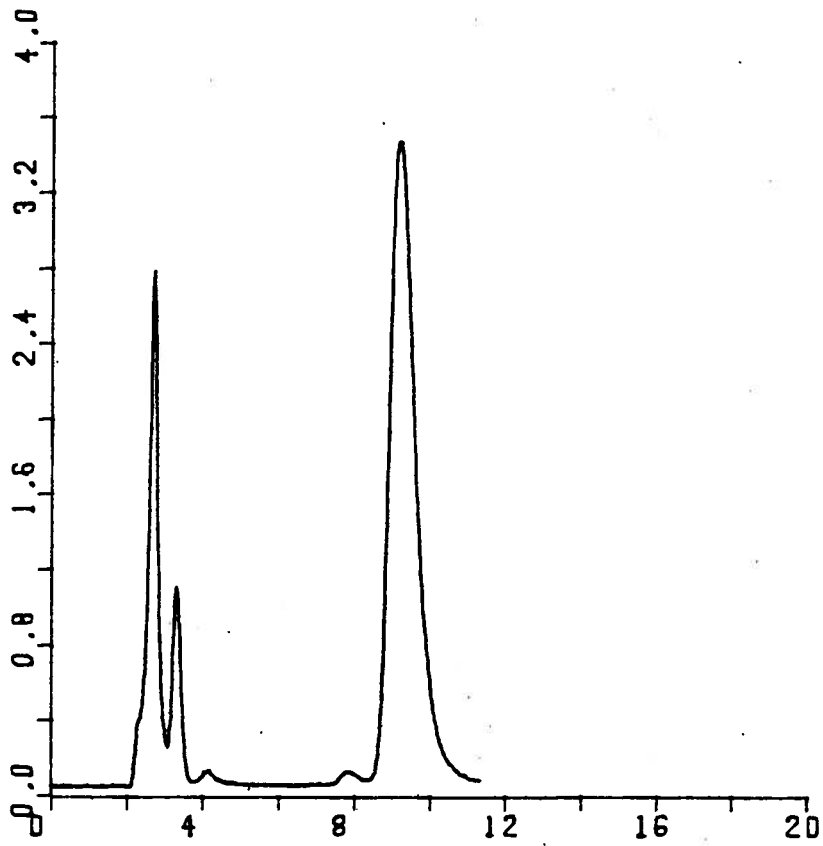In this form the graph will appear as in Figure 6.2.

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
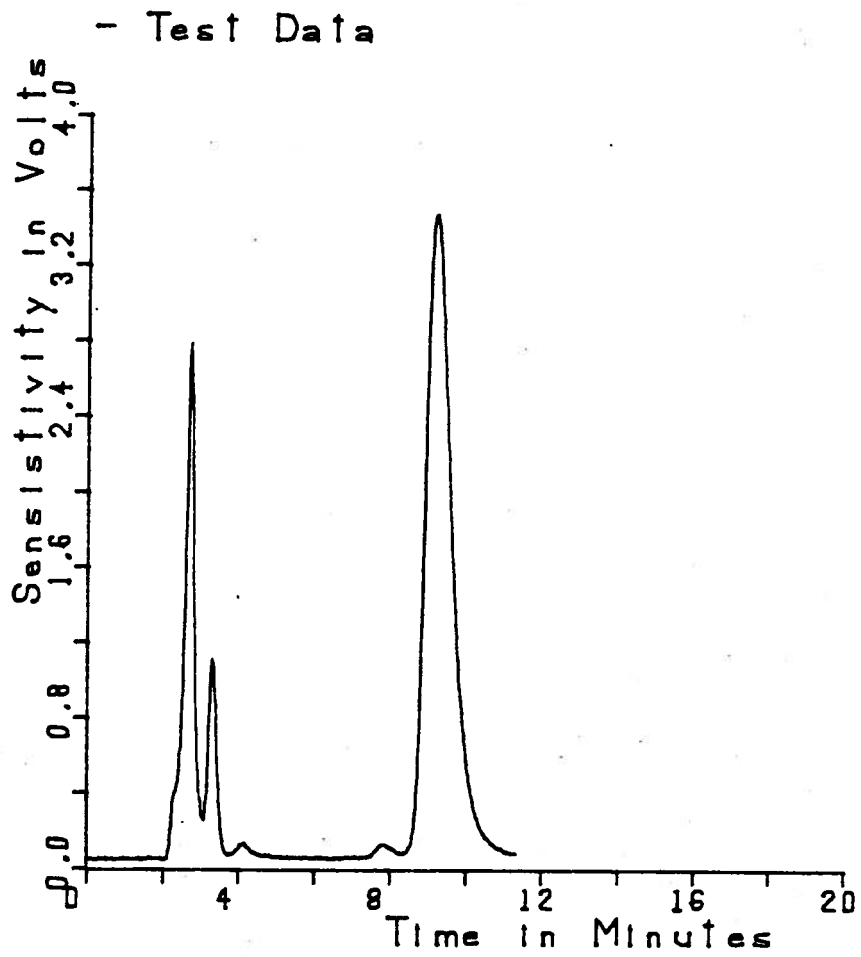
- Test Data

Fig. 3 - Annotated Plot

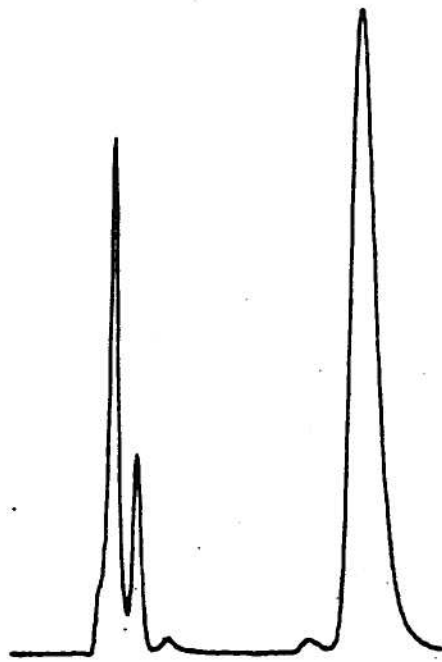Figure 6.3 Graph with Annotation

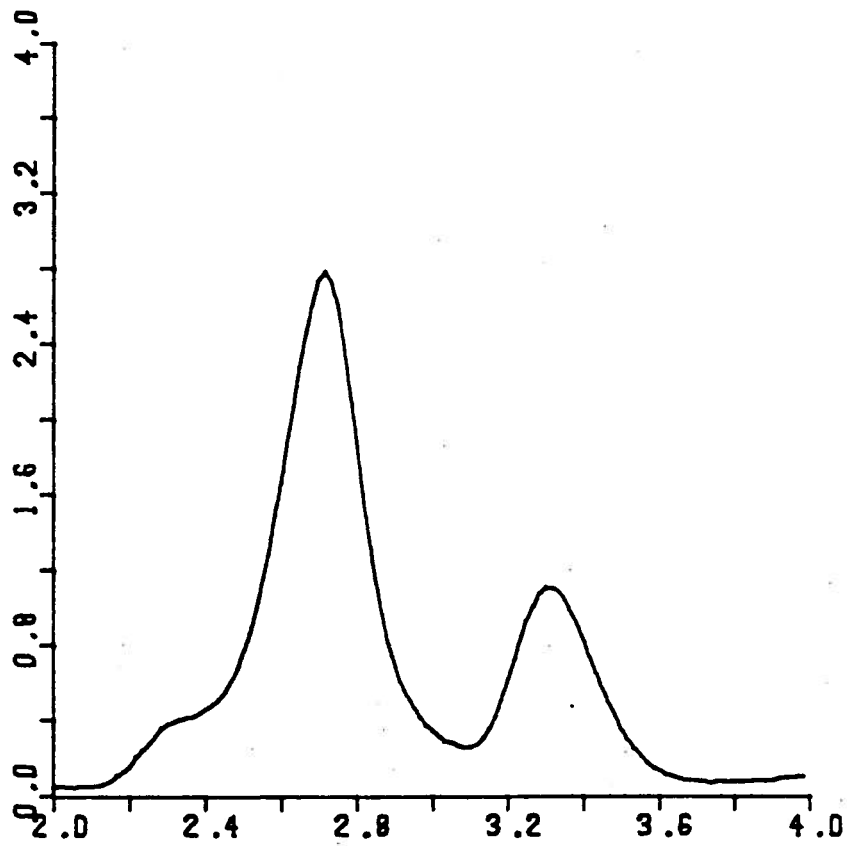Figure 6.4   Graph without Axis

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:
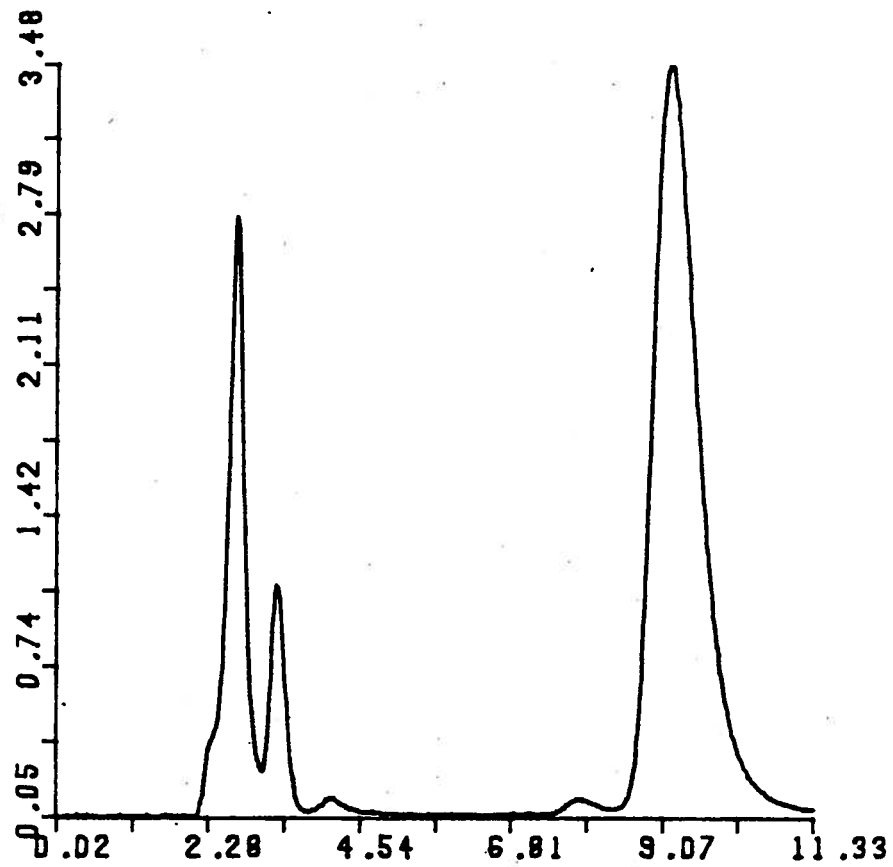
Fig. 5 - Exact Axis Scaling

Figure 6.6   Graph with Exact Axis Scaling

Fig 7. - Plotting Symbols

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
```
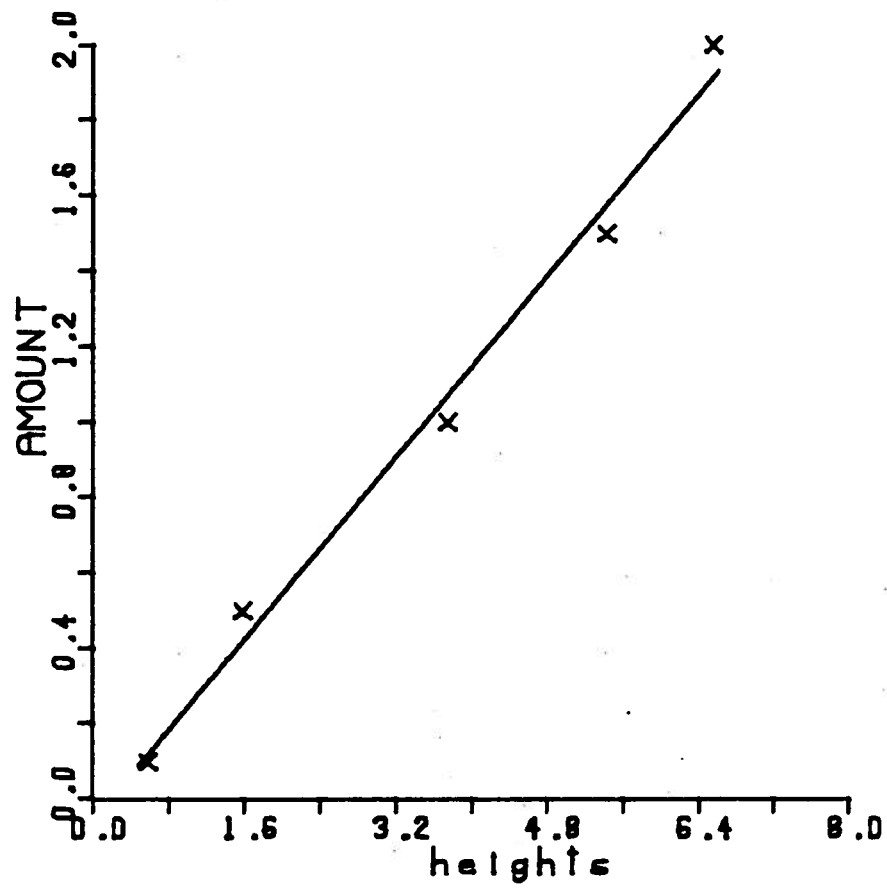
Fig. 9 — Data and Curve Fitting Overlay

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

        KEYWORD   TYPE   DESCRIPTION

        GRAPH.NAME   CHAR(20)   graph name

EXAMPLE

        To delete a plot:

        RLS>SHOW PLOTS

        LINE   GRAPH.NAME   DESCRIPTION

          1   picture1   "figure 1 - lab data"
          2   picture2   "bitumen sample"
          3   test   "curve fit data"

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

        LINE   GRAPH.NAME   DESCRIPTION

          1   picture1   "figure 1 - lab data"
          3   test   "curve fit data"

        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 specifiying an arbitrary scale FACTOR.

KEYWORDS

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

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   MBOL 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:

        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

        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

        GRAPH.NAME     CHAR(20)        graph data set name
        DEVICE         CHAR(10)        output device name
        FACTOR         REAL            scaling factor

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
*/
```

```
/*
NAME

        SHOW PLOTS

ACTION

        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

        LINE    GRAPH.NAME      DESCRIPTION

          1     picture1        "figure 1 - lab data #1"
          2     picture2        "figure 9 - bitumen sample"

        RLS>SHOW PLOTS GRAPH.NAME PICTURE1

        LINE    GRAPH.NAME      DESCRIPTION

        1       picture1        "figure 1 - lab data #1"

        LINE      XMIN      XMAX      YMIN      YMAX

        1       0.000e+00  1.000e+01  0.000e+00  2.000e+03

*/
```

/*
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

        KEYWORD   TYPE   DESCRIPTION

        INPUT-FILE   CHAR(40)   input file name
        GRAPH.NAME   CHAR(20)   plot descriptor name
        HEIGHT   REAL   character height in cm
        PEN   INTEGER   pen number

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:

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

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

LINE	NAME	FORM	DESCRIPTION
1	fn1	y=a+b*x	"linear fit"
2	fn1	y=a+b/x	"non-linear fit"
3	calib	y=a*x^b	"calibration curve fit"

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

LINE	NAME	FORM	DESCRIPTION
1	fn1	y=a+b/x	"non-linear fit"

LINE	COEFFICIENT
1	1.
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

LINE	NAME	FORM	DESCRIPTION

```
1        fn1               y=a+b*x "linear fit"
3        calib             y=a*x^b "calibration curve fit"

RLS>
```

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:

```
    FORM                  DESCRIPTION

    N-POLYNOMIAL      general polynomial of order N
    Y=A*X             straight line through (0,0)
    Y=A+B*X           straight line
    Y=A*EXP(B*X)      exponential curve
    Y=1/(A+B*X)
    Y=A+B/X
    Y=A+B*LOG(X)      log base 10 curve
    Y=A*X^B           power curve
    Y=X/(A+B*X)
    Y=A+B*LN(X)       natural logarithm
    Y=A*B^X           power curve
```

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

LINE	DATA	DESCRIPTION
1	WESTWOOD	"Westwood Company"

LINE	"Lot Size" "units"	"Labour" "man-hours"
1	30	73
2	20	50
3	60	128
4	80	170
5	40	87
6	50	108
7	60	135
8	30	69
9	70	148
10	60	132

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 ·   1.00000e+01
2   2.00000e+00

RLS>

The coefficients in the above list are displayed in the order of increasing signficance. For the function forms that are specified in the format 'Y=' the A coefficient is listed first and the B coefficient is second. ie. 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.
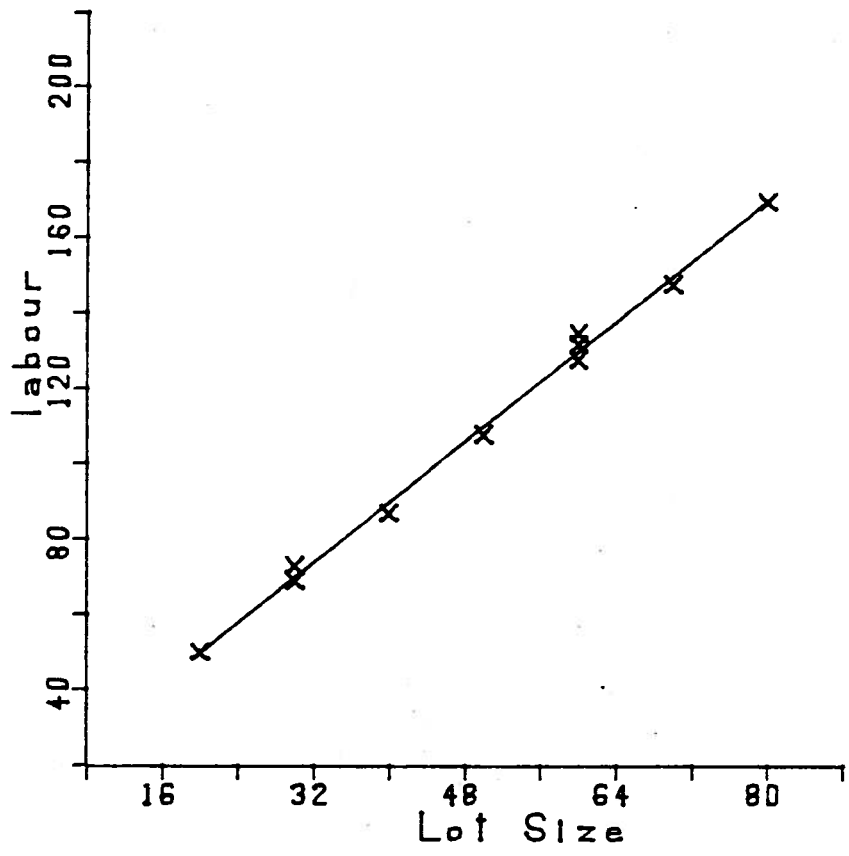
Figure 7.1 Data with Fitted Curve

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

   1 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 ALPHA the F-VALUE should be compared to the F statistic from a table such that if:

F-VALUE < F(ALHPA;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 devications
     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:

     $r(i,j) = cov(i,j) / sqrt(var(i)*var(j))$

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-VALUE = COEFFICIENT(i) / 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:

     ABS(T-VALUE) < T(1-ALHPA/2;DF.RES) then conclude C1
     ABS(T-VALUE) > T(1-ALPHA/2;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*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:

"Applied Linear Statistical Models", J.Neter and W.Wasserman,
      Richard D. Irwin, Inc., 1974.

"Numerical Methods", G.Dahlquist and A.Bjorck,
      Prentice-Hall, N.J., 1974.

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          FUNCTION      FUNCTION
 #   SET           NAME          FORM

   1 westwood      westwood      1-polynomial
```

VARIABLES

VARIABLE	MEAN	VARIANCE	ST.DEV
X	5.00000e+01	3.40000e+03	5.83095e+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 COEFF.	LINEARIZED COEFF.	ST.ERROR	T-VALUE
1	1.00000e+01	1.00000e+01	2.50294e+00	3.99530e+00
2	2.00000e+00	2.00000e+00	4.69668e-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             9.95608e-01
```

COVARIANCE MATRIX

```
 6.26471e+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	1.08000e+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+
                Figure                    s Report
```

```
Y=A*X                no transformation

Y=A+B*X              no transformation

Y=A*EXP(B*X)         take the natural logarithm of both
                     sides of the equation:
                     LN(Y)=LN(A)+B*X, Y > 0
                     Y'=A'+B*X
                     A=EXP(A')

Y=1/(A+B*X)          take the inverse of Y
                     1/Y=A+B*X, Y > 0
                     Y'=A+B*X

Y=A+B/X              take the inverse of X
                     Y=A+B*(1/X), X > 0
                     Y=A+B*X'

Y=A+B*LOG(X)         take the logarithm base 10 of X
                     Y=A+B*LOG(X), X > 0
                     Y=A+B*X'

Y=A+X^B              take the natural logarithm of both sides
                     of the equation
                     LN(Y)=LN(A)+B*LN(X), X,Y > 0
                     LN(Y)=A'+B*LN(X)
                     A=EXP(A')

Y=X/(A+B*X)          take inverse of X and Y
                     1/Y=A/X+B, X,Y > 0

Y=A+B*LN(X)          take the natural logarithm of X
                     Y=A+B*LN(X), X > 0
                     Y=A+B*X'

Y=A*B^X              take the natural logarithm of both sides
                     of the equation
                     LN(Y)=LN(A)+LN(B)*X
                     Y'=A'+B'*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

        KEYWORD                    TYPE              DESCRIPTION

        COEFFICIENT.NAME           CHAR(20)          function name

EXAMPLE

        RLS>ADD FUNCTION COEFFICIENT FN1
        enter FORM                 y=a+b*x           :y=a*exp(b*x)
        enter description          ""                :exponential fit
        enter coefficient #1       0.                :1.
        enter coefficient #2       0.                :2.3
        RLS>SHOW FUNCTION COEFFICIENT FN1

        LINE    FUNCTION        FORM              DESCRIPTION

        1       FN1             y=a*exp(b*x)      exponential fit

        LINE    COEFFICIENT

        1       1.
        2       2.3

        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:

FROM	TO
lpa-11 a/d counts	volts
lps-11 a/d counts	volts
minutes	seconds
seconds	minutes
microvolts	volts
millivolts	volts
volts	lpa-11 a/d counts
volts	lps-11 a/d counts
volts	microvolts
volts	millivolts

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

KEYWORD	DESCRIPTION
LPA-11	lpa-11 a/d counts
LPS-11	lps-11 a/d counts
MICROVOLTS	microvolts
MILLIVOLTS	millivolts
MINUTES	time in minutes
SECONDS	time in seconds
VOLTS	voltage

KEYWORDS

SIGNAL-FILE	file	x-y data file name
NEWX	string	new units for x data
NEWY	string	new units for y data
XUNITS	string	current units for x data
YUNITS	string	current units for y data
STEPSIZE	float	stepsize for equidistant x-y data

EXAMPLE

        If a signal file has been collected from the "SAMPLE ANALOG"
        command with the x axis in units of SECONDS then
        the foll ing 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

LINE	FUNCTION	FORM	DESCRIPTION
1	FN1	y=a*x	"test function"
2	FN1	y=a+b/x	"non-linear fit"
3	FN2	y=a+b*x	"linear fit"

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

LINE	FUNCTION	FORM	DESCRIPTION
1	FN1	y=a*x	"test function"
2	FN2	y=a+b*x	"linear fit"

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

COEFFICIENT.NAME	CHAR(20)	function name
FORM	CHAR(15)	function form
X-Y.NAME	CHAR(20)	name of resulting x-y data set
XMIN	REAL	starting x value
XMAX	REAL	ending x value
NPOINTS	INTEGER	number of points to evaluate

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

COEFFICIENT.NAME	CHAR(20)	function name
FORM	CHAR(15)	function form
X-Y.NAME	CHAR(20)	data set name
RESIDUAL.NAME	CHAR(20)	new X-Y data set
VERSUS	CHAR	X or Y

EXAMPLE

      RLS>GENERATE RESIDUALS COEFFICIENT FN1 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:

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

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

X-Y.NAME	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)   fu   tion name
        FORM   CHAR(15)   f   ion form
        X-Y.NAME   CHAR(20)   X   ata set nam
        OUTPUT-FILE   CHAR(20)   o   file nam
        FULL   LOGICAL   y   r full lis   ng

EXAMPLE

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

```
*/
```

```
/*
NAME

        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 FIT1

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

COEFFICIENT.NAME	CHAR(20)	function name
FORM	CHAR(15)	function form
OUTPUT-FILE	CHAR(40)	output file name

EXAMPLE

RLS>SHOW FUNCTIONS

LINE	FUNCTION	FORM	DESCRIPTION
1	FN1	y=a*x	"test line"
2	FN2	y=a+b/x	"non-linear fit"
3	CURVE	y=a*exp(b*x)	"exponential curve"

RLS>SHOW FUNCTION COEFFICIENT FN2

LINE	FUNCTION	FORM	DESCRIPTION
1	FN2	y=a+b/x	"non-linear fit"

LINE	COEFFICIENT
1	1.
2	2.3

```
*/
```

CHAPTER 8

DATA ENTRY

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

VERB	OBJECT	DESCRIPTION
ADD	DATASET	enter an x-y data set
CHANGE	DATASET	change an x-y data set
DELETE	DATASET	delete an x-y data set
SHOW	DATASET	display an x-y data set

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

LINE	DATA	DESCRIPTION
1	lab1	"lab set #1"
2	lab2	"lab set #2"
3	xytest	"xy test data"

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

LINE	DATA	DESCRIPTION

```
1        xytest             "xy test data"

LINE     NROWS     NCOLS

1        5         2

LINE     X         Y

1        3.4       6.5
2        4.2       5.9
3        5.1       10.2
4        6.3       9.4
5        7.2       8.1

RLS>
```

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

LINE     DATA             DESCRIPTION

1        lab1             "lab set #1"
2        lab2             "lab set #2"
3        xytest           "xy test data"

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

LINE     DATA             DESCRIPTION

1        lab1             "lab set #1"
2        xytest           "xy test data"

RLS>
```

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
```

```
xlabel                  ""          :amount injected
xunits                  ""          :volts
ylabel                  ""          :detector response
yunits                  ""          :ppm
x(1)                                :10
y(1)                                :2.453e-01
x(2)                                :20
y(2)                                :5.321e-01
x(3)                                :40
y(3)                                :1.921e+00
x(4)                                :

RLS>
```

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

```
RLS>
```

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"       :
```

```
xlabel            "amount injected"         :
xunits            volts                     :ppm
ylabel            "detector response        :
yunits            ppm                       :volts
x(1)              10                        :
y(1)              2.453e-01                 :
x(2)              20                        :30
y(2)              5.321e-01                 :
x(3)              40                        :
y(3)              1.921e+00                 :

RLS>
```

8.5   COMMAND DEFINITIONS

```
/*
COMMAND

        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

        KEYWORD           TYPE                 DESCRIPTION

        X-Y.NAME          CHAR(20)             x-y data set name

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

KEYWORD	TYPE	DESCRIPTION
X-Y.NAME	CHAR(20)	x-y data set name

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.      :4.
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

KEYWORD	TYPE	DESCRIPTION
X-Y.NAME	CHAR(20)	X-Y data set name

EXAMPLE

        To delete an x-y data set:

        RLS>SHOW DATASET

LINE	DATA	DESCRIPTION
1	test	"lab data"
2	xydata	"bitumen sample"

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

LINE	DATA	DESCRIPTION
1	xydata	"bitumen sample"

        RLS>

```
*/
```

```
/*
NAME

        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

        KEYWORD           TYPE              DESCRIPTION

        X-Y.NAME          CHAR(20)          X-Y data set name
        OUTPUT-FILE       CHAR(40)          output file name

EXAMPLE

        To obtain the directory listing of data sets:

        RLS>SHOW DATASET

        LINE    DATA              DESCRIPTION

          1     test1             "lab data #1"
          2     test2             "bitumen sample"

        RLS>SHOW DATASET X-Y.NAME TEST2

        LINE    DATA              DESCRIPTION

         1      test2             "lab data #1"

        LINE      X               Y

         1       1.0             3.5
         2       2.0             7.9
         3       3.0             5.2
         4       4.0             9.2

*/
```

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.