POLYMATH

VERSION 4.1
Provides System Printing from Windows 3.X, 95, 98 and NT

USER-FRIENDLY NUMERICAL ANALYSIS PROGRAMS

- SIMULTANEOUS DIFFERENTIAL EQUATIONS
- SIMULTANEOUS ALGEBRAIC EQUATIONS
- SIMULTANEOUS LINEAR EQUATIONS
- POLYNOMIAL, MULTIPLE LINEAR AND NONLINEAR REGRESSION

for IBM and Compatible Personal Computers

Internet: http://www.polymath-software.com

Users are encouraged to obtain the latest general information on POLYMATH and its use from the above Internet site. This will include updates on this version and availability of future versions.

Michael B. Cutlip and Mordechai Shacham, the authors of POLYMATH, have published a new book entitled ***Problem Solving in Chemical Engineering with Numerical Methods***. This book is a companion book for students and professional engineers who want to utilize the POLYMATH software to effectively and efficiently obtain solutions to realistic and complex problems. Details on this Prentice Hall book, ISBN 0-13-862566-2, can be found on the preceding POLYMATH www site or at www.prenhall.com.

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HARDWARE REQUIREMENTS

POLYMATH runs on the IBM Personal Computer and most compatibles. A floating-point processor is required. Most graphics boards are automatically supported. The minimum desirable application memory is 450 Kb plus extended memory for large applications. POLYMATH works with PC and MS DOS 3.0 and above. It can also execute as a DOS application under Windows 3.1, Windows 95, Windows 98, and Windows NT. It is important to give POLYMATH as much of the basic 640 Kb memory as possible and up to 2048 Kb of extended memory during installation. This version of POLMATH supports only the Windows printers that are available to your operating system.

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INTRODUCTION

POLYMATH OVERVIEW

POLYMATH is an effective yet easy to use computational system which has been specifically created for professional or educational use. The various programs in the POLYMATH series allow the user to apply effective numerical analysis techniques during interactive problem solving on a personal computer. Whether you are student, engineer, mathematician, scientist, or anyone with a need to solve problems, you will appreciate the ease in which POLYMATH allows you to obtain solutions. Chances are very good that you will seldom need to refer to this manual beyond an initial reading because POLYMATH is so easy to use.

With POLYMATH, you are able to focus your attention on the problem at hand rather than spending your valuable time in learning how to use or reuse the program. You are encouraged to become familiar with the mathematical concepts being utilized in POLYMATH. These are discussed in most textbooks concerned with numerical analysis.

The available programs in POLYMATH include:

- *SIMULTANEOUS DIFFERENTIAL EQUATION SOLVER*
- *SIMULTANEOUS ALGEBRAIC EQUATION SOLVER*
- *SIMULTANEOUS LINEAR EQUATION SOLVER*
- *POLYNOMIAL, MULTIPLE LINEAR AND NONLINEAR REGRESSION*

Whether you are a novice computer user or one with considerable computer experience, you will be able to make full use of the programs in POLYMATH which allow numerical problems to be solved conveniently and interactively.

If you have limited computer experience, it will be helpful for you to read through this manual and try many of the QUICK TOUR problems. If you have considerable personal computer experience, you may only need to read the chapters at the back of this manual on the individual programs and try some of the QUICK TOUR problems.

This manual will be a convenient reference guide when using POLYMATH.

MANUAL OVERVIEW

This manual first provides general information on features which are common to all of the POLYMATH programs. Particular details of individual programs are then presented. Major chapter topics are outlined below:

INTRODUCTION

The introduction gives an overview of the POLYMATH computational system and gives general instructions for procedures to follow when using individual POLYMATH programs.

GETTING STARTED

This chapter prepares you for executing POLYMATH the first time, with information about turning on the computer, loading POLYMATH, and making choices from the various menu and option screens.

HELP

On-line access to a general help section is discussed.

UTILITIES

This chapter discusses features that all programs have available. These include a scientific calculator and a convenient conversion for units and dimensions. This chapter discusses saving individual problems, data and/or result files on a floppy or hard disk. It also describes the use of the problem library for storing, retrieving and modifying problems on a disk. Options for the printing and plotting of results are explained.

The remaining chapters of the manual present a QUICK TOUR of <u>each individual POLYMATH program</u> and are organized according to the following subsections:

1. PROGRAM OVERVIEW
This subsection gives general details of the particular program.
2. QUICK TOUR
You can use this subsection to see how easy it is to enter and solve a problem with a particular POLYMATH program.

APPENDIX

Detailed installation instructions and additional output options are presented for advanced users.

DISPLAY PRESENTATION

Throughout this manual, a full screen is indicated by a total enclosure:

An upper part of screen is contained within a partial enclosure:

A lower part of screen is shown by a partial enclosure:

An intermediate part of a screen is given between vertical lines:
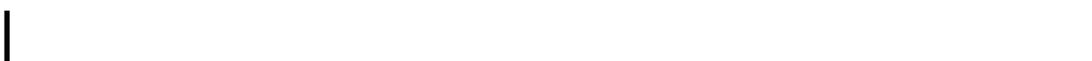
The option box is given by:
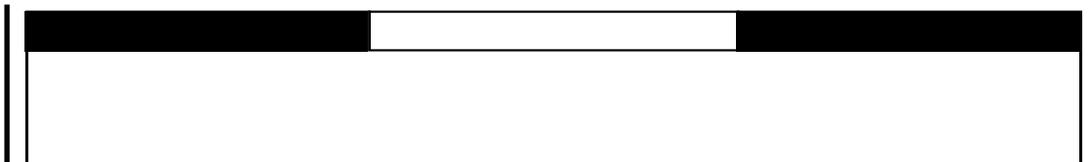
KEYBOARD INFORMATION

When using POLYMATH, it is not necessary to remember a complex series of keystrokes to respond to the menus, options, or prompts. The commands available to you are clearly labeled for easy use on each display. Normally the keystrokes which are available are given on the display as indicated on the PROBLEM OPTIONS display shown below.

```
                          PROBLEM OPTIONS                          NUM
a/d/c/u. to add/delete/change/duplicate an equation.        t.  to enter title.
i. to specify root search interval.
                        ⇧ F7 to solve the problem.
⇧ F8 for file and library options.     F6 for help.      F3 to print problem.
```
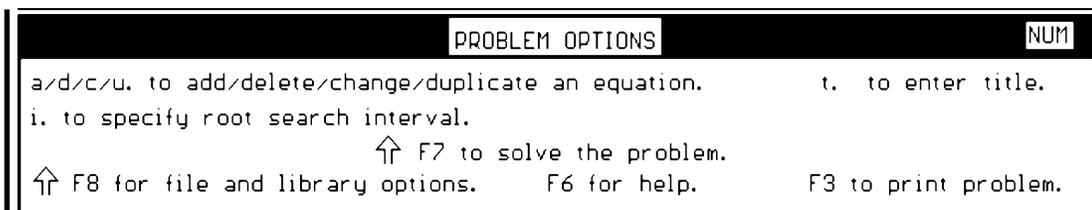
USING THE ↵ KEY

In this manual as in POLYMATH, the ↵ symbol is used to indicate the carriage return key which is also called the enter key. Usually when you are responding to a menu option, the enter key is not required. However, when data or mathematical functions are being entered, the enter key is used to indicate that the entry is complete.

SHIFTED KEYPRESSES

Some options require that several keys be pressed at the same time. This is indicated in POLYMATH and in this manual by a dash between the keys such as a ⇑ F8 which means to press and hold the ⇑ or "shift" key, then press the F8 function key and finally release both keys.

THE EDITING KEYS

Use the left and right arrow keys to bring the cursor to the desired position, while editing an expression. Use the Del key to delete the character above the cursor or the ← (Back Space) key to delete the first character to the left of the cursor. Typed in characters will be added to the existing expression in the first position left to the cursor.

BACKING UP KEYS

Press either the **F8** or the **Esc** key to have POLYMATH back up one program step.

ENTERING VARIABLE NAMES

A variable may be called by any alphanumeric combination of characters, and the variable name MUST start with a lower or upper case letter. Blanks, punctuation marks and mathematical operators are not allowed in variable names.

Note that POLYMATH distinguishes between lower and upper case letters, so the variables 'MyVar2' and 'myVar2' are not the same.

ENTERING NUMBERS

All numbers should be entered with the upper row on the key board or with the numerical keypad activated. Remember that zero is a number from the top row and not the letter key from the second row. The number 1 is from the top row while letter l is from the third row.

The results of the internal calculations made by POLYMATH have at least a precision of eight digits of significance. Results are presented with at least four significant digits such as xxx.x or x.xxx . All mathematical operations are performed as floating point calculations, so it is not necessary to enter decimal points for real numbers.

MATHEMATICAL SYMBOLS

You can use familiar notation when indicating standard mathematical operations.

Operator	Meaning	Symbol	Entry
+	addition	+	+
-	subtraction	-	-
x	multiplication	*	*
÷	division	/	/
	power of 10	$x.x10^a$	x.xea
			x.xEa
(x.x is numerical with a decimal and a is an integer)			
	exponentiation	r^s	r**s or r^s

MATHEMATICAL FUNCTIONS

Useful functions will be recognized by POLYMATH when entered as part of an expression. The arguments must be enclosed in parentheses:

ln   (base e)
abs (absolute value)
sin
arcsin
sinh
log (base 10)
int (integer part)
cos
arccos
cosh
exp
frac (fractional part)
tan
arctan
tanh

exp2(2^x)
round (rounds value)
sec
arcsec
arcsinh
exp10 (10^x)
sign (+1/0/-1)
csc
arccsc
arccosh
sqrt (square root)
cbrt (cube root)
cot
arccot
arctanh

LOGICAL EXPRESSIONS

An "if" function is available during equation entry with the following syntax: if (condition) then (expression) else (expression). The parentheses are required, but spaces are optional. The condition may include the following operators:

>	greater than
<	less than
>=	greater than or equal
<=	less than or equal
==	equals
<>	does not equal
|	or
&	and

The expressions may be any formula, including another "if" statement. For example:

a=if(x>0) then(log(x)) else(0)

b=if (T<minT) then(minT) else (if (T>maxT) then (maxT) else (T))

POLYMATH MESSAGES

There are many POLYMATH messages which may provide assistance during problem solving. These messages will tell you what is incorrect and how to correct it. All user inputs, equations and data, are checked for format and syntax upon entry, and feedback is immediate. Correct input is required before proceeding to a problem solution.

HARD COPY

If there is a printer connected to the computer, hard copy of the problem statements, tabular and graphical results etc. can be made by pressing F3 key wherever this option is indicated on the screen. This version of POLYMATH allows printing from the Windows printers, and the Windows meta files can also be used in various documents. See pages 9-2 and 9-4 for more details.

Problem statements and results can be also printed by saving them as a file and printing this file after leaving POLYMATH.

GRAPHICS

POLYMATH gives convenient displays during problem entry, modification and solution. Your computer will always operate in a graphics mode while you are executing POLYMATH.

GETTING STARTED

This chapter provides information on the hardware requirements and discusses the installation of POLYMATH.

HARDWARE REQUIREMENTS

POLYMATH 4.1 runs on IBM compatible personal computers that support the Windows-based operating systems. Most graphics boards are automatically supported. The minimum application memory requirement is approximately 450Kb, and extended memory is used when it is available. POLYMATH 4.1 runs as a DOS application under Windows 3.X, Windows 95, Windows 98, and Windows NT. Printing is accomplished by a separate program operating under Windows. This allows the printing from POLY-MATH to be done by any printer that can be used with the particular Windows operating system.

POLYMATH SOFTWARE

The complete set of POLYMATH application programs with a general selection menu is available on a single 3-1/2 inch 1.44 Mb floppy in compressed form. It is recommended that a backup disk be made before attempting to install POLYMATH onto a hard disk. Installation is available via an install program which is executed from any drive.

INSTALLATION TO INDIVIDUAL COMPUTERS AND NETWORKS

POLYMATH executes best when the software is installed on a hard disk or a network. There is a utility on the POLYMATH distribution disk which is called "install". **Detailed installation instructions are found in the Appendix of this manual.** Experienced users need to simply put the disk in the floppy drive, typically A or B. Type "install" **at the prompt of your installation floppy drive**, and press return. Follow the instructions on the screen to install POLYMATH on the particular drive and directory that you desire. Note that the default drive is "C:" and the default directory is called "POLYMAT4". Network installation will require responses to additional questions during installation. Latest detailed information can be found on the README.TXT file found on the installation disk.

FIRST TIME EXECUTION OF POLYMATH

The execution of **POLYMATH** is started by first having your current directory set to the subdirectory of the hard disk where **POLYMATH** version 4.1 is stored. This is assumed to be C:\POLYMAT4

C:\POLYMAT4 >

Execution is started by entering "polymath" at the cursor

C:\POLYMAT4 > polymath

and then press the Return (◄┘) key.
The Program Selection Menu should then appear:

```
POLYMATH

1. Simultaneous Differential Equation Solver

2. Simultaneous Algebraic Equation Solver

3. Linear Equation Solver

4. Polynomial, Multiple Linear and
   Nonlinear Regression

        Enter your choice or F8 to exit


POLYMATH is available from:
   The CACHE Corporation
   P.O.Box 7939, Austin TX 78713
   (512) 471-4933
```
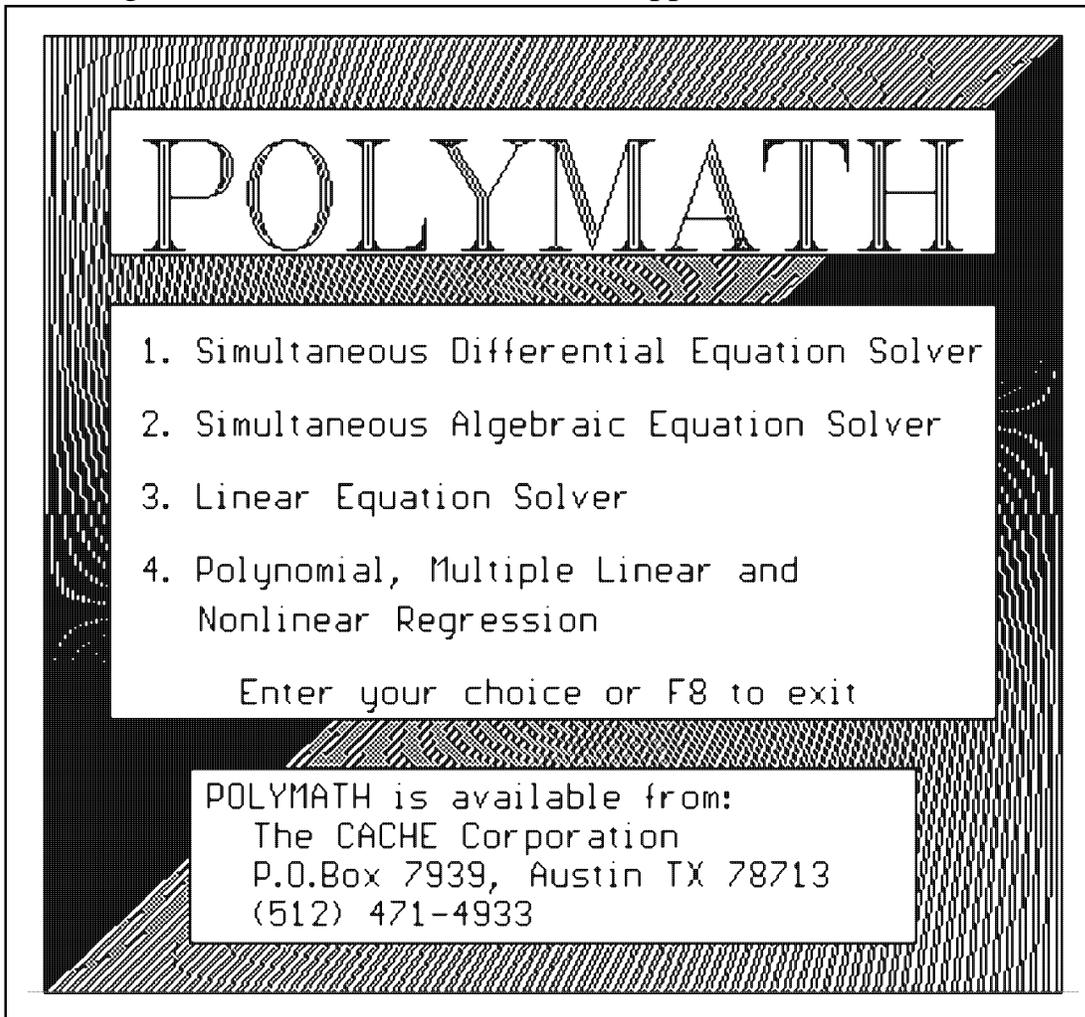
The desired **POLYMATH** program is then selected by entering the appropriate letter. You will then taken to the Main Program Menu of that particular program. Individual programs are discussed in later chapters of this manual.

EXITING POLYMATH PROGRAM

The best way to exit POLYMATH is to follow the instructions on the program display. However, a Shift-¡F10 keypress (⇑F10) will stop the execution of POLYMATH at any point in a program and will return the user to the Polymath Program Selection Menu. *THIS ACTION WILL DELETE THE EXISTING PROBLEM* so be sure to store your problem as an individual file or in the library before exiting the program in this manner. A query is made to determine if the user really wants to end the program in this manner while losing the current problem.

This ⇑ F10 keypress is one of the few POLYMATH commands which is not always indicated in the various Display Menus. It is worth remembering.

$$\boxed{\textbf{HELP}}$$

MAIN HELP MENU

Each individual POLYMATH program has a detailed help section which is available from many points in the program by pressing F6 when indicated. The Help Menu allows the selection of the topic area for specific help as shown below for the Differential Equation Solver:

```
    SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

          (Explanations and examples)
┌──────────────────────────────────────────────────────┐
│                    HELP MENU                           │
└──────────────────────────────────────────────────────┘

   Select a topic to study from the list below

     a.   Entering the equations.

     b.   Integration algorithms.

     c.   Results storage algorithm.

     d.   Troubleshooting.




                  F8 to return
```

For example, pressing "a" gives a discussion on entering the equations.

```
        ENTERING THE EQUATIONS INTO THE PROGRAM (page 1 of 6)


    The purpose of this program is to help you solve systems of first-order
ordinary differential equations.  The system may contain up to 31 differential
and supporting explicit algebraic equations.

    The differential equations should be entered in the following form:

        d(x)/d(t)= an expression
    or  d(x)= an expression.
```

Once the current topic is completed, the Help Options Menu provides for additional options as shown below:

```
┌─────────────────────────── HELP OPTIONS ───────────────────────────┐
│                                                                     │
│   ↵  for next page.              ⇑ ↵    for next topic.              │
│   F6 for help menu.              F8 to return to the program.        │
└─────────────────────────────────────────────────────────────────────┘
```
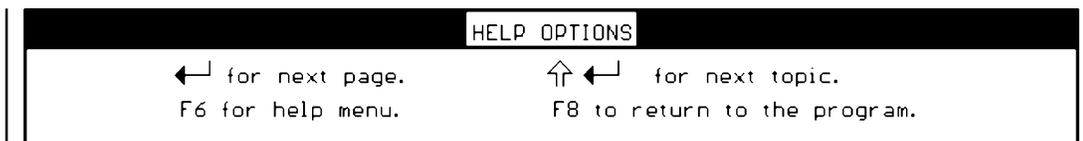
The ⇑ - F8 option to return to the program will take you to the display where you originally requested HELP

ACCESSING HELP BEFORE PROBLEM ENTRY

The Main Help Menu is reached during the startup of your **POLYMATH** program from the Main Menu as shown below and from the Problem Options Menu by pressing F6.

```
┌─────────────────────────────────────────────────────────────┐
│  ┌───────────────────────────┐   ┌─────────────────────────┐ │
│  │                           │   │                         │ │
│  │      POLYMATH             │   │                         │ │
│  │                           │   │                         │ │
│  │                           │   │                         │ │
│  │     Simultaneous          │   │                         │ │
│  │       Ordinary            │   │                         │ │
│  │     Differential          │   │                         │ │
│  │   Equation Solver         │   │                         │ │
│  │                           │   │  The following keys are │ │
│  │                           │   │     always active:      │ │
│  │  ↵  to begin.             │   │  ─────────────────────  │ │
│  │  F6 for HELP menu.        │   │  ⇑ F10 to return to     │ │
│  │  F7 for sample problems.  │   │         this display    │ │
│  │  F8 for POLYMATH menu.    │   │  F4 for calculator      │ │
│  │  F9 for file options.     │   │  F5 for unit converter  │ │
│  │  ⇑ F9 for the credits.    │   │                         │ │
│  └───────────────────────────┘   └─────────────────────────┘ │
└─────────────────────────────────────────────────────────────┘
```
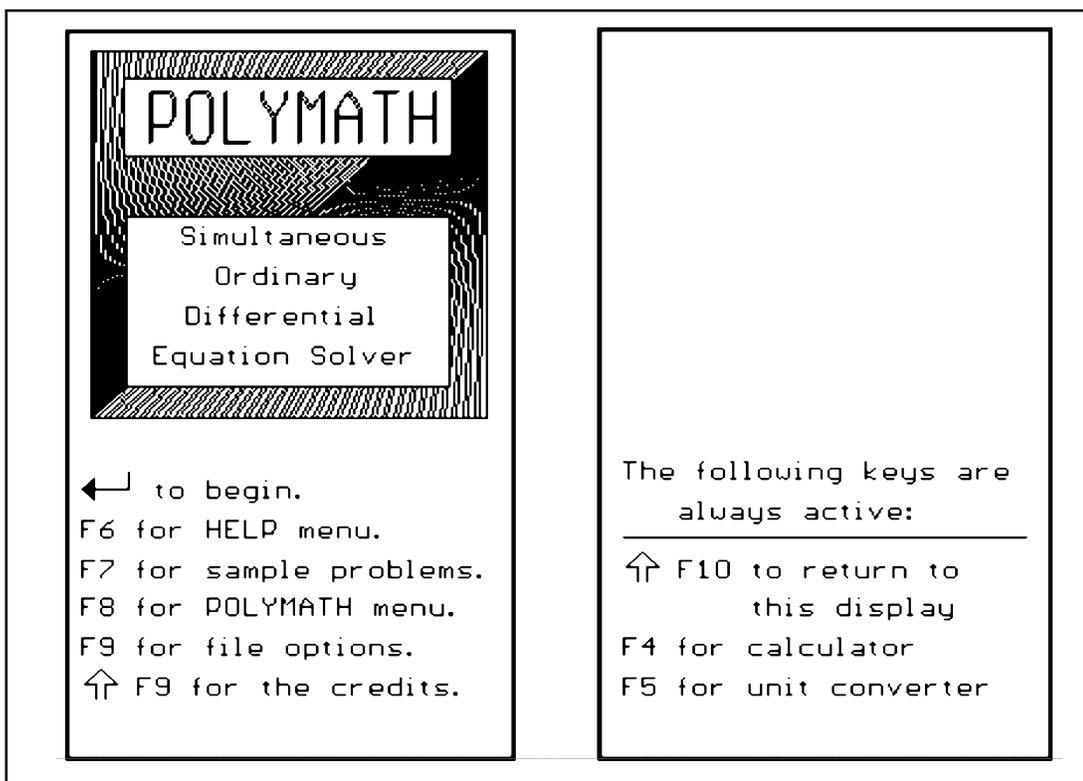
ACCESSING HELP DURING PROBLEM ENTRY

When you are entering a problem, the HELP MENU is available from the Problem Options Menu. This will allow you to obtain the necessary help and return to the same point where the HELP MENU was originally requested. As an example, this access point is shown in the Problem Options Menu shown on the next page.

```
┌─────────────────────────────────────────────────────────────────────┐
│                        PROBLEM OPTIONS                          NUM   │
├─────────────────────────────────────────────────────────────────────┤
│ a/d/c/u. to add/delete/change/duplicate an equation.      t.  to change title. │
│ i/f. to specify initial/final values.          ↑,↓, PgUp, PgDn to move pointer. │
│                      ⇧ F7 to solve the problem.                       │
│ ⇧ F8 for file and library options.    F6 for help.      F3 to print problem. │
└─────────────────────────────────────────────────────────────────────┘
```

CALCULATOR HELP

A detailed discussion of the POLYMATH Calculator is given in Chapter 4 of this manual. The Calculator can be accessed from by pressing F4 from any point in a POLYMATH program.

```
┌─────────────────────────────────────────────────────────────────────┐
│ ⟫_                                                                    │
│                                                                       │
│ CALCULATOR: Enter an expression and press <ENTER> to evaluate it.     │
│     Press <ESC> to leave or press F6 for information.                 │
└─────────────────────────────────────────────────────────────────────┘
```

An F6 keypress brings up the same page help which provides a brief instruction inside the Calculator window.

UNIT CONVERSION HELP

The Unit Conversion Utility is discussed in Chapter 4 of this manual. There is no on-line help for this utility.

UTILITIES

CALCULATOR

A sophisticated calculator is always available for use in a POLY-MATH program. This calculator is accessed by pressing the F4 key. At this time a window will be open in the option box area which will give you access to the calculator.

> ≫_
>
> CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
> Press <ESC> to leave or press F6 for information
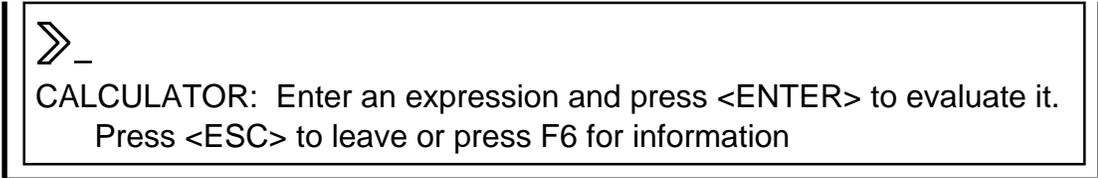
The POLYMATH calculator allows you to enter an expression to be evaluated. After the expression is complete, press ← to have it calculated. You may then press ← again to clear the expression, or you may edit your expression using the standard editing functions. When you wish to leave the calculator, just press the F8 or Esc key.

CALCULATOR EXPONENTIATION

Numbers may also be entered in scientific notation. The calculator will recognize E or e as being equivalent to the notation *10**. Either ** or ^ indicates general exponentiation. For example, the following three expressions are equivalent for a particular value of A:

$$4.71*10**A = 4.71eA = 4.71*10^A$$

AVAILABLE FUNCTIONS

A number of standard functions are available for use in the calculator. The underlined portion of the following functions is all that is required provided that all arguments are enclosed in parentheses. The arguments may themselves be expressions or other functions. The nesting of function is allowed.

ln ( ) or alog ( ) = natural logarithm to the base e
log ( ) or alog10 ( ) = logarithm to the base 10
exp ( ) = exponential (e^x)
exp2 ( ) = exponential of 2 (2^x)
exp10 ( ) = exponential of 10 (10^x)
sqrt ( ) = square root
abs ( ) = absolute value

int ( ) or ip ( ) = integer part
frac ( ) = or fp ( ) = fractional part
round ( ) = rounded value
sign ( ) = returns + 1 or 0 or -1
N! = factorial of integer part of number N (this only operates on a
    number)
sin ( ) = trigonometric sine with argument in radians
cos ( ) = trigonometric cosine with argument in radians
tan ( ) = trigonometric tangent with argument in radians
sec ( ) = trigonometric secant with argument in radians
csc ( ) = trigonometric cosecant with argument in radians
cot ( ) = trigonometric cotangent with argument in radians
arcsin ( ) = trigonometric inverse sine with result in radians,
        alternates arsin ( ) and asin ( )
arccos ( ) = trigonometric inverse cosine with result in radians,
        alternates arcos ( ) and acos ( )
arctan ( ) = trigonometric inverse tangent with result in radians,
        alternate atan ( )
arcsec ( ) = trigonometric inverse secant with result in radians
arccsc ( ) = trigonometric inverse cosecant with result in radians
arccot ( ) = trigonometric inverse cotangent with result in radians
sinh ( ) = hyperbolic sine
cosh ( ) = hyperbolic cosine
tanh ( ) = hyperbolic tangent
arcsinh ( ) = inverse hyperbolic sine
arccosh ( ) = inverse hyperbolic cosine
arctanh ( ) = inverse hyperbolic tangent

You should note that the functions require that their arguments be enclosed in parentheses, but that the arguments do not have to be simple numbers. You may have a complicated expression as the argument for a function, and you may even nest the functions, using one function (or an expression including one or more functions) as the argument for another.

ASSIGNMENT FUNCTIONS

The assignment function is a way of storing your results. You may specify a variable name in which to store the results of a computation by first typing in the variable name, then an equals sign, then the expression you wish to store. For example, if you wish to store the value of sin (4/3) ^{2} in variable 'a', you would enter:

$$a = \sin (4/3)**2$$

Variable names must start with a letter, and can contain letters and digits. There is no limit on the length of the variable names, or on the number of variables you can use. You can then use the variable 'a' in other calculations. **These variables are stored only as long as you remain in the current POLYMATH program. Please note that all stored values are lost when the particular program is exited. Calculator information is not retained during problem storage.**

CALCULATOR EXAMPLES

Example 1. In this example the vapor pressure of water at temperatures of 50, 60, and 70 °C has to be calculated using the equation:

$$\log_{10} P = 8.10765 - \frac{1750.29}{235.0 + T}$$

For T = 50 the following expression should be typed into the calculator:

$\gg$ 10^(8.10675 - 1750.29 / (235+50))

CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
   Press <ESC> to leave or press F6 for information.

Pressing ↵ brings up the desired answer which is 92.3382371 mm Hg at 50 ° C. To change the temperature use the left arrow to bring the cursor just right to the zero of the number 50, use the ← (BkSp or delete) key to erase this number and type in the new temperature value.

Example 2. In this example the pressure of carbon dioxide at temperature of T = 400 K and molal volume of $\widehat{V}$ = 0.8 liter is calculated using the following equations:

$$P = \frac{RT}{\widehat{V} - b} - \frac{a}{\widehat{V}^2}$$

Where
$$a = \frac{27}{64} \left(\frac{R^2 T_c^2}{P_c} \right) \qquad b = \frac{RT_c}{8 P_c}$$

$$R = 0.08206, \quad T_c = 304.2 \quad \text{and } P_c = 72.9.$$

One way to carry out this calculation is to store the numerical values in the named variables. First you can type in Pc = 72.9 and press ◄┘ to store this value as shown below.

> Pc=72.9
CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
=72.9.

After that you can type in Tc = 304.2 and R = 0.08206. To calculate b, you must type in the complete expression as follows:

> b=R*Tc/(8*Pc)
CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
=0.0428029012

The value of a is calculated in the same manner yielding a value of 3.60609951. Finally P can be calculated as shown:

> P=R*400/(0.8-b)-a/(0.8*0.8)
CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
=37.7148168

UNIT CONVERSION

A utility for unit conversion is always available for use within a POLYMATH program. Unit Conversion is accessed by pressing F5 wherever you desire. This will result in the following window in the option box area:

```
Type the letter of the physical quantity for conversion.
a) Energy     b)  Force       c) Length     d) Mass       e) Power
f) Pressure   g) Volume      h) Temperature     F8 or ESC to exit
```

The above listing indicates the various classes of Unit Conversion which are available in POLYMATH. A listing of the various units in each class is given below:

ENERGY UNITS: joule, erg, cal, Btu, hp hr, ft lb_f, (liter)(atm), kwh

FORCE UNITS: newton, dyne, kg, lb, poundal

LENGTH UNITS: meter, inch, foot, mile, angstrom, micron, yard

MASS UNITS: kilogram, pound, ton (metric)

POWER UNITS: watts, hp (metric), hp (British), cal/sec, Btu/sec, ft lb_f/sec

PRESSURE UNITS: pascal, atm, bar, mm Hg (torr), in Hg, psi [lb_f /sq in]

VOLUME UNITS: cu. meter, liter, cu. feet, Imperial gal, gal (U.S.), barrel (oil), cu. centimeter

TEMPERATURE UNITS: Celsius, Fahrenheit, Kelvin, Rankine

PREFIXES FOR UNITS
It is convenient to also specify prefixes for any units involved in a Unit Conversion. This feature provides the following prefixes:

deci 10^{-1} centi 10^{-2} milli 10^{-3} micro 10^{-6} deka 10

hecto 10^2 kilo 10^3 mega 10^6 giga 10^9

UNIT CONVERSION EXAMPLE

Suppose you want to convert 100 BTU's to kilo-calories. First you should access the Unit Conversion Utility by pressing F5. This will bring up the following options

```
Type the letter of the physical quantity for conversion.
a) Energy    b) Force      c) Length     d) Mass       e) Power
f) Pressure  g) Volume    h) Temperature    F8 or ESC to exit
```

Press "a" to specify an Energy conversion:

```
From units:  Type in a letter  (F9 to set a prefix first)
a. joule       b. erg        c.  cal        d. Btu         e. hp hr
f. ft lb_f       g. (liter)(atm) h. kwh
```

Type a "d" to specify Btu:

```
From units :  Btu            To units:      (F9 for a prefix)
a. joule       b. erg        c.  cal        d. Btu         e. hp hr
f. ft lb,       g. (liter)(atm) h. kwm
```

Use F9 to indicate a Prefix:

```
Press the number of the needed prefix or F9 for none.
1) deci 10^{-1}     2) centi 10^{-2}     3) milli 10^{-3}      4) micro 10^{-6}
5) deka 10    6) hecto 10^2   7) kilo 10^3   8) mega 10^6     9) giga 10^9
```

Please indicate kilo by pressing the number 7.

```
From units:  Btu                      To units:  kilo -
a. joule         b. erg         c. cal        d. Btu         e. hp hr
f. ft lb_f g. (liter)(atm)       h. kwh
```

Complete the units by pressing "c" for calories. Indicate the numerical value to be 100 and press enter:

```
From units:  Btu                      To units: kilo-cal
Numerical value:  100
100.00 Btu  =  25.216 kilo-cal
```

PROBLEM STORAGE

POLYMATH programs can be stored for future use as either DOS files or in a "Library" of problems. The Library has the advantage that the titles are displayed for only the problems for the particular POLYMATH program which is in use. Both the DOS files and the Library can be placed in any desired subdirectory or floppy disk. In both cases, only the problem and **not** the solution is stored. The storage options are available from the Task Menu which is available from POLYMATH programs by pressing either F9 from the Main Menu or ⇑ F8 from the Problem Options Menu.

```
┌──────────────────────────────────────────────────────────┐
│                        TASK MENU                          │
│                                                           │
│      ⇑↵    to continue working on your current problem.   │
│                                                           │
│       ↵    to enter a new problem.                        │
│                                                           │
│      F7    for SAMPLE PROBLEMS MENU.                       │
│                                                           │
│      F9    for LIBRARY OPTIONS.                            │
│                                                           │
│   DOS file options:                                       │
│                                                           │
│        S. Save current problem on file.                   │
│                                                           │
│        L. Load problem from file.                         │
│                                                           │
└──────────────────────────────────────────────────────────┘
```
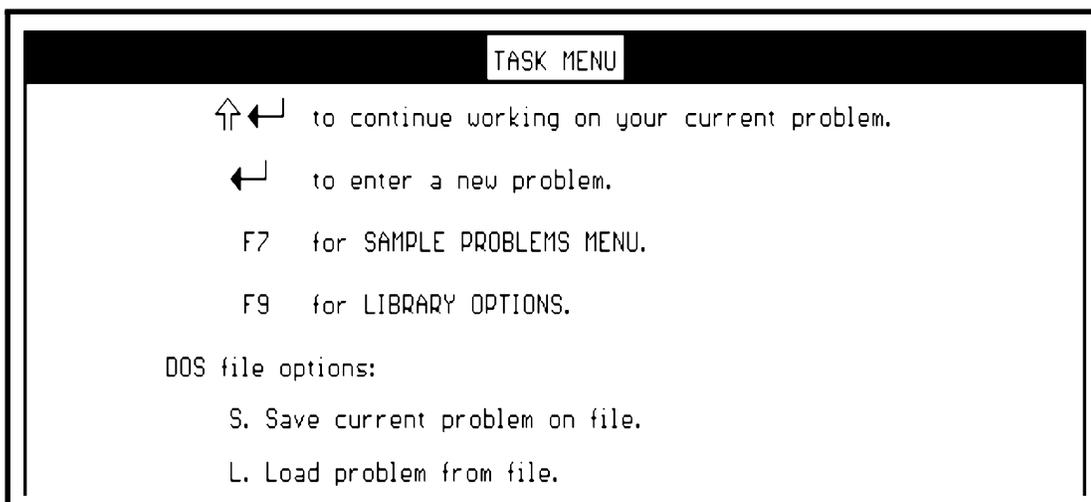
FILE OPERATIONS

A current problem can be saved to a DOS file by selecting "S" from the Task Menu. The desired directory and DOS file name can be specified from the window given below:

```
┌──────────────────────────────────────────────────────────┐
│ Enter DOS filename to write to:      Directory: C:\POLYMAT4│
│                                                           │
│ ≫ _                                                       │
│                                                           │
│ Press F6 for directory listing, F9 to change directory, F8 to return. │
└──────────────────────────────────────────────────────────┘
```
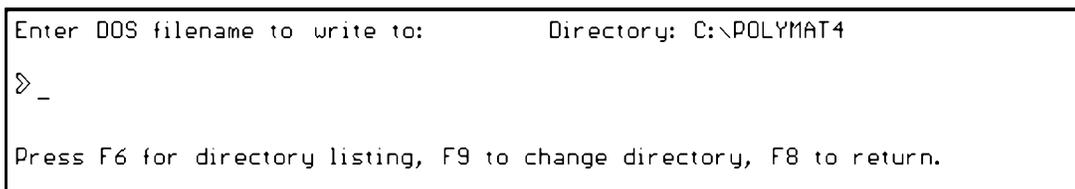
Note that the path to the desired directory can also be entered along with the file name as in "A:\MYFILE.POL" which would place the DOS file on the Drive A.

A previously stored problem in a DOS file can be loaded into POLYMATH from the Task Menu by selecting "L". A window similar to the one above will allow you to load the problem from any subdirectory or floppy disk. An F6 keypress gives the contents of the current directory for help in identifying the file name for the desired problem.

LIBRARY OPERATIONS

The Library is **highly recommended for storing problems** as the titles of the problems are retained and displayed which is a considerable convenience. Also, only the problems for the particular POLYMATH program in current use are displayed. The Library is accessed from the Task Menu by pressing F9 as shown below:

```
┌──────────────────────────────────────────────────────────────────────┐
│        ┌───────────────────────────────────────────────────┐          │
│        │ Regression Library directory: C:\POLYMAT4          │          │
│        │                                                               │
│        File name       Problem title                                   │
│  →  1) REG01    .POL    Sample Problem 1                                │
│     2) REG02    .POL    Sample Problem 2                                │
│     3) REG03    .POL    Sample Problem 3                                │
│     4) REG04    .POL    Sample Problem 4                                │
│                                                                        │
│                        ┌─────────────────┐                             │
│                        │ LIBRARY OPTIONS │                             │
│          S.   Store current problem.        C.   Change library directory │
│               or: Use ↑ or ↓ to move problem pointer and press:        │
│          L.   Load problem.                 D.   Delete problem.   F8 to return │
└──────────────────────────────────────────────────────────────────────┘
```

If there is no current Library on the desired subdirectory or floppy disk, then a Library is created.

LIBRARY STORAGE

The Library Options menu allows the current POLYMATH problem to be stored by simply entering "S". The title as currently defined in the active problem will be displayed. The user must choose a file name for this particular problem; however, it will then be displayed along with the Problem title as shown above.

LIBRARY RETRIEVAL

The Library Options window allows the current POLYMATH problem to be recalled by first using the cursor keys to direct the arrow to the problem of interest and then entering "L". A window will confirm the library retrieval as shown below:

```
┌──────────────────────────────────────────────────────────────────────┐
│ Reading problem from file REG04.POL...                                 │
│                                                                        │
│                                                                        │
│ Load done, press F8 to remain in library                               │
│                                                                        │
│              any other key for problem options                         │
│                                                                        │
└──────────────────────────────────────────────────────────────────────┘
```

Problems may be deleted from the Library by using the arrow to identify the problem, and then selecting "D" from the Library Options menu. Users are prompted to verify problem deletion.

PROBLEM OUTPUT AS PRINTED GRAPHICS

One of the most useful features of POLYMATH is the ability to create graphical plots of the results of the numerical calculations. The command to print graphical output is F3. The first step in printing graphical output is to display the desired output variables. The POLYMATH programs allow the user to make plots of up to four variables versus another variable.

An example which will be used to demonstrate plotting is the Quick Tour Problem 1 from the next chapter. Here the POLYMATH Differential Equation Solver has produced a numerical solution to three simultaneous ordinary differential equations. The calculations are summarized on a Partial Results display which has the following Display Options Menu:

```
┌─────────────────────────────────────────────────────────────────────┐
│                        │ DISPLAY OPTIONS │                    │ NUM │ │
│ g. Other variables in GRAPH form.          t. Same variables in TABULAR form. │
│ d. Write results to file.     s. Summary table.    F3 to prepare to print graph. │
│ ⇧ F8 for new problem or library.                   ⇧ ← to make changes.  │
└─────────────────────────────────────────────────────────────────────┘
```

SIMPLE SCREEN PLOT

The selection of "g" from the Display Options Menu allows the user to select desired variables for plotting. A plot of variables A, B, and C versus the independent variable t can be obtain by entering "A,B,C" at the cursor and pressing the Return key (←).

```
┌─────────────────────────────────────────────────────────────────────┐
│ Type in the names of up to four (4) variables separated by commas (,) │
│ and optionally one  independent  variable preceded by a slash (/).    │
│ For example,     myvar1,myvar2/timevar                                 │
│ ≫ A,B,C_                                                               │
└─────────────────────────────────────────────────────────────────────┘
```

The resulting graph is automatically scaled and presented on the screen.

Quick Tour Problem 1
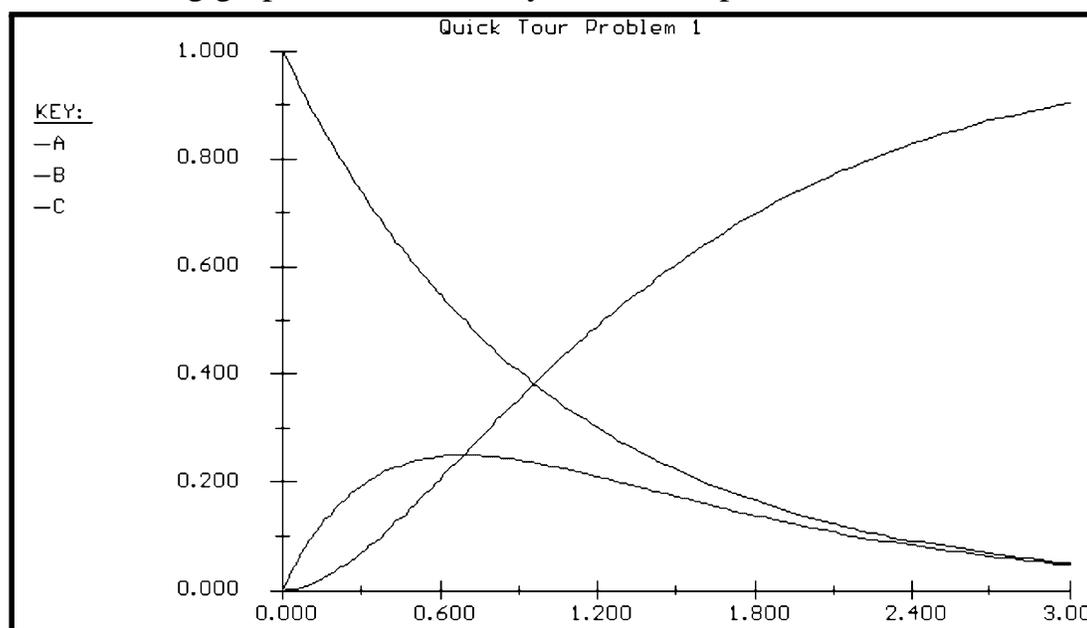
OPTIONAL SCREEN PLOT

The selection of "g" from the Display Options Menu with the entry of "B/A" results in B plotted versus A. This demonstrates that dependent variables can be plotted against each other.

PRESENTATION PLOT

A simple plot can be printed directly or it can be modified before printing by using options from the Graph Option Menu shown below:

```
┌────────────────────────────────────────────────────────────┐
│                      GRAPH OPTIONS                          │
│        s.  Change X axis scale.    S.  Change Y axis scale. │
│  l.  Add label to X axis.    L.  Add label to Y axis.    t. change graph title. │
│          F3  to print the graph          F8 for display options. │
└────────────────────────────────────────────────────────────┘
```
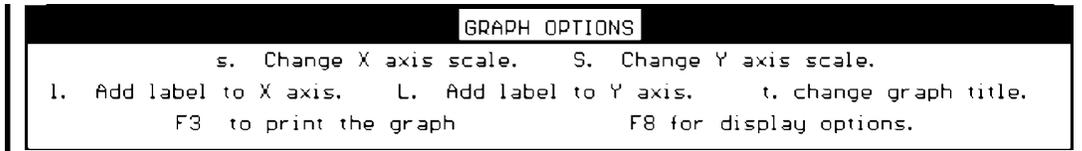
This menu allow the user to modify the plot before printing as desired to obtain a final presentation graphic with specified scaling and labels.

PROBLEM OUTPUT TO SCREEN AND AS PRINTED TABLES

The Display Options Menu also allows the user to select tabular output from the Partial Results Display by pressing "t":

```
┌────────────────────────────────────────────────────────────┐
│                   DISPLAY OPTIONS                     NUM   │
│  g. Other variables in GRAPH form.        t. Same variables in TABULAR form. │
│  d. Write results to file.    s. Summary table.    F3 to prepare to print graph. │
│  ⇧ F8 for new problem or library.              ⇧ ⏎  to make changes. │
└────────────────────────────────────────────────────────────┘
```
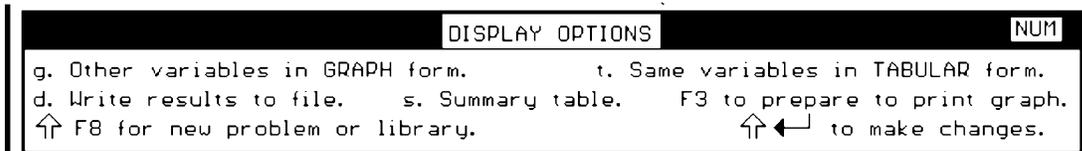
This is shown below for the same entry of "A, B, C" for the Quick Tour Problem 1 from the next chapter on differential equations.

t	A	B	C
0	1	0	0
0.3	0.74081822	0.19200658	0.067175195
0.6	0.54881164	0.24761742	0.20357094
0.9	0.40656966	0.24127077	0.35215957
1.2	0.30119421	0.21047626	0.48832953
1.5	0.22313016	0.17334309	0.60352675
1.8	0.16529889	0.13797517	0.69672595
2.1	0.12245643	0.10746085	0.77008272
2.4	0.090717953	0.082488206	0.82679384
2.7	0.067205513	0.062688932	0.87010556
3	0.049787068	0.047308316	0.90290462

The output shown above gives variable values for the integration interval at selected intervals. The maximum number of points is determined by the numerical integration algorithm. Output variable values for a smaller number of points are determined by interpolation. A Screen Table can be printed by using F3.

PROBLEM OUTPUT AS DOS FILES

The output from many of the POLYMATH programs can also be stored for future use as DOS files for use in taking results to spreadsheets and more sophisticated graphics programs. Typically this is done after the output has been sent to the screen. This is again accomplished with option "d" from the Display Options Menu.

```
┌──────────────────────────────────────────────────────────────────┐
│                        DISPLAY OPTIONS                       NUM   │
│ g. Other variables in GRAPH form.      t. Same variables in TABULAR form. │
│ d. Write results to file.   s. Summary table.   F3 to prepare to print graph. │
│ ⇑ F8 for new problem or library.              ⇑ ⟵  to make changes. │
└──────────────────────────────────────────────────────────────────┘
```
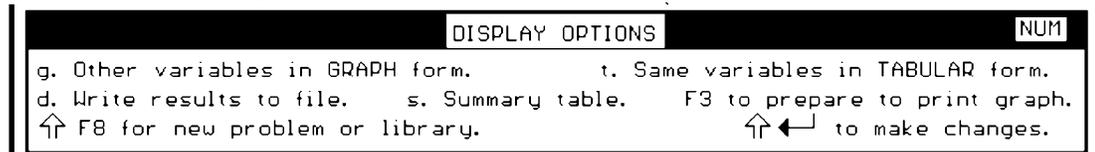
This option take the user to a display where the name and location of the DOS data file is entered:

```
┌──────────────────────────────────────────────────────────────────┐
│ Enter DOS filename to write to:       Directory: C:\POLYMAT4      │
│                                                                    │
│ ≫ _                                                                │
│                                                                    │
│ Press F6 for directory listing, F9 to change directory, F8 to return. │
└──────────────────────────────────────────────────────────────────┘
```
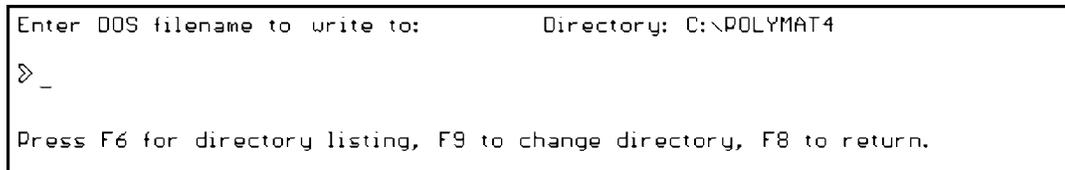
Please note that the user can change the drive and the directory to an desired location. One the location is indicated and the file name is entered, the desired variable names must be provided and the number of data points to be saved. The file shown below was created as shown for the request of "A,B,C" and 10 data points for Quick Tour Problem 1 from the next chapter:

t	A	B	C
0	1	0	0
0.3	0.74081822	0.19200658	0.067175195
0.6	0.54881164	0.24761742	0.20357094
0.9	0.40656966	0.24127077	0.35215957
1.2	0.30119421	0.21047626	0.48832953
1.5	0.22313016	0.17334309	0.60352675
1.8	0.16529889	0.13797517	0.69672595
2.1	0.12245643	0.10746085	0.77008272
2.4	0.090717953	0.082488206	0.82679384
2.7	0.067205513	0.062688932	0.87010556
3	0.049787068	0.047308316	0.90290462

Note that the separate columns of data in this DOS output file are separated by tabs which is suitable format for input to various spreadsheet or graphics programs.

PROBLEM OUTPUT AS GRAPHICS FILES

This 4.1 version of POLYMATH creates Windows Meta files (WMFs) that can be printed or entered into documents. These files are normally printed directly by special MetaFile Print programs for Windows 3.X (MFP16) or for Windows 95, 98, and NT (MFP32) . If these special print programs are not running, the generated WMFs are found in the SPOOL subdirectory under the POLYMAT4 directory. Thus the user can place these file directly into word processors and desktop publishing software. Details of this option are found in Chapter 9 of this manual. A typical example would be to create the following output in a WMF file for inclusion in a written reporting using word processing or desktop publishing. The problem is again the for Quick Tour Problem 1 from the next chapter. Note that the figure below has utilized the title and axis definition options.

CONCENTRATION PROFILES IN A BATCH REACTOR
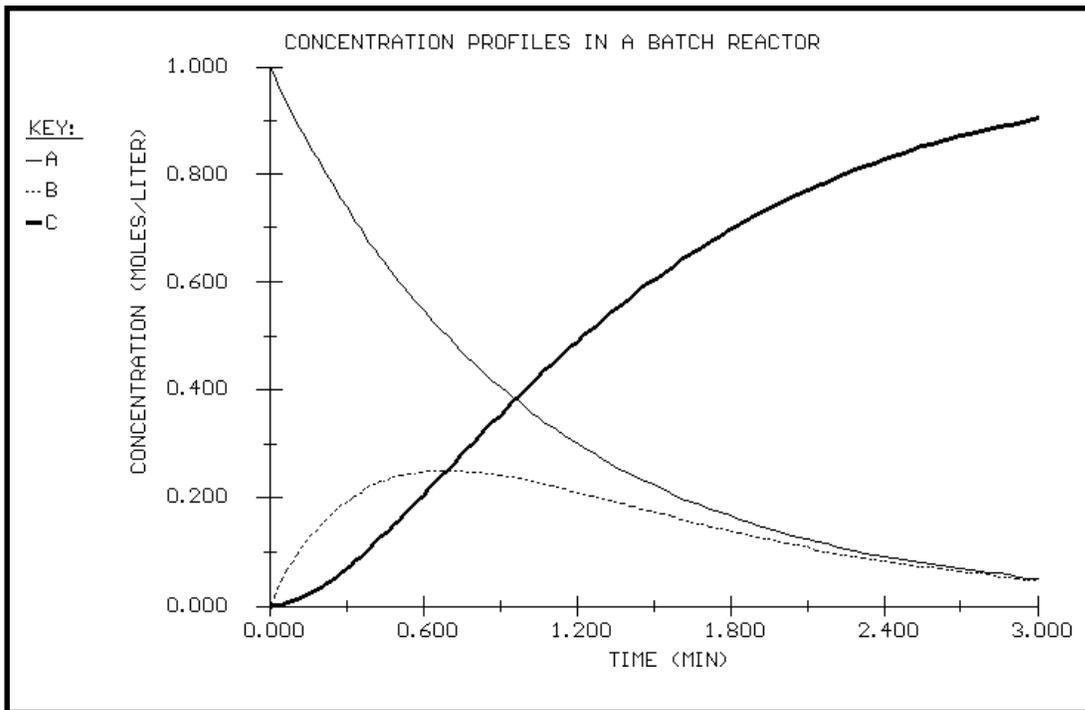
DIFFERENTIAL EQUATION SOLVER

QUICK TOUR

This section is intended to give you a very quick indication of the operation of the POLYMATH Differential Equation Solver Program.

DIFFERENTIAL EQUATION SOLVER

The program allows the numerical integration of up to 31 simultaneous nonlinear ordinary differential equations and explicit algebraic expressions. All equations are checked for syntax upon entry. Equations are easily modified. Undefined variables are identified. The integration method and stepsize are automatically selected; however, a stiff algorithm may be specified if desired. Graphical output of problem variables is easily obtained with automatic scaling.

STARTING POLYMATH

To begin, please have POLYMATH loaded into your computer as detailed in Chapter 2. Here it is assumed that your computer is set to the hard disk subdirectory or floppy drive containing the POLYMATH package. At the prompt (assumed C:\POLYMAT4 here), you should enter "polymath"

C:\POLYMATH4 > polymath

then press the Return (⏎) key. The Program Selection Menu should then appear, and you should enter "1" to select the Simultaneous Differential Equation Solver. This should bring up the Main Program Menu:

```
       POLYMATH

      Simultaneous
        Ordinary
       Differential
     Equation Solver


 ⏎   to begin.            The following keys are
 F6 for HELP menu.            always active:
 F7 for sample problems.
 F8 for POLYMATH menu.    ⇧ F10 to return to
 F9 for file options.            this display
 ⇧ F9 for the credits.    F4 for calculator
                          F5 for unit converter
```

Now that POLYMATH is loaded, please press F6 and then the letter "a" to get information on "Entering the equations". The first page of the Help Section should be on your screen as shown here:

```
            ENTERING THE EQUATIONS INTO THE PROGRAM (page 1 of 6)


    The purpose of this program is to help you solve systems of first-order
ordinary differential equations.  The system may contain up to 31 differential
and supporting explicit algebraic equations.

    The differential equations should be entered in the following form:

        d(x)/d(t)= an expression
    or   d(x)= an expression.

    Here t is the independent variable and x is a dependent variable.
Variable names must begin with an alphabetic character, and can contain
an unlimited number of alphabetic and numeric characters.  Variable names
are case-sensitive, meaning 't' and 'T' are two different variables.


    Auxiliary algebraic equations may be entered in the form:

       x= an expression
    where the same naming rules apply.




                                    HELP OPTIONS
       ⏎ for next page.           ⇧ ⏎   for next topic.
       F6 for help menu.            F8 to return to the program.
```

Please press F8 to return from the Help to the program, and then press the Enter key (◄─┘)to continue this Quick Tour example.

SOLVING A SYSTEM OF DIFFERENTIAL EQUATIONS

Let us now enter and solve a system of three simultaneous differential equations:

$$d(A) / d(t) = - k_A (A)$$
$$d(B) / d(t) = k_A (A) - k_B (B)$$
$$d(C) / d(t) = k_B (B)$$

In these equations, the parameter k_A is to be constant at a value of 1.0 and the parameter k_B is to be constant at the value of 2.0. The initial condition for dependent variable "A" is to be 1.0 when the initial value of the independent variable "t" is zero. The initial conditions for dependent variables "B" and "C" are both zero. The solution for the three differential equations is desired for the independent variable "t" between zero and 3.0. Thus this problem will be entered by using the three differential equations as given above along with two expressions for the values for k_A and k_B given by:

$$k_A = 1.0; \qquad k_B = 2.0$$

ENTERING THE EQUATIONS

The equations are entered into POLYMATH by first pressing the "a" option from the Problem Options Menu. The following display gives the first equation as it should be entered at the arrow. (Use the Backspace key, to correct entry errors after using arrow keys to position cursor.) Press the Return key (⏎) to indicate that the equation is to be entered. Don't be concerned if you have entered an incorrect equation, as there will soon be an opportunity to make any needed corrections.

```
Differential Equations:  0              Auxiliary Equations:  0

》  d(A)/d(t)=-ka*A_
```

The above differential equation is entered according to required format which is given by:

$$d(x)/d(t) = \text{an expression}$$

where the dependent variable name "x" and the independent variable name "t" must begin with an alphabetic character and can contain any number of alphabetic and numerical characters. In this Quick Tour problem, the dependent variables are A, B and C for the differential equations, and the independent variable is t. Note that POLYMATH variables are case sensitive. The constants k_A and k_B are considered to be variables which can be defined by explicit algebraic equations given by the format:

$$x = \text{an expression}$$

In this problem, the variables for k_A and k_B will have constant values. Note that the subscripts are not available in POLYMATH, and in this problem the variable names of ka and kb will be used.

Please continue to enter the equations until your set of equations corresponds to the following:

```
Equations:
→  d(A)/d(t)=-ka*A
   d(B)/d(t)=ka*A-kb*B
   d(C)/d(t)=kb*B
   ka=1
   kb=2
```

As you enter the equations, note that syntax errors are checked prior to being accepted, and various messages are provided to help to identify input errors. Undefined variables are also identified by name during equation entry.

ALTERING THE EQUATIONS

After you have entered the equations, please press ⬅ with no equation at the arrow to go to the Problem Options display which will allow needed corrections:

```
 Equations

→ d(A)/d(t)=-ka*A

  d(B)/d(t)=ka*A-kb*B

  d(C)/d(t)=kb*B

  ka=1

  kb=2


     Differential Equations:  3          Auxiliary Equations:  2

                          PROBLEM OPTIONS                          NUM
 a/d/c/u. to add/delete/change/duplicate an equation.     t.  to enter title.
 i/f. to specify initial/final values.        ↑,↓, PgUp, PgDn to move pointer.
                       ⇧ F7 to solve the problem.
 ⇧ F8 for file and library options.    F6 for help.    F3 to print problem.
```

The Problem Options Menu allows you to make a number of alterations on the equations which have been entered. Please make sure that your equations all have been entered as shown above. Remember to first indicate the equation that needs altering by using the arrow keys. When all equation are correct, press ⇧ F7 (keep pressing shift while pressing F7) to continue with the problem solution.

ENTERING THE BOUNDARY CONDITIONS

At this point you will be asked to provide the initial values for the independent variable and each of the dependent variables defined by the differential equations.

```
  Enter initial value for t
  ≫ _
```

Please indicate this value to be the number "0" and press Return.

The next initial value request is for variable "A". Please this value as the value "1."

```
  Enter initial value for A
  ≫ 1 _
```

The initial values for B and C will be requested if they have not been previously entered. Please enter the number "0" for each of these variables.

Next the final value for t, the independent variable, will be requested. Set this parameter at "3":

```
Enter final value for t
≫ 3 _
```

As soon as the problem is completely specified, then the solution will be generated. However, if you corrected some of your entries, then you may need to press ⇑ F7 again to request the solution. Note that a title such as "Quick Tour Problem 1" could have been entered from the Problem Option Menu.

SOLVING THE PROBLEM

The numerical solution is usually very fast. For slower computers, an arrow will indicate the progress in the independent variable during the integration. Usually the solution will be almost instantaneous. The screen display after the solution is given below:

```
                          Quick Tour Problem 1
   Equations                                                Initial values

 → d(A)/d(t)=-ka*A                                                1
   d(B)/d(t)=ka*A-kb*B                                            0
   d(C)/d(t)=kb*B                                                 0
   ka=1
   kb=2
   t₀ = 0,    t_f = 3


    ┌─────────────────────────────────────────────────────┐
    │  Solution process complete.                          │
    │                                                      │
    │  Press any key to display results.                   │
    │                                                      │
    └─────────────────────────────────────────────────────┘



    ┌─────────────────────────────────────────────────────┐
    │    Differential Equations:  3        Auxiliary Equations:  2 │
    └─────────────────────────────────────────────────────┘

    Solution progress - independent variable value
                                                            ↓
   ├──────┼──────┼──────┼──────┼──────┼──────┼──────┤
   0                          1.5                         3
```
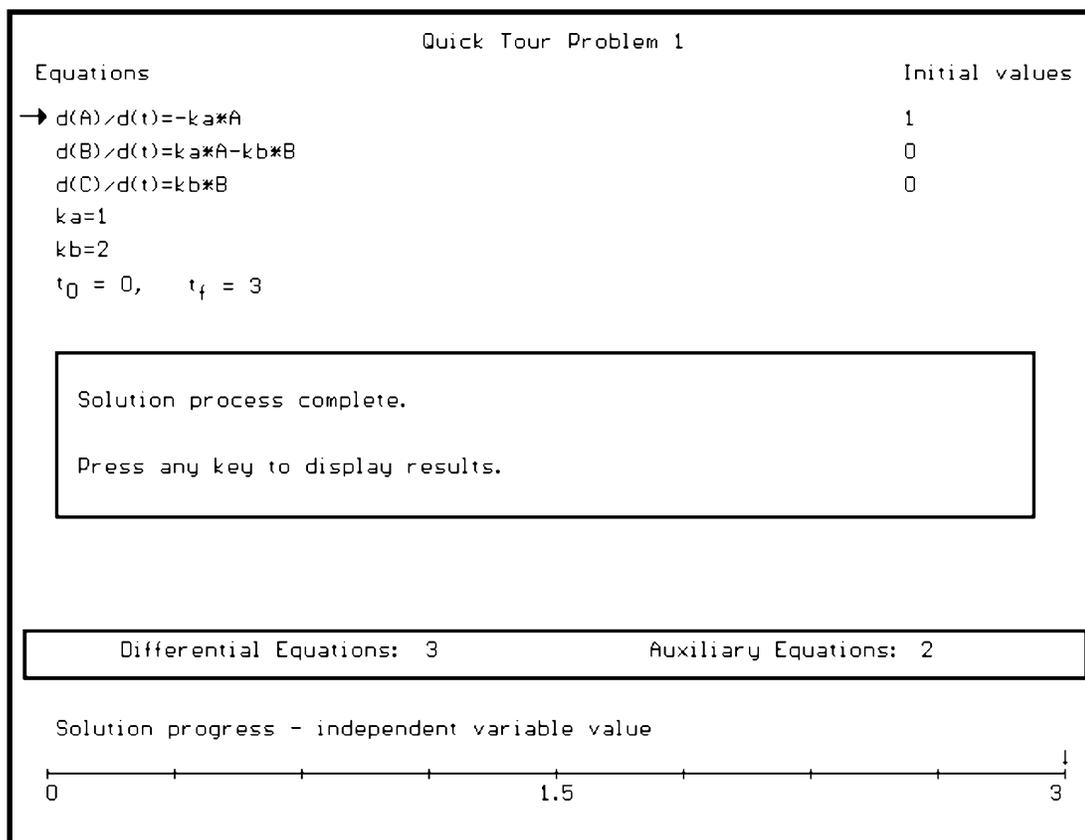
Another Return keypress gives the partial Results Table which summarizes the variables of the problem as shown below:

```
                         Quick Tour Problem 1
    Variable      Initial value     Maximum value     Minimum value     Final value
    t             0                 3                 0                 3
    A             1                 1                 0.0497871         0.0497871
    B             0                 0.249993          0                 0.0473083
    C             0                 0.902905          0                 0.902905
    ka            1                 1                 1                 1
    kb            2                 2                 2                 2
```

```
┌─────────────────────────── DISPLAY OPTIONS ─────────────────┤ NUM ├┐
│    t. Results in TABULAR form.          g. Results in GRAPHICAL form.│
│    d. Output results to DOS file.       F3 to print this summary table.│
│  ⇧ F8 for new problem or library.         ⇧ ⏎  to make changes.      │
└──────────────────────────────────────────────────────────────────────┘
```

The Partial Results Table shown above provides a summary of the numerical simulation. To display or store the results you can enter "t" (tabular display), "g" (graphical display), or "d" (storing the results on a DOS file). This Table may be printed with the function key F3.

PLOTTING THE RESULTS

Let us now plot the variable from this Problem 1 by entering "g" for a graphical presentation. When asked to type in the variable for plotting, please enter the input indicated below at the arrow:

```
┌──────────────────────────────────────────────────────────────────┐
│  Type in the names of up to four (4) variables separated by commas (,)│
│  and optionally one 'independent' variable preceded by a slash(/). │
│  For example,  myvar1, myvar2/timevar                             │
│                                                                    │
│  ≫ A, B, C __                                                      │
└──────────────────────────────────────────────────────────────────┘
```

A Return keypress (⏎) will indicate the end of the variables and should generate the graphical plot on the next page of the specified variables A, B, and C versus t, the independent variable, for this example.

```
                    Quick Tour Problem 1
        1.000 ─┬
KEY:
─A
─B      0.800 ─┼
─C
        0.600 ─┼

        0.400 ─┼

        0.200 ─┼

        0.000 ─┼
            0.000    0.600    1.200    1.800    2.400    3.00
                                    t
```

DISPLAY OPTIONS   **NUM**

g. Other variables in GRAPH form.   t. Same variables in TABULAR form.
d. Write results to file.   s. Summary table.   F3 to prepare to print graph.
⇧ F8 for new problem or library.   ⇧ ⏎ to make changes.
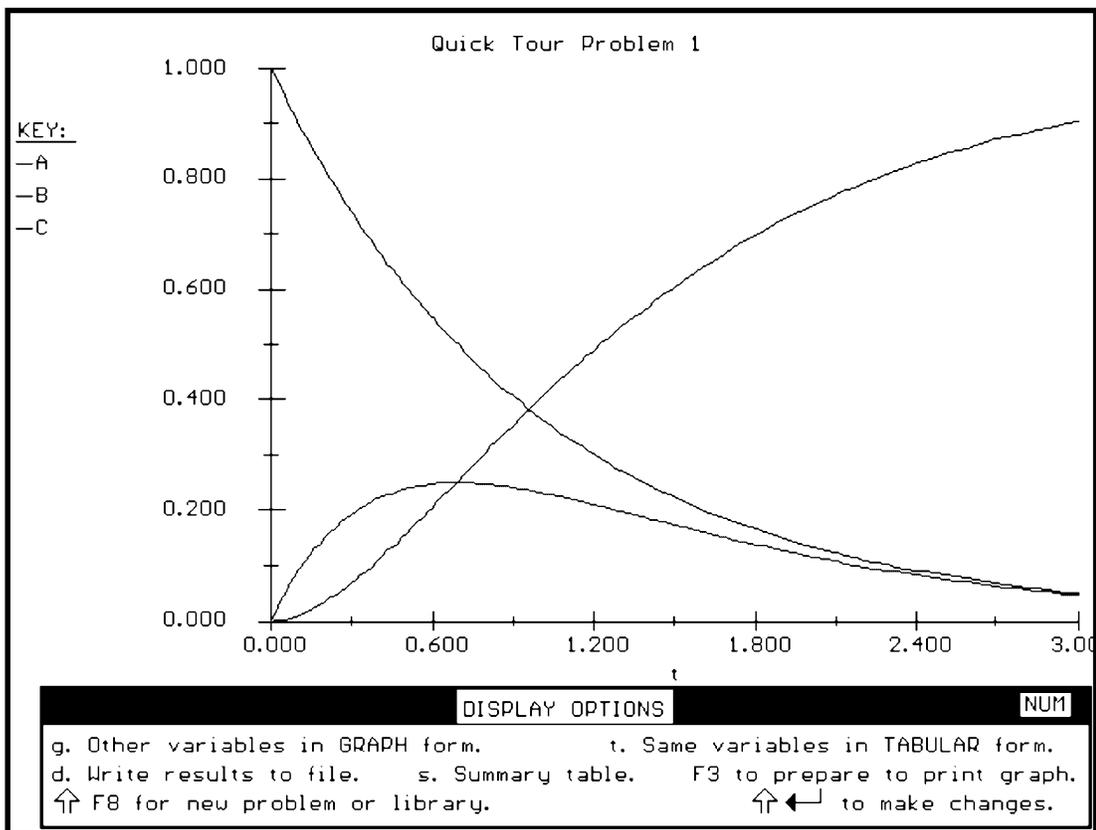
Suppose that you want to plot variable B versus variable A. Select the option "g" from the Display Options Menu and enter B/A when asked for the variable names.

Type in the names of up to four (4) variables separated by commas (,) and optionally one 'independent' variable preceded by a slash(/).
For example, myvar1, myvar2/timevar

≫ B/A

This will results in a scaled plot for variable B versus variable A.

This concludes the Quick Tour problem using the Differential Equation Solver. If you wish to stop working on POLYMATH, please follow the exiting instructions given below.

EXITING OR RESTARTING POLYMATH

A ⇧ - F10 keypress will always stop the operation of POLYMATH and return you to the Program Selection Menu. THIS *ACTION WILL DELETE THE EXISTING PROBLEM.* The program can be exited or restarted from the Program Selection Menu.

INTEGRATION ALGORITHMS

The program will first attempt to integrate the system of differential equations using the Runge-Kutta-Fehlberg (RKF) algorithm. A detailed discussion of this algorithm is given by Forsythe et al.* This algorithm monitors the estimate of the integration error and alters the step size of the integration in order to keep the error below a specified threshold. The default values for both relative and absolute (maximal) errors are less than 10^{-10}. If this cannot be attained, then the absolute and relative errors are set as necessary to 10^{-7} and then to 10^{-4}.

If it is not possible to achieve errors of 10^{-4}, then the integration is stopped, and the user is given a choice to continue or to try an alternate integration algorithm for stiff systems of differential equations. Under these circumstances, the system of equations is likely to be "stiff" where dependent variables may change in widely varying time scales, and the user is able to initiate the solution from the beginning with an alternate "stiff" integration algorithm The algorithm used is the semi-implicit extrapolation method of Bader-Deuflhard**, and the maximal errors are again started at 10^{-10}.

When the integration is very slow, the F10 keypress will allow the selection of the stiff algorithm, and the problem will be solved from the beginning.

* Frosythe, B. E., M. A. Malcolm, and C. B. Moler, **Computer Methods for Mathematical Computation**, Prentice-Hall, Englewood Cliffs, NJ, 1977.
** Press, W. H., P. B. Flannery, S. A. Teukolsky, and W. T. Vetterling, **Numerical Recipes**, 2nd Ed., Cambridge University Press, 1992, pp. 735-739.

TROUBLE SHOOTING

SPECIFIC ERROR MESSAGES

Most error messages given by POLYMATH are self-explanatory, and they suggest the type of action which should be taken to correct the difficulty.

NONSPECIFIC ERROR MESSAGES

"Circular dependency detected."

This message appears during the inputting of equations when the equations are not all explicit. For example, an attempt to define y=z/x when z has been previously defined will cause this error message to appear. This version of POLYMATH Differential Equations Solver can only solve variables which can be explicitly expressed as a function of other variables.

"The expression ... is undefined at the starting point."

This common problem can be solved by starting the integration from t=eps where eps is a very small number and t represents the independent problem variable.

"Solution process halted due to a lack of memory."

This message may result when the default Runge-Kutta-Fehlberg algorithm is used for a stiff system of differential equations, and thus very small step sizes are taken. Consequently, a large number of data points for possible plotting of the results. **Use the F10 to stop the integration and switch to the stiff algorithm.** If the message persists, then take the following steps to resolve the difficulty:

(1) If you are running under Windows, make sure the PIF for POLYMATH specifies 640K of conventional memory and 1024K or more of XMS(see the Appendix for more details).
(2) Remove other memory-resident programs from your computer.
(3) Reduce the number of equations. This is most easily accomplished by introducing the numerical values of the constants into the equations, instead of defining them separately.
(4) Reduce the integration interval.

"Solution process halted because it was not going anywhere."

This message usually appears when the problem is very stiff, and the default RKF algorithm is used for integration. The stiff algorithm should be used, or the interval of integration should be reduced. If the error message persists, there are probably errors in the problem setup or input. Please check for errors in the basic equation set, the POLYMATH equation entry, and the numerical values and the units of the variables.

.

ALGEBRAIC EQUATION SOLVER

QUICK TOUR

This chapter is intended to give a very brief discussion of the operation of the POLYMATH Nonlinear Algebraic Equation Solver.

NONLINEAR ALGEBRAIC EQUATION SOLVER

The user can solve up to a combination of 32 simultaneous nonlinear equations and explicit algebraic expressions. Only real (non-complex) roots are found. All equations are checked for correct syntax and other errors upon entry. Equations can be easily be modified, added or deleted. Multiple roots are given for a single equation.

STARTING POLYMATH

To begin, please have POLYMATH loaded into your computer as detailed in Chapter 2. Here it is assumed that your computer is set to the hard disk subdirectory or floppy drive containing the POLYMATH package. At the prompt (assumed C:\POLYMAT4 here), you should enter "polymath"

| C:\POLYMAT4>polymath |

then press the Return (⬅) key. The Main Program Menu should then appear: The Program Selection Menu should then appear, and you should enter "2" to select the Simultaneous Algebraic Equation Solver.

```
 POLYMATH

   Simultaneous
    Nonlinear
     Algebraic
  Equation Solver


⬅  to begin.
F6 for HELP menu.
F7 for sample problems.
F8 for POLYMATH menu.
F9 for file options.
⇧ F9 for the credits.
```

```
The following keys are
    always active:

⇧ F10 to return to
        this display
F4 for calculator
F5 for unit converter
```

Once that POLYMATH is loaded, please utilize the Help Menu by pressing F6 and then the letter "a" to obtain details on in order to learn how to input the equations. The first page of this Help Section is given below:

```
            ENTERING THE EQUATIONS INTO THE PROGRAM (page 1 of 5)

    The purpose of this program is to help you to solve systems of nonlinear
algebraic equations.  The system may contain up to 32 nonlinear simultaneous
and supporting auxiliary equations.  Only real roots (non-complex) can be found.

    Variable names must begin with an alphabetic character and can contain
alphabetic and numeric characters.  Variable names are case-sensitive,
meaning 't' and 'T' are two different variables.

    Nonlinear equations requiring simultaneous solution (implicit equations)
may be entered in the following form:
        f(x)= an expression.
  where 'x' is named according to the rules given above, and f(x) is an
expression to have the value of zero.

    In addition to the implicit equations, auxiliary equations can be defined.
The auxiliary equations are solved sequentially.  They are of the form:
        x= an expression
  where 'x' is any variable name.


                            ┌─────────────┐
                            │ HELP OPTIONS│
    ←┘ for next page.           ⇧ ←┘   for next topic.
    F6 for help menu.           F8 to return to the program.
```

This Help Section gives detailed information for entering the nonlinear and auxiliary equations. Press F8 to return from the Help Section to the program, and then press the Enter key (◄─┘) to enter an equation for the first Quick Tour example. The Problem Options Menu at the bottom of your display allows entry of equations with the keypress of "a". Now you are ready for the first problem.

```
   Nonlinear Equations:  0              Auxiliary Equations:  0
                           ┌────────────────┐
                           │ PROBLEM OPTIONS│
   a. to add an equation.                        t.  to enter title.

                        ⇧ F7 to solve the problem.
  ⇧ F8 for file and library options.          F6 for helpful information.
```

SOLVING ONE NONLINEAR EQUATION

The first nonlinear equation to be solved as Quick Tour Problem 1 is:

$$x^2 - 5x + 6 = 0$$

The solution is to be obtained over the range of x between 1 and 4. This equation is entered into POLYMATH using the equation entry guidelines where the equation is to be zero at the solution. The following display gives the equation as it should be entered at the arrow: (Use the ← or the delete key to erase entered characters. Standard DOS editing is available at the cursor.)

```
        Nonlinear Equations: 1              Auxiliary Equations:  0


  ⟩ f(x)=x^2-5*x+6_
```

The format for the above equation for f(x) is that the left side of the equation will be equal to zero when the solution has been obtained. The variable which is to be determined is set as an argument within the parentheses for the function f( ).

Thus in this case, the variable is x and the function to be solved as being zero is x^2-5x+6. Also note that in POLYMATH one way of entering x^2 is x^2. An alternative entry is x**2.

After you have correctly typed the equation at the arrow, please press ←⏎ once to enter it and **then ←⏎ again** to end equation entry. This should result in the Problem Options Menu at the bottom of the display and the equation at the top:

```
  Equations

  → f(x)=x^2-5*x+6

        Nonlinear Equations: 1              Auxiliary Equations:  0

                          PROBLEM OPTIONS                        NUM
  a/d/c/u. to add/delete/change/duplicate an equation.       t.  to enter title.
  i. to specify initial values.
                        ⇑ F7 to solve the problem.
  ⇑ F8 for file and library options.     F6 for help.     F3 to print problem.
```

The Problem Options Menu indicates which options are now available for you to carry out a number of tasks. In this case, the problem should be complete, and these options for the equation at the arrow will not be needed. If an equation needed to be changed, then you would enter a "c" at the above display. (The arrow is moved by the arrow keys on the keyboard.)

Once you have the equation entered properly, please press ⇑F7 to solve the problem. You will then be asked to provide the interval over which you wish to find solutions for the equation. This interval is only requested during the solution of a single nonlinear equation.

```
Enter minimal value for x

》_
```

Please indicate the x_{min} to be 1 and press (←). Then indicate x_{max} to be 4 and press (←).

```
Enter maximal value for x

》4_
```

The entire problem is then display above the Problem Options Menu:

```
  Equations

→ f(x)=x^2-5*x+6

  x_min = 1,   x_max = 4
```

For this single equation, the solution is presented graphically over the search range which you indicated. The solution is where the function f(x) is equal to zero. POLYMATH has the ability to determine multiple solutions to a single equation problem, and the first of two solutions is shown below:

Single Nonlinear Equation - Quick Tour

Solution 1:   x = 2

DISPLAY OPTIONS

← for next solution
⇑← to make changes   F3 to print this graph
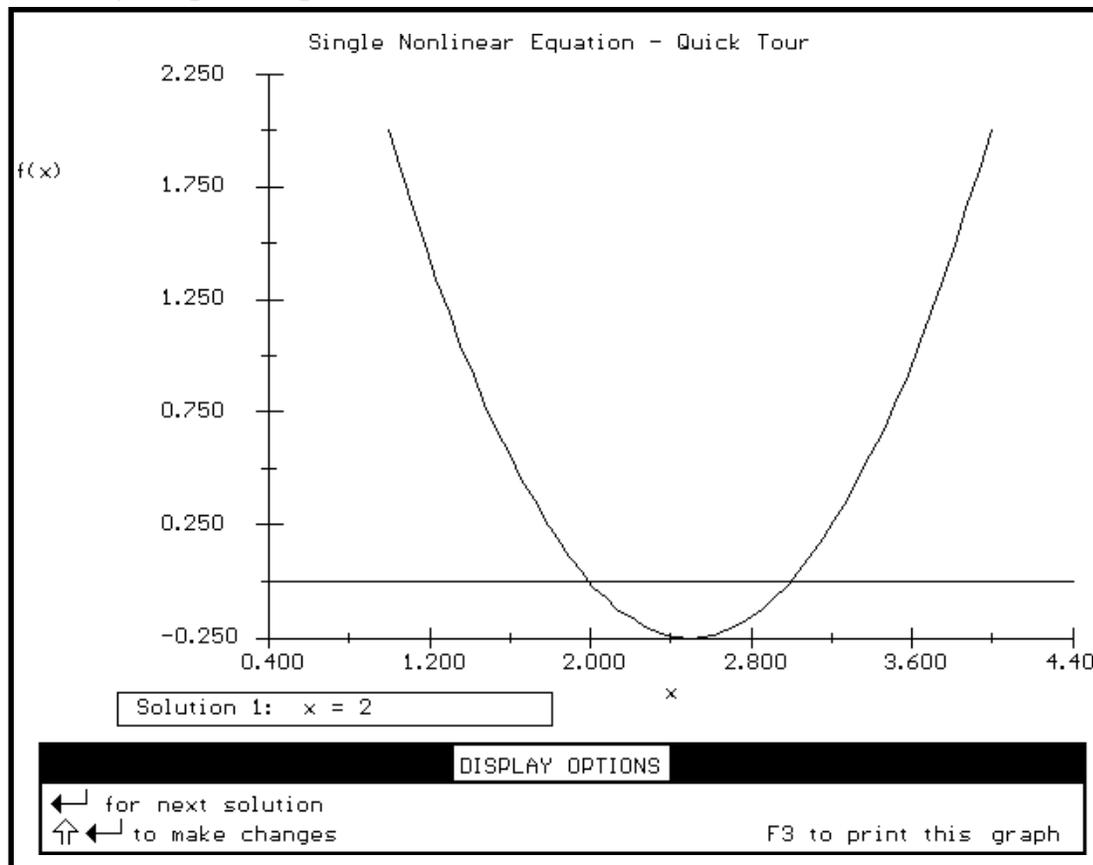
Press enter (⏎) for the second solution.

```
Solution 2:  x = 3
```

A shift-return (⇧⏎) will return you to the Problem Options Display.

SOLVING A SYSTEM OF NONLINEAR EQUATIONS

Next, you will solve two nonlinear equations with two unknowns. To enter this new set of equation press ⇧ F8 for a new problem, then press ⏎ followed by "y" to enter a new problem.

The equations that will be solved are:

$$k\,C_{A1}^2 = \frac{v\,(C_{Af} - C_{A1})}{V} \qquad \text{and} \qquad k\,C_{A2}^2 = \frac{v\,(C_{A1} - C_{A2})}{V}$$

where k = 0.075; v = 30; C_{Af} = 1.6 ; C_{A2} = 0.2C_{Af} .
Thus there are two unknowns: C_{A1} and V.

To solve this system of equations, each nonlinear equation must be rewritten in the form f(x) = (an expression that is to have the value of zero at the solution). The appropriate forms for these equations are:

$$f\,(C_{A1}) = kC_{A1}^2 - \frac{v\,(C_{Af} - C_{A1})}{V}$$

and

$$f\,(V) = kC_{A2}^2 - \frac{v\,(C_{A1} - C_{A2})}{V}$$

All equations can be entered into POLYMATH as shown below. Note that each of the problem unknowns (C_{A1} and V) should appear once and only once inside the brackets in the left of the equal sign. The unknown variable may not be in that particular equation. POLYMATH just needs to know the variable names that you are using in your problem. The explicit algebraic equations may be entered directly. Please enter the equations as given below. The order of the equation is not important as POLYMATH will order the equations during problem solution.

```
Equations
      f(Ca1)=k*Ca1^2-v*(Caf-Ca1)/V
      f(V)=k*Ca2^2-v*(Ca1-Ca2)/V
      k=0.075
      Caf=1.6
      v=30
      Ca2=0.2*Caf
```

Press ⇧F7 to solve this system of equations.

For two or more nonlinear equations, POLYMATH requires an initial estimate to be specified for each unknown.

```
Enter initial value for Ca1
 >_
```

While the solution method used is very robust, it often will not be able to find the solution if unreasonable initial estimated are entered. In this example, physical considerations dictate that C_{A1} must be smaller than C_{A0} and larger than C_{A2}. So please enter initial estimate of Ca1 as 1.0. As for V, any positive value up to about V=3900 can be a reasonable estimate. Please use the initial value of 300 for V in this Quick Tour example.

After entering the initial values, this example problem should be:

```
 Equations                                              Initial values

→ f(Ca1)=k*Ca1^2-v*(Caf-Ca1)/U                                1
  f(U)=k*Ca2^2-v*(Ca1-Ca2)/U                                 300
  k=0.075
  v=30
  Caf=1.6
  Ca2=0.2*Caf
```

Please press ⇧-F7 to solve the problem. The solution process will start and its progress will be indicated on the screen by an arrow moving along a ruler scale. For most computers, the solution is so fast that the display of the iterations in the numerical solution to a converged solution will not be seen. When visible, the arrow indicates how far from zero the function values are at a particular stage of the solution on a logarithmic scale. Details are given in the Help Section by pressing F6.

The results are given after any keypress as shown below:

	Solution	
Variable	Value	f()
Ca1	0.601997	-2.04e-15
U	1101.55	-6.739e-16
k	0.075	
v	30	
Caf	1.6	
Ca2	0.32	

Please note that the values of the various nonlinear equation functions (nearly zero) are given along the with values of all the problem variables.

This concludes the Quick Tour problem using the Simultaneous Nonlinear Algebraic Equation Solver. If you wish to stop working on POLYMATH, please follow the exiting instructions given below.

EXITING OR RESTARTING POLYMATH

A ⇑ - F10 keypress will always stop the operation of POLYMATH and return you to the Program Selection Menu. THIS _ACTION WILL DELETE THE EXISTING PROBLEM._ The program can be exited or restarted from the Program Selection Menu.

SELECTION OF INITIAL ESTIMATES FOR THE UNKNOWNS

The solution algorithm requires specification of initial estimates for all the unknowns. Generally speaking, closer initial estimates have a better chance of converging to the correct solution.

If you wish to solve only a single nonlinear equation, the program will plot the equation so that the location of the roots (if any) can be seen. The program will then show the roots. If no roots exist in the chosen range, the plot will indicate what range should be explored to have the nonlinear function f( ) cross zero.

When several equations are to be solved, the selection of the initial values is more complicated. First, the user should try to find the limiting values for the variables using physical considerations. (For example: The mole or mass fraction of a component can neither be negative nor greater that 1; the temperature of cooling water can be neither below freezing nor above boiling; etc.) Typical initial estimates are taken to be mid range.

Users should be particularly careful no to select initial estimates where some of the functions may be undefined. (For example, $f(xa)=1/(xa-xb)+...$ is undefined whenever $xa=xb$; $f(xb)=\log(1-xb)$ is undefined whenever $xb>=1$; etc.) The selection of such initial estimates will stop the POLYMATH solution, and an error message will be displayed.

METHOD OF SOLUTION

For a single nonlinear equation, the user must specify an interval in which the real root(s) can be found. The program will first attempt to locate points or regions where the function is undefined inside this interval*. If the equations are too complicated for determination of discontinuity points, a warning message is issued.

_____

*For details of the method, see Shacham, O. and Shacham, M., Acm. Trans. Math. Softw., **16** (3), 258-268 (1990).

The function is plotted and smaller intervals in which root(s) are located by a sign change of the function. The Improved Memory Method*, which employs a combination of polynomial interpolation and bisection, is used to converge to the exact solution inside those intervals. Iterations are stopped when the relative error is $<10^{-10}$. Numerical pertubation is used to calculate needed derivatives.

For solving a system equations, the bounded Newton-Raphson (NR) method is used. The NR direction is initially used, but the distance is limited by the possible discontinuities **. The progress in iteration will be either the full NR step or close to the first point of discontinuity in that direction. The logarithm of the Euclidean norm of the function residuals is displayed during solution. Norm values below 10^{-5} are not shown. Iterations end when the norm of the relative error is $< 10^{-10}$.

TROUBLE SHOOTING

Most error messages are self-explanatory and suggest needed action. Other less obvious error messages and suggested actions are given below:

"Circular dependency detected."

This message appears while inputting equations when an attempt is made to define a variable as a function of another variable that was already defined as a function of the new variable. For example, attempting to define y=z/x, when z is already defined as a function of y, will cause this error. This can be prevented by writing the equation in a implicit form: f(y)=y-z/x.

"Solution process halted because ..."

This message for simultaneous nonlinear equations suggests that:
1. The system contains equations which are very nonlinear.
2. The initial estimates are too far from the solution.
or 3. **The problem has no solution.**

Equations can be made less nonlinear by eliminating division by unknowns (multiplying both sides of the equation by the expression that contains the unknowns). Often, substitution and reordering can bring the system of equations to a form that only one equation is implicit. Realistic initial estimates can often help achieve a solution. Finally, nonconvergence may indicate that the set of equations set has no solution. Check the problem setup in this case and pay particular attention to the units.

---

*For details of this method, see Shacham, M., Computers & Chem. Engng., 14 (6), 621-629 (1990)

For details of the method, see Shacham, O. and Shacham, M., Acm. Trans. Math. Softw., **16 (3), 258-268 (1990).

LINEAR EQUATION SOLVER

QUICK TOUR

This chapter is intended to give a very brief discussion of the operation of the POLYMATH Linear Equation Solver.

LINEAR EQUATION SOLVER

The user can solve up to a combination of 32 simultaneous linear equations. The equations are entered in matrix form.

STARTING POLYMATH

To begin, please have POLYMATH loaded into your computer as detailed in Chapter 2. Here it is assumed that your computer is set to the hard disk subdirectory containing the POLYMATH package. At the prompt (assumed C:\POLYMAT4 here), you should enter "polymath"

C:\POLYMAT4>polymath

then press the Return (⬅⎯) key. The Main Program Menu should then appear: The Program Selection Menu should then appear, and you should enter "3" on the keyboard to select the Linear Equation Solver.

```
   POLYMATH


      Linear
      Equation
      Solver




 ⬅⎯  to begin.
F6 for HELP menu.
F7 for sample problems.
F8 for POLYMATH menu.
F9 for file options.
⇧ F9 for the credits.
```

```
The following keys are
    always active:

⇧ F10 to return to
       this display
F4 for calculator
F5 for unit converter
```

Once that POLYMATH is loaded, please utilize the Help Menu by pressing F6 for information regarding the use of the Linear Equation Solver. This Help Section is given below:

```
        ENTERING DATA INTO THE LINEAR EQUATION SOLVER
        _____

    The purpose of this program is to solve systems of up to 32 linear equations,
where the coefficients and constants are entered in matrix form.

    On the main data screen, the matrix of coefficients (up to 6 columns and 18
rows of it) and the vector of coefficients (up to 18 rows of it) are displayed.
Each equation (row) is indicated by a number, and each column by a variable name
(x1, x2, ..., xn, b).

    At any given time, one of the boxes is highlighted.  This is the current box.
You can move the highlight by using the arrow keys (↑,↓,→,←) and the Home,
End, PageUp and PageDown keys (if you use the numeric keypad keys, make sure
NumLock is off).  The Home and End keys function as Page Left and Page Right,
respectively.

    To enter or modify a value in a data cell, move the highlight to the
appropriate box and either start typing in a number, or press <Enter> to edit
the value already in the box.  When you are done typing in the number, you may
press the <Tab> key to move to the next box in the current row, the ↑ or ↓ key
to move to the box above or below the current one, or <Enter> to move to the
first box in the next row.  Note that if you started editing by pressing <Enter>,
pressing <Enter> when done will not move the highlight.

    Column names may not be changed.
```

This Help Section gives detailed information for entering a system of linear equations. Press any key to return from the Help Section to the program, and your display should be at the Main Menu for the Linear Equation Solver. (An alternate command to reach the Main Menu is the ⇑F10 keypress.)

To begin the first Quick Tour example, please press the Return key (◀─┘) from the Main Menu. This will give the Task Menu as shown below:

```
┌──────────────────────────────────────────────────────┐
│                    ▐ TASK MENU ▌                       │
│                                                        │
│                                                        │
│        ◀─┘    to enter a new problem.                  │
│                                                        │
│        F7    for SAMPLE PROBLEMS MENU.                  │
│                                                        │
│        F9    for LIBRARY OPTIONS.                      │
│                                                        │
│    DOS file options:                                   │
│                                                        │
│        S. Save current problem on file.                │
│                                                        │
│        L. Load problem from file.                      │
│                                                        │
│          ⇑  F10 for the MAIN MENU                      │
│                                                        │
└──────────────────────────────────────────────────────┘
```

SOLVING FIVE SIMULTANEOUS LINEAR EQUATIONS

A typical problem for simultaneous linear equations is given below for the variables x1 through x5:

$$x1 + 0.5\,x2 + 0.333333\,x3 + 0.25\,x4 + 0.2\,x5 = 0.0$$
$$0.5\,x1 + 0.333333\,x2 + 0.25\,x3 + 0.2\,x4 + 0.166667\,x5 = 1.0$$
$$0.333333\,x1 + 0.25\,x2 + 0.2\,x3 + 0.166667\,x4 + 0.142857\,x5 = 0.0$$
$$0.25\,x1 + 0.2\,x2 + 0.166667\,x3 + 0.142857\,x4 + 0.125\,x5 = 0.0$$
$$0.2\,x1 + 0.166667\,x2 + 0.142857\,x3 + 0.125\,x4 + 0.111111\,x5 = 0.0$$

The above problem in stored as a Sample Problem in POLYMATH. To recall the above problem, press F7 from the Task Menu of the Linear Equation Solver. Then select problem number "2" to obtain the Problem Options Menu shown below:

```
                              Sample Problem 2
Name      x1        x2        x3        x4        x5              b
   1 |        1 |      0.5 | 0.333333 |     0.25 |      0.2 |               0 |
   2 |      0.5 | 0.333333 |     0.25 |      0.2 | 0.166667 |               1 |
   3 | 0.333333 |     0.25 |      0.2 | 0.166667 | 0.142857 |               0 |
   4 |     0.25 |      0.2 | 0.166667 | 0.142857 |    0.125 |               0 |
   5 |      0.2 | 0.166667 | 0.142857 |    0.125 | 0.111111 |               0 |

                          PROBLEM OPTIONS
   ←┘  to edit current box.    ↑,↓,→,←, PgUp, PgDn, Home, End to move pointer.
                           T.  to enter title
  ⇧ F7 to solve this problem.              F6 for helpful information.
  ⇧ F8 for file and library options.              F3 to print problem.
```

Solve this system of equations by pressing ⇧F7 which should yield the results and the Display Options Menu on the next page. Remember that this keypress combination is accomplished by pressing and holding the Shift key and then pressing the F7 function key.

```
                        Sample Problem 2
                            Solution

                    Variable      Value

                       x1        -300
                       x2        4800
                       x3        -18900
                       x4        26880
                       x5        -12600

                          DISPLAY OPTIONS
     d. Output results to DOS file.              F3 to print results.
   ⇧ F8 for new problem or library              ⇧ ←┘   to make changes.
```

Lets explore making changes to this system of equations. This is accomplished by first pressing ⇑◄─┘ to "make changes" to the problem. Use the arrow keys to take the highlighted box to the top of the "b" of constants for the equation. Please delete the 0 and enter 1.0 in this box which corresponds to changing the first linear equation to:

$$x1 + 0.5\ x2 + 0.333333\ x3 + 0.25\ x4 + 0.2\ x5 = 1.0$$

This involves using the arrow key and pressing the return key (◄─┘) when the highlighted box is in the desired location as shown.

```
              b
        ┌──────────────┐
        │            0 │
        ├──────────────┤
        │            1 │
        ├──────────────┤
        │            0 │
        ├──────────────┤
        │            0 │
        ├──────────────┤
        │            0 │
        └──────────────┘
```

Then enter the new value at the cursor:

```
  ┌────────────────────────┐
  │ ⟩ 1_                    │
  │                        │
  │ Tab: next column        │
  └────────────────────────┘
```

Please solve the problem by pressing ⇑F7. The results are shown below:

Sample Problem 2

Variable	Solution Value
x1	-275
x2	4500
x3	-17850
x4	25480
x5	-11970

This concludes the Quick Tour Problem for Simultaneous Linear Equations. When you are ready to leave this program and return to the Program Selection Menu, use the ⇑ F10 keypress which is discussed below.

EXITING OR RESTARTING POLYMATH

A ⇑ F10 keypress will always stop the operation of POLYMATH and return you to the Program Selection Menu. THIS *ACTION WILL DELETE THE EXISTING PROBLEM.* The program can be exited or restarted from the Program Selection Menu.

REGRESSION

QUICK TOUR

This chapter is intended to give a very brief overview of the operation of the POLYMATH Polynomial, Multiple Linear and Nonlinear Regression program.

REGRESSION PROGRAM

This program allows you to input numerical data into up to 30 columns, with up to 100 data points in each column. The data can be manipulated by defining expressions containing the names of previously defined columns. Relationships between different variables (columns of data) can be found using polynomial, multiple linear and nonlinear regression as well as cubic spline interpolation. Fitted curves can be interpolated, differentiated and integrated. Graphical output of the fitted curves and expressions is presented, and a statistical analysis of the parameters found during the regressions is given.

STARTING POLYMATH

To begin, please have POLYMATH loaded into your computer as detailed in Chapter 2. Here it is assumed that your computer is set to the hard disk subdirectory or floppy drive containing the POLYMATH package. At the prompt (assumed C:\POLYMAT4 here), you should enter "polymath"

                C:\POLYMAT4 > polymath

then press the Enter (↵) key. The Program Selection Menu should then appear, and you should enter "4" on the keyboard to select the Polynomial, Multiple Linear and Nonlinear Regression program. This should bring up the Main Program Menu as given in the next page.

In order to save time in entering data points during this quick tour, we will use sample problems which have been stored in POLYMATH. Press F7 to access the Sample Problems Menu from the Main Program Menu.

QUICK TOUR PROBLEM 1

Let us consider a fairly typical application of the Regression Program in which some data are available. When these data are fitted to a polynomial

within POLYMATH, the polynomial expression has the form:

$$P(x) = a_0 + a_1x + a_2x^2 + ... + a_nx^n$$

where y is the dependent variable, x is the independent variable, and the parameters are a_0 ...a_n. Variable "n" here represents the degree of the polynomial. In POLYMATH, the maximum degree which is shown is 5. The above polynomial expression gives a relationship between the dependent variable and the independent variable which is obtained by determining the parameters according to a least squares objective function. Data points are usually available which give x and y values from which the parameters a_0... a_n can be determined.

```
 POLYMATH

    Polynomial,
  Multiple Linear
   and Nonlinear
    Regression

←┘  to begin.
F6 for HELP menu.
F7 for sample problems.
F8 for POLYMATH menu.
F9 for file options.
⇧ F9 for the credits.
```

```
The following keys are
   always active:

⇧ F10 to return to
        this display
F4 for calculator
F5 for unit converter
```

RECALLING SAMPLE PROBLEM 3

After pressing F7 at the Main Program Menu, the Sample Problems Menu should appear on your screen as shown on the next page.. The sample problem to be discussed should be retrieved by pressing "3" on the keyboard. This will result in the Problem Options Display which includes 10 data points of x and y as shown on the next page.

```
┌─────────────────────────────────────────────────────────────┐
│                    SAMPLE PROBLEMS MENU                      │
│  1   One independent variable fitted to an equation of the form │
│          Y = a₀Xᵃ1      linearized to:                      │
│          lnY = a0 + a1*lnX                                   │
│  ──────────────────────────────────────────────────────────  │
│  2   One independent variable fitted to a nonlinear equation:  │
│          Y = 10 { a₀ + a₁/(X+z) }                           │
│  ──────────────────────────────────────────────────────────  │
│  3   One independent variable fitted to a polynomial.          │
│  ──────────────────────────────────────────────────────────  │
│  4   Two independent variables fitted to a linear equation:    │
│          Y = a₀ + a₁X₁ + a₂X₂                               │
│  ──────────────────────────────────────────────────────────  │
│  5   Two independent variables fitted to an equation of the form: │
│          Y = a₀X₁ᵃ1X₂ᵃ2      linearized and regressed as:   │
│          lnY = a0 + a1*lnX1 + a2*lnX2                        │
│  ──────────────────────────────────────────────────────────  │
│  6   Three independent variables fitted to an equation of the form: │
│          Y = 1000 X₁/(a₀ + a₁X₁ + a₂X₂ + a₃X₃)             │
│              linearized to:                                   │
│          1000/Y = a1 + a0*(1/X1) + a2*(X2/X1) + a3*(X3/X1)   │
│              regressed as:                                    │
│          y = a1 + a0*x1 + a2*x2 + a3*x3                      │
│  ──────────────────────────────────────────────────────────  │
│                       F8 to return                          │
└─────────────────────────────────────────────────────────────┘
```

Menu items rendered:

1 One independent variable fitted to an equation of the form
$$Y = a_0 X^{a1} \quad \text{linearized to:}$$
$$lnY = a0 + a1*lnX$$

2 One independent variable fitted to a nonlinear equation:
$$Y = 10^{\{ a_0 + a_1/(X+z) \}}$$

3 One independent variable fitted to a polynomial.

4 Two independent variables fitted to a linear equation:
$$Y = a_0 + a_1 X_1 + a_2 X_2$$

5 Two independent variables fitted to an equation of the form:
$$Y = a_0 X_1^{a1} X_2^{a2} \quad \text{linearized and regressed as:}$$
$$lnY = a0 + a1*lnX1 + a2*lnX2$$

6 Three independent variables fitted to an equation of the form:
$$Y = 1000\, X_1/(a_0 + a_1 X_1 + a_2 X_2 + a_3 X_3)$$
linearized to:
$$1000/Y = a1 + a0*(1/X1) + a2*(X2/X1) + a3*(X3/X1)$$
regressed as:
$$y = a1 + a0*x1 + a2*x2 + a3*x3$$

F8 to return

Sample Problem 3

Name	X	Y					
1	0.23	5.64					
2	1.01	7.83					
3	2.29	17.04					
4	2.87	21.38					
5	4.15	24.56					
6	5.36	16.21					
7	5.51	14.57					
8	6.36	0.78					
9	6.84	-7.64					
10	7	-12.52					
11							
12							
13							
14							
15							
16							
17							
18							

```
┌──────────────────── PROBLEM OPTIONS ──────────────────[NUM]─┐
│  ←┘  to edit current box.    ↑,↓,→,←, PgUp, PgDn, Home, End to move pointer. │
│  ⇧←┘ for row/column options.                    T.  to change title. │
│  ⇧F7 to fit a curve or do regression.      F6 for helpful information. │
│  ⇧F8 for file and library options.              F3 to print problem. │
└─────────────────────────────────────────────────────────────┘
```

FITTING A POLYNOMIAL

The Problem Options Menu includes problem editing, library, printing, help and solution options. To fit a polynomial to the data of Y versus X you should select the "⇑ F7 to fit a curve or do regression" option. After pressing ⇑ F7 the following "Solution Options" menu appears:

```
┌────────────────────────────────────────────────────────────────┐
│                      SOLUTION OPTIONS                            │
├────────────────────────────────────────────────────────────────┤
│  l. Do linear regression.   L. Linear regression without free parameter. │
│  p. Fit a polynomial.       P. Polynomial passing through origin. │
│  s. Fit a cubic spline.     R. Do nonlinear regression.          │
│              ⇧ ⏎ or F8 for problem options                      │
└────────────────────────────────────────────────────────────────┘
```

After pressing "p" (lower case), you should be asked for the name of the independent variable's column, as shown below:

```
┌────────────────────────────────────────────────────────────────┐
│  Enter independent column name ( ⏎ to cancel):                 │
│  ≫ _                                                            │
└────────────────────────────────────────────────────────────────┘
```

You should enter a capital "X" (upper case) as name of the independent variable and press ⏎. The same question regarding the dependent variable will be presented. Please enter a capital "Y" (upper case) at the arrow. The following display should appear:

Deg.	1	2	3	4	5
a0	18.2007	-2.41992	3.68736	6.31569	6.21607
a1	-2.2623	15.8712	4.23908	-4.23011	-3.78885
a2		-2.41526	1.63518	6.95477	6.52291
a3			-0.368083	-1.49302	-1.33232
a4				0.0760754	0.0508872
a5					0.00140166
var.	135.88	12.263	1.49732	0.257127	0.319264

```
┌────────────────────────────────────────────────────────────────┐
│                      DISPLAY OPTIONS                            │
├────────────────────────────────────────────────────────────────┤
│  1, 2, 3, 4, 5 to choose a polynomial   r. Residuals plot   s. save results │
│        x.  Y value for specific X       y.  X value for specific Y │
│        i.  Integrate polynomial         d.  differentiate polynomial │
│  F9 for statistical analysis.    F3 to edit graph    F8 for problem options │
└────────────────────────────────────────────────────────────────┘
```

On this display the coefficients of the polynomial P(x), up to the fifth order are shown together with the value of the variance. One of the polynomials is highlighted by having a box around it. This is the lowest order polynomial, such that higher order polynomial does not give significantly better fit. The same polynomial is also plotted versus the experimental data. Other polynomials can be highlighted and plotted by pressing a number between 1 and 5. There are many additional calculations and other operations that can be carried out using the selected polynomial. Please make sure the highlighted box is on the 4th degree polynomial. Let us find the value of X for Y = 10. To do that you should press "y" and enter after the prompt regarding the value of Y: "10". The following display results:

Deg.	1	2	3	4	5
a0	18.2007	-2.41992	3.68736	6.31569	6.21607
a1	-2.2623	15.8712	4.23908	-4.23011	-3.78885
a2		-2.41526	1.63518	6.95477	6.52291
a3			-0.368083	-1.49302	-1.33232
a4				0.0760754	0.0508872
a5					0.00140166
var.	135.88	12.263	1.49732	0.257127	0.319264

DISPLAY OPTIONS
```
Y = 10
X = 1.36962, 5.83496
Press any key to continue.
```
F9 for statistical analysis.   F3 to edit graph   F8 for problem options
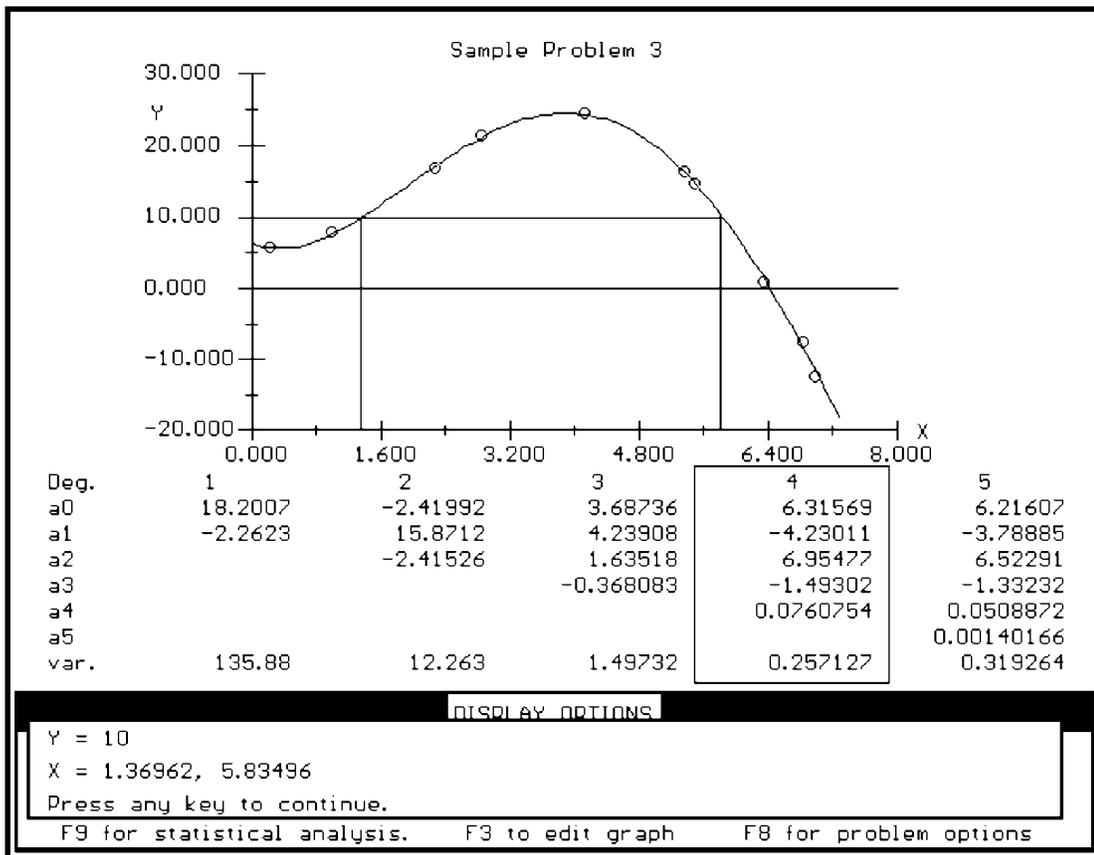
The resultant X values are shown both graphically and numerically. For Y = 10 there are two X values, X = 1.36962 and X = 5.83496.

FITTING A CUBIC SPLINE

We will now fit a cubic spline to these data of Sample Problem 3. Please press F8 two times to return to the Problems Options Menu. Then press ⇑ F7 to "fit a curve or do regression". The Solutions Options Menu should appear.

```
┌─────────────────────────────────────────────────────────────┐
│                    SOLUTION OPTIONS                          │
│  l. Do linear regression.   L. Linear regression without free parameter. │
│  p. Fit a polynomial.       P. Polynomial passing through origin.        │
│  s. Fit a cubic spline.     R. Do nonlinear regression.                  │
│                             ⇧ ◀┘ or F8 for problem options              │
└─────────────────────────────────────────────────────────────┘
```

Enter "s" (lower case) for a cubic spline followed by "X" and then "Y". The following display should present the results:

Sample Problem 3

```
┌─────────────────────────────────────────────────────────────┐
│                    DISPLAY OPTIONS                           │
│    x.  Y value for specific X.      y.  X value for specific Y │
│       i.  Integrate spline.         d.  Differentiate spline.  │
│  F6 for HELP      F3 to edit graph    ⇧ ◀┘  or F8 for problem options │
└─────────────────────────────────────────────────────────────┘
```
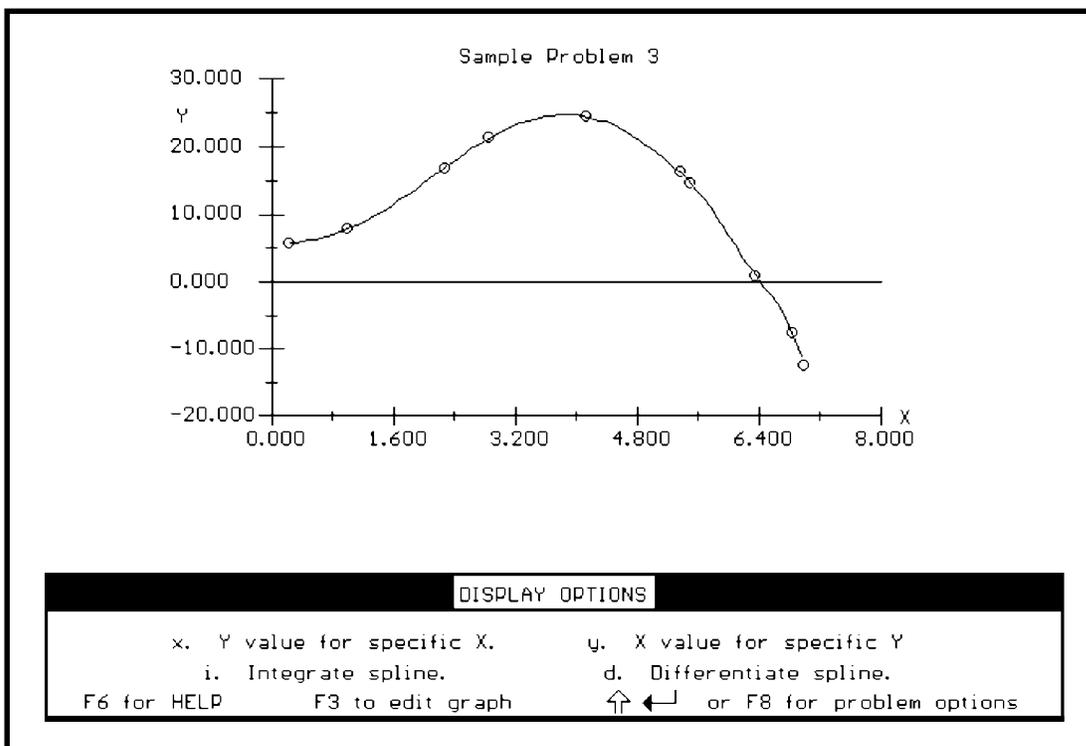
EVALUATION OF AN INTEGRAL WITH THE CUBIC SPLINE

Please take options "i" and request the initial value for the integration to be "1" at the arrow:

```
║  Enter first value for X :》1_                              ║
```

Press ◀┘ and then enter "6" at the arrow for the find value of the integration.

```
║  Enter second value for X :》6_                             ║
```

Press ◀┘ to have the resulting integration shown on the next display with both graphical and numerical results:

Sample Problem 3

```
        30.000 ┬
          Y
        20.000 ┼
        10.000 ┼
         0.000 ┼
       -10.000 ┼
       -20.000 ┴┬────┬────┬────┬────┬────┬ X
              0.000  1.600  3.200  4.800  6.400  8.000
```

```
                        ┌──────────DISPLAY OPTIONS──────────┐
                        │ x₁ = 1          x₂ = 6            │
              x.   Y    │ Integral = 90.579             ic Y │
               i.       │ Press any key to continue.    ne.  │
       F6 for HELP      F3 to edit graph      ⇧ ⏎    or F8 for problem options
```
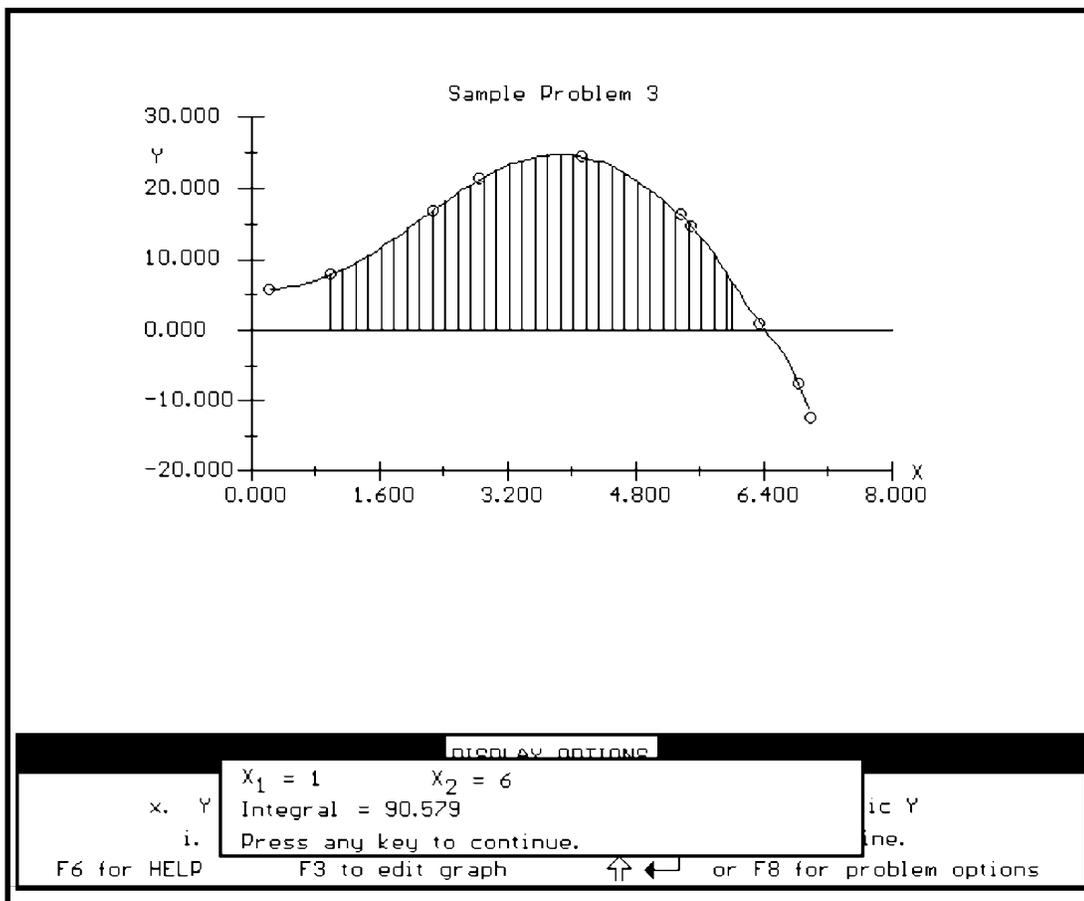
Please press any key to end this Sample Problem 3.

MULTIPLE LINEAR REGRESSION

It will often be useful to fit a linear function of the form:

$$y(\underline{x}) = a_0 + a_1 x_1 + a_2 x_2 + ... + a_n x_n$$

where x_1, x_2, ..., x_n are n independent variables and y is the dependent variable, to a set of N tabulated values of $x_{1,i}$, $x_{2,i}$, ... and y ($\underline{x}_i$). We will examine this option using Sample Problem 4.

RECALLING SAMPLE PROBLEM 4

First exit to the main title page by pressing ⇧ F10. Press F7 to access the Sample Problems Menu, and select problem number 4 by pressing "4". (The problem display is shown on the next page).

```
                          Sample Problem 4
Name │   X1   │   X2   │    Y   │        │        │        │
  1  │    78  │    1   │   1.5  │        │        │        │
  2  │  113.5 │   3.2  │    6   │        │        │        │
  3  │   130  │   4.8  │   10   │        │        │        │
  4  │   154  │   8.4  │   20   │        │        │        │
  5  │   169  │   12   │   30   │        │        │        │
  6  │   187  │  18.5  │   50   │        │        │        │
  7  │   206  │  27.5  │   80   │        │        │        │
  8  │   214  │   32   │  100   │        │        │        │
  9  │        │        │        │        │        │        │
 10  │        │        │        │        │        │        │
 11  │        │        │        │        │        │        │
 12  │        │        │        │        │        │        │
 13  │        │        │        │        │        │        │
 14  │        │        │        │        │        │        │
 15  │        │        │        │        │        │        │
 16  │        │        │        │        │        │        │
 17  │        │        │        │        │        │        │
 18  │        │        │        │        │        │        │
                          PROBLEM OPTIONS                    NUM
  ⏎ to edit current box.   ↑,↓,→,←, PgUp, PgDn, Home, End to move pointer.
  ⇧ ⏎ for row/column options.                    T.  to change title.
  ⇧ F7 to fit a curve or do regression.          F6 for helpful information.
  ⇧ F8 for file and library options.             F3 to print problem.
```

SOLVING SAMPLE PROBLEM 4

After you press ⇧ F7 "to fit a curve or do regression", the following Solution Options Menu should appear:

```
                          SOLUTION OPTIONS
  l. Do linear regression.   L. Linear regression without free parameter.
  p. Fit a polynomial.       P. Polynomial passing through origin.
  s. Fit a cubic spline.     R. Do nonlinear regression.
                          ⇧ ⏎ or F8 for problem options
```

This time press "l" (lower case letter "l") to do "linear regression". You will be prompted for the first independent variable (column) name.

```
                          SOLUTION OPTIONS
  l.│ Enter 1st independent column name ( ⏎ to end):       │r.
  p.│ ≫ X1_                                                 │
  s.│                                                       │
                          ⇧ ⏎ or F8 for problem options
```
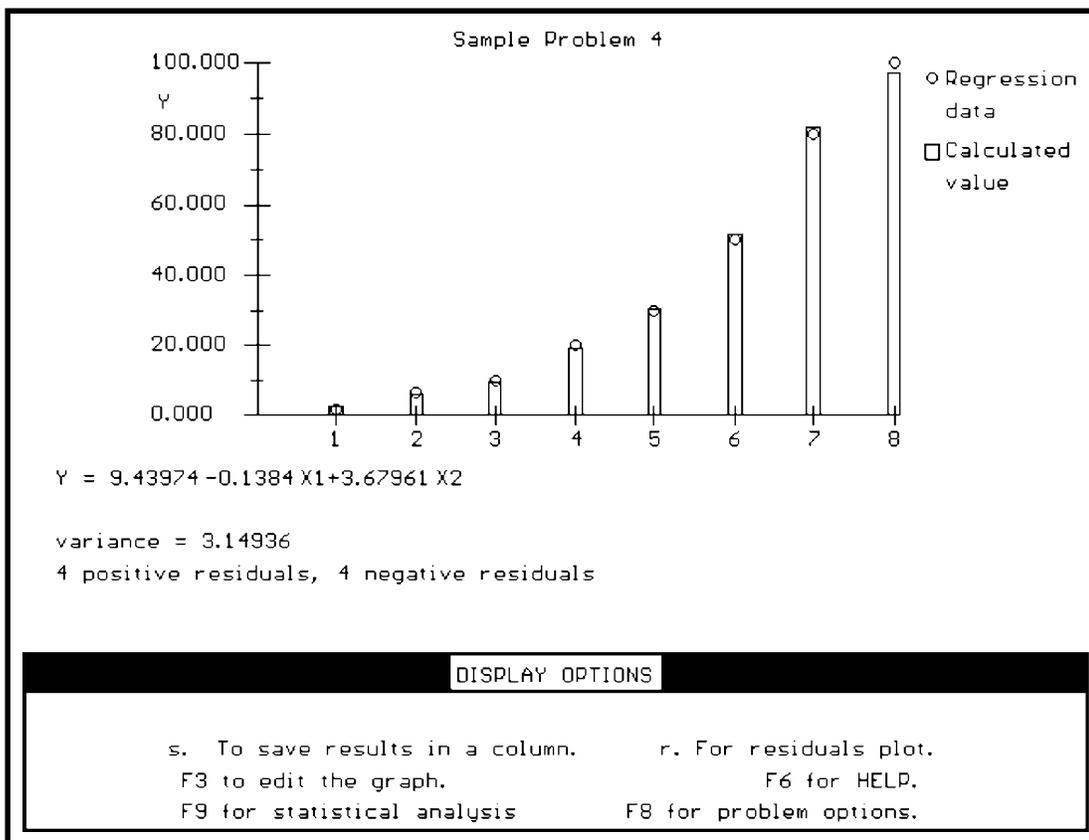
Please type in "X1" at the arrow and press ⏎. You will be prompted for the 2nd independent variable. Enter "X2" as the second independent variable name and press ⏎ once again. A prompt for the 3rd independent variable will appear. You should press ⏎ here without typing in anything else, since there are no additional independent variables.

At the prompt for the dependent variable (column) name shown below you should type "Y" and press ←⎦.

```
┌──────────────────────────────────────────────────────────────┐
│                      SOLUTION OPTIONS                          │
│  1. ┌─────────────────────────────────────────────┐           │
│     │ Enter dependent column name ( ←⎦ to cancel):│       r. │
│  p. │ ≫ Y_                                         │           │
│     └─────────────────────────────────────────────┘           │
│  s.                                                            │
│                      ↑↑ ←⎦ or F8 for problem options           │
└──────────────────────────────────────────────────────────────┘
```

Once the calculations are completed, the linear regression (or correlation) is presented in numerical and graphical form.

Sample Problem 4

Y = 9.43974 −0.1384 X1+3.67961 X2

variance = 3.14936
4 positive residuals, 4 negative residuals

DISPLAY OPTIONS

s. To save results in a column.   r. For residuals plot.
F3 to edit the graph.   F6 for HELP.
F9 for statistical analysis   F8 for problem options.

Please note that the correlation the equation for variable "Y" has the form of the linear expression: $Y = a_0 + a_1X_1 + a_2X_2$ where $a_0 = 9.43974$, $a_1 = -0.1384$ and $a_2 = 3.67961$. This graphical display of Sample Problem 4 presents the regression data versus the calculated values from the linear regression. The numerical value of the variance and the number of the positive and negative residuals give an indication regarding the validity of the assumption that Y can be represented as linear function of X1 and X2. The results in this case indicate a good fit between the observed data and the correlation function.

The Display Options Menu allows the user to use an "s" keypress "to save results in a column". This refers to saving the calculated value of Y from the linear regression to the Problems Options Display under a column name provided by the user. The "r" keypress from the Display Options Menu give a statistical residual plot as shown below:

```
                          Sample Problem 4
      2.500  ┬                                              o

     error   ┼
      1.500  ┼
             ┼            o       o
      0.500  ┼    o
             ├──────────────────────────────────────────────
                              o
     -0.500  ┼
            ┼o
     -1.500  ┼
             ┼                        o
                                                o
     -2.500  ┼──┼────┼────┼────┼────┼────┼────┼────┼────┼  Y
            0.000   20.000   40.000   60.000   80.000  100.000

  error = Y - (9.43974 -0.1384 X1+3.67961 X2)
```
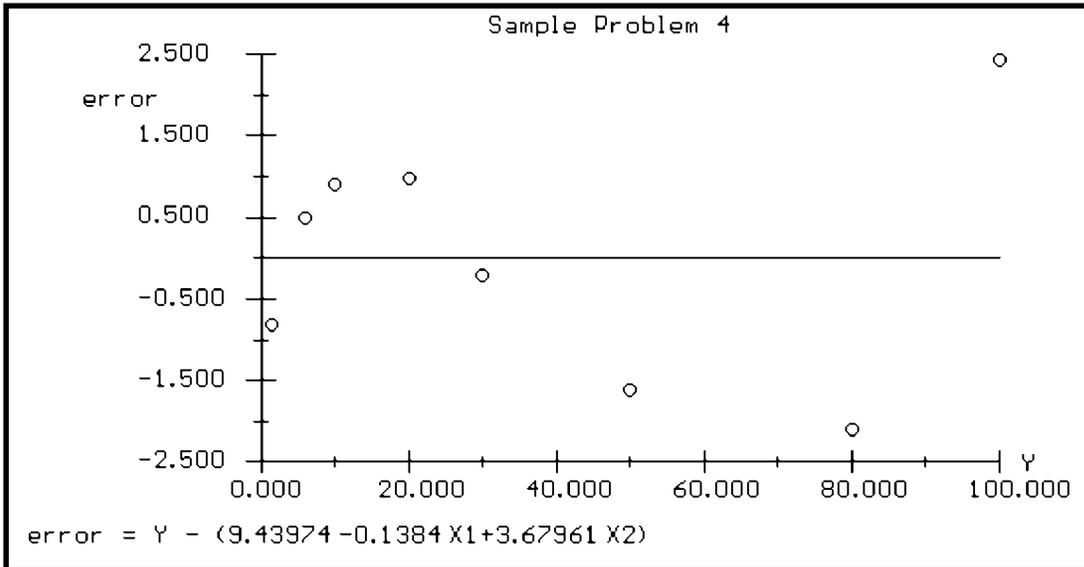
The "F9" keypress from the Display Options Menu give a statistical summary:

```
                         Sample Problem 4

    Matrix of correlation coefficients for the linear correlation equation
              1              2              3
  1 │1             │-0.973045     │0.8467        │
  2 │-0.973045     │1             │-0.935468     │
  3 │0.8467        │-0.935468     │1             │
```

		0.95 conf.	lower	upper
Param.	Value	interval	limit	limit
1	9.43974	11.1725	-1.73278	20.6123
2	-0.1384	0.103488	-0.241888	-0.0349122
3	3.67961	0.423457	3.25615	4.10307

The confidence intervals given in the statistical summary are very useful in interpreting the validity of the linear regression of data.

This concludes Sample Problem 4 which illustrated multiple linear regression.

TRANSFORMATION OF VARIABLES

A nonlinear correlation equation can be often brought into a linear form by a transformation of the data. For example, the nonlinear equation:

$$Y = a_0 \, X_1^{a_1} \, X_2^{a_2}$$

can be linearized by taking logarithm of both sides of the equation:

$$\ln Y = \ln a_0 + a_1 \ln X_1 + a_2 \ln X_2.$$

To demonstrate this option please recall Sample Problem 5. To do this, please press ⇑ F10 to get to the Main Program Menu, F7 to access the Sample Problems Menu and select Sample Problem number 5. This should result in the Problem Option Display below:

```
                           Sample Problem 5
Name │    X1    │    X2    │    Y     │   lnX1    │   lnX2    │    lnY    │
   1 │  0.475   │  0.475   │  1.063   │ -0.74444  │ -0.74444  │ 0.0610951 │
   2 │  0.465   │  0.465   │  1.05    │ -0.765718 │ -0.765718 │ 0.0487902 │
   3 │  0.421   │  0.42    │  1.2     │ -0.865122 │ -0.867501 │ 0.182322  │
   4 │  0.32    │  0.52    │  0.6     │ -1.13943  │ -0.653926 │ -0.510826 │
   5 │  0.54    │  0.54    │  0.9375  │ -0.616186 │ -0.616186 │ -0.06454  │
   6 │  0.57    │  0.37    │  2.063   │ -0.562119 │ -0.994252 │ 0.724161  │
   7 │          │          │          │           │           │           │
   8 │          │          │          │           │           │           │
   9 │          │          │          │           │           │           │
  10 │          │          │          │           │           │           │
  11 │          │          │          │           │           │           │
  12 │          │          │          │           │           │           │
  13 │          │          │          │           │           │           │
  14 │          │          │          │           │           │           │
  15 │          │          │          │           │           │           │
  16 │          │          │          │           │           │           │
  17 │          │          │          │           │           │           │
  18 │          │          │          │           │           │           │

                           PROBLEM OPTIONS
  ↵   to edit current box.    ↑,↓,→,←, PgUp, PgDn, Home, End to move pointer.
 ⇑ ↵  for row/column options.                      T.  to change title.
 ⇑ F7 to fit a curve or do regression.         F6 for helpful information.
 ⇑ F8 for file and library options.            F3 to print problem.
```
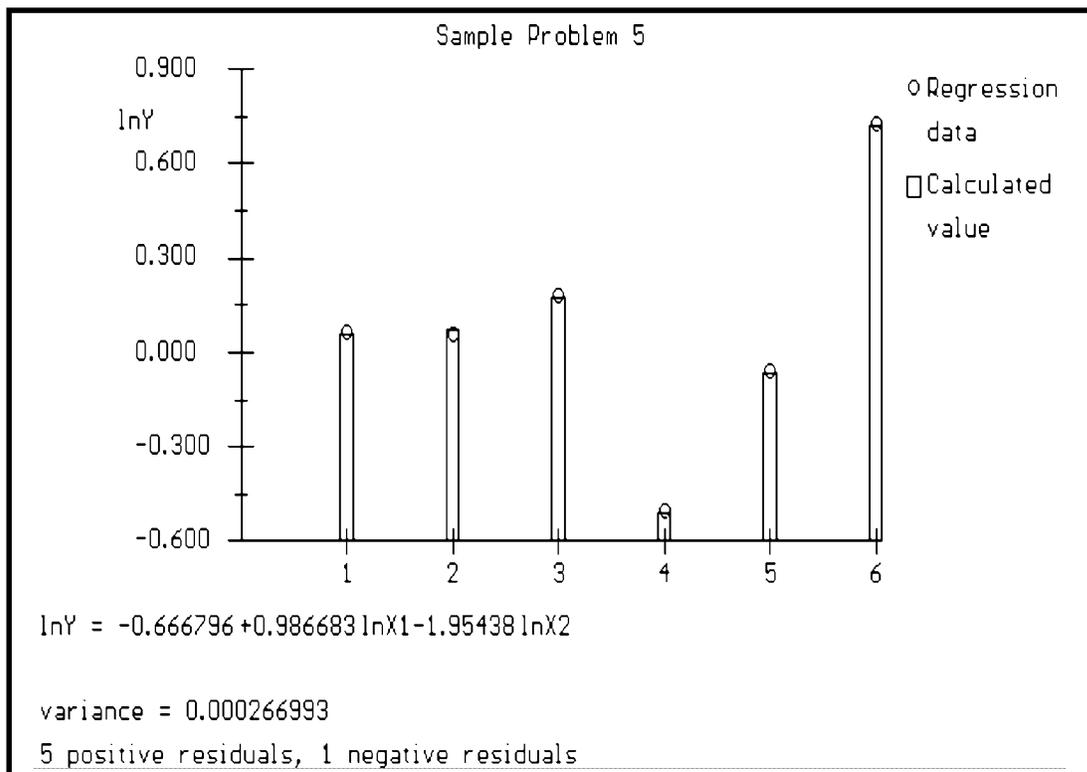
In this display X1, X2 and Y represent the original data, the variables (columns) lnX1, lnX2 and lnY represent the transformed data. You can see the definition of ln X1 , for example, by moving the cursor (the highlighted box), which located in row number 1 of the first column, into the box containing "lnX1" (using the arrow keys) and press ↵ .

The following window is brought up:

```
Enter column definition:
≫ lnX1=ln(X1)_
```

Note that the expression in the right hand side of the column definition equation must be a valid algebraic expression, and any function arguments used in the expression should be enclosed within parentheses.

Since we do not want to change this expression, please press ⬅ to close the window. Now press ⇑ F7 to do regression, then "1" to do linear regression. Type in "lnX1" as the name of the first independent variable, "lnX2" as the name of the second independent variable and "lnY" as the name of the dependent variable. The results should be displayed as shown below:

Sample Problem 5

$lnY = -0.666796 + 0.986683 \, lnX1 - 1.95438 \, lnX2$

variance = 0.000266993

5 positive residuals, 1 negative residuals

All of the statistical analyses are available for the transformed variable.

Please note that the results indicate that the equation for variable "Y" can be written as: $Y = a_0 \, X_1^{a_1} \, X_2^{a_2}$ where $a_0 = \exp(-0.666796) = 0.5133$, $a_1 = 0.986683$ and $a_2 = -1.95438$.

This concludes the transformation of variable and the multiple linear regression for Sample Problem 5.

NONLINEAR REGRESSION

It is often desirable to fit a general nonlinear function model to the independent variables as indicated below:

$$y(\underline{x}) = f(x_1, x_2, ..., x_n; a_0, a_1, ..., a_m)$$

In the above expression, x_1, x_2, ..., x_n are n independent variables, y is the dependent variable, and a_0, a_1, ..., a_m are the model parameters. The data are represented by a set of N tabulated values of $x_{1,i}$, $x_{2,i}$, ... and $y(\underline{x}_i)$. The regression adjusts the values of the model parameters to minimize the sum of squares of the deviations between the calculated $y(\underline{x})$ and the data $y(\underline{x}_i)$.

The nonlinear regression capability of POLYMATH allows a general nonlinear function to be treated directly without any transformation. Lets return to Sample Problem 5 and this time treat the model for Y directly where

$$Y = a_0\, X_1^{a_1}\, X_2^{a_2}\quad .$$

Please recall Sample Problem 5. From the Problem Options Display press ⇑ F7 and then enter "R" (upper case R) to "Do nonlinear regression." The user is then prompted to:

```
Enter the model equation ( ⬅   to cancel) :
≫ _
```

The user can then enter the model equation using any of the variables from the columns of the Problem Options Display and any unknown parameters (maximum of five) which are needed. For this example, please enter

```
Enter the model equation ( ⬅   to cancel) :
≫ Y=k*X1^alpha*X2^beta_
```

Thus in this problem, the unknown parameters are k, alpha, and beta. The next query for the user is to supply initial estimates for each of the unknown parameter in turn:

```
Enter initial guess for  k :
≫ _
```

It is good practice to provide good initial parameter estimates from either reasonable physical/chemical model values or from a linearized treatment of the nonlinear model. In this example however, please set all initial guesses for the parameters as unity, "1.0". Then POLYMATH will provide a summary of the problem on the Regression Option Display as shown on the next page.

```
                        Sample Problem 5

 Nonlinear regression model equation:

 Y=k*X1^alpha*X2^beta

 Initial estimates:

 k = 1
 alpha = 1
 beta = 1




 ┌──────────────────────────────────────────────────────────────────────────┐
 ███████████████████████████████│REGRESSION OPTIONS│████████████████████████████
 │            e.  Change the model equation.                                  │
 │            i.  Change the initial guesses.                                  │
 │                 ⇧ F7 to solve.                                             │
 │              F8 for the problem options.                                   │
 └──────────────────────────────────────────────────────────────────────────┘
```

The Regression Options Menu gives several useful options for model changes and alterations to initial parameter guesses; however, please press ⇧F7 to solve this problem. The program search is shown to the user and the converged solution is indicated below:

```
                        Sample Problem 5

 Nonlinear regression model equation:

 Y=k*X1^alpha*X2^beta

 Initial estimates:                      Current values:

 k = 1                                    k = 0.509711
 alpha = 1                                alpha = 0.987817
 beta = 1                                 beta = -1.96425




 ┌─────────────────────────────────────────────────────────────────────┐
 │ Log of sum of squares:                                                │
 │-3 ┌─────────────────────────────────────────────────────────────┐    │
 │   │                                                             │    │
 │   │                                                             │    │
 │   │                                                             │    │
 │-4 └─────────────────────────────────────────────────────────────┘    │
 │ Sum of squares =     0.000903922                                      │
 ├───────────────────────────────────────────────────────────────────────┤
 │ Solution process complete.                                            │
 │ Press any key to see the graph of the results.                        │
 └───────────────────────────────────────────────────────────────────────┘
```

There are a number of options from the Display Options Menu (not shown here). Perhaps the most useful is the "statistical analysis" which is given on the next page.

```
                          Sample Problem 5

     Matrix of correlation coefficients for the nonlinear correlation equation
                     k              alpha            beta
          k   | 1            | 0.839634     | 0.917385     |
       alpha  | 0.839634     | 1            | 0.565458     |
        beta  | 0.917385     | 0.565458     | 1            |



             Converged       0.95 conf.        lower           upper
  Param.       Value         interval          limit           limit
  k           0.509711       0.110869         0.398842        0.62058
  alpha       0.987817       0.149894         0.837924        1.13771
  beta       -1.96425        0.163335        -2.12759        -1.80092


    Model: Y=k*X1^alpha*X2^beta
    k = 0.509711                    beta = -1.96425
    alpha = 0.987817
    5 positive residuals, 1 negative residuals.  Sum of squares = 0.000903922

  ████████████████████████ DISPLAY OPTIONS ████████████████████████
                     F3 to print this page.
       F9 to return to the graph.                    F6 for HELP.
       F8 for regression options.        ⇧F8 for problem options.
```

This concludes the Quick Tour section dealing with nonlinear regression and the Chapter on the Polynomial, Multiple Linear and Nonlinear Regression Program. Remember, when you wish to stop POLYMATH, please follow the exiting instructions given below.

EXITING OR RESTARTING POLYMATH

A ⇧ F10 keypress will always stop the operation of POLYMATH and return you to the Program Selection Menu. *THIS ACTION WILL DELETE THE EXISTING PROBLEM.* The program can be exited or restarted from the Program Selection Menu.

SOLUTION METHODS

When fitting a polynomial of the form

$$P(x) = a_0 + a_1x + a_2x^2 +...+a_nx^n$$

to N points of observed data, the minimum sum of square error correlation of the coefficients $a_0, a_1, a_2...a_n$ can be found by solving the system of linear equation (often called normal equations):

$$\mathbf{X^T X A = X^T Y}$$

where

$$
\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_N \end{bmatrix}
\qquad
\mathbf{A} = \begin{bmatrix} a_o \\ a_1 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix}
\qquad
\mathbf{X} = \begin{bmatrix}
x_1^0 & x_1^1 & \cdot & \cdot & \cdot & \cdot & x_1^n \\
x_2^0 & x_2^1 & \cdot & \cdot & \cdot & \cdot & x_2^n \\
x_N^0 & x_N^1 & \cdot & \cdot & \cdot & \cdot & x_N^n
\end{bmatrix}
$$

and where y_1, y_2...y_N are N observed values of dependent variable, and x_1, x_2...x_N are N observed values of the independent variable.

Multiple linear regression can also be expressed in the same form except that the matrix **X** is redefined as follows:

$$
\mathbf{X} = \begin{bmatrix}
1 & x_{1,1} & x_{2,1} & \cdot & \cdot & \cdot & x_{n,1} \\
1 & x_{1,2} & x_{2,2} & \cdot & \cdot & \cdot & x_{n,2} \\
1 & x_{1,N} & x_{2,N} & \cdot & \cdot & \cdot & x_{n,N}
\end{bmatrix}
$$

where $x_{i,j}$ is the j-th observed value of the i-th independent variable.

When polynomial or multiple linear regression are carried out without the free parameter (a_0), the first element in vector **A** and the first column in matrix **X** must be removed.

In POLYMATH the normal equations are solved using the Gauss-Jordan elimination. It is indicated in the literature that direct solution of normal equations is rather susceptible to round off errors. Practical experience has should this method to sufficiently accurate for most practical problems.

The nonlinear regression problems in POLYMATH are solved using the Levenberg-Marquardt method. A detailed description of this method can be found, for example, in the book by Press et al.*

---

*Press, W. H., P. B. Flannery, S. A. Teukolsky, and W. T. Vetterling, **Numerical Recipes**, 2nd Ed., Cambridge University Press, 1992, pp. 678-683.

APPENDIX

INSTALLATION AND EXECUTION INSTRUCTIONS FOR VARI-OUS OPERATING SYSTEMS

This Appendix provides complete instructions for the installation and execution of POLYMATH for Windows 3.X, Windows 95, Windows 98, and Windows NT operating systems. Detailed information is also provided for advanced options. Latest updates will be on the README.TXT file.

WINDOWS 3.X INSTALLATION
1. Put the diskette in the appropriate drive such as "A:".
2. Double click on the Main icon in the Program Manager window.
3. Double click on the MS-DOS Prompt icon.
4. Change the directory to the floppy drive where installation diskette is located. For example, if the drive to be used is A, then insert "A:" at the cursor and press Enter.
5. At the A:\> prompt, enter "dir".
6. There should be three files: Readme.txt, Install.exe, and Pmunzip.exe
7. At the A:\> prompt, enter "install"
8. Follow the instructions on the screen.
9. At the A:\> prompt enter "exit" to return to Windows

CONTINUE STEPS BELOW TO CREATE A PIF FILE FOR POLYMATH ONLY IF POLYMATH DOES NOT EXECUTE PROPERLY

10. From the Program Manager Window click on Main.
11. From the Main Window double click on PIF Editor.
12. Please enter the following in the PIF Editor:
    Program Filename: POLYMATH.BAT
    Window Title: POLYMATH 4.0
    Startup Directory: C:\POLYMAT4
    Video Memory: Low Graphics
    Memory Requirements: -1   -1
    EMS Memory: 0   1024
    XMS Memory: 1024   1024
    Display Usage: Full Screen
13. From File use Save As "POLYMAT4.PIF".

WINDOWS 3.X EXECUTION*

This 4.1 version of POLYMATH is a DOS program, but it creates Windows Meta files (WMFs) that can be printed or entered into documents. A special MetaFile Print program for Windows 3.X (MFP16) prints only POLYMATH WMF files that are generated upon printing requests from within POLYMATH. These generated WMFs are normally placed in the SPOOL subdirectory under the POLYMAT4 directory. Thus the user must first run the MFP16 Windows program before POLYMATH to insure that all requests to Print will be printed on the Windows printer. The MFP16 program produces a small blue printer icon on the bottom right of the desktop. A right mouse click on this icon gives the options which can be executed by a left mouse click.

1. Click on the File options in the Program Manager Window, select Run.
2. Enter the Command Line for the Metafile Print program such as "c:\polymat4\mfp16.exe"
3. The Command Line for your POLYMATH location should then be entered such as "c:\polymat4\polymath.bat".
4. Click on "OK"
5. If POLYMATH does not run properly, then create a PIF file starting with Step 10 as given in the preceding Windows 3.X Installation section.
6. Always end POLYMATH by exiting from the Program Selection Menu.

* A Program Group and a Program Item can be created under Windows to allow POLYMATH.bat and MFP16.exe to be executed conveniently from the desktop.

WINDOWS 3.X SHUTDOWN
1. POLYMATH can be terminated at any time by pressing Shift-F10 to return to the Program Selection Menu and then by pressing F8 to exit.
2. The MFP16 program can be terminated by a right click with the mouse on the small blue printer icon followed by a left mouse click on "terminate."

USING PRINT METAFILES IN DOCUMENTS FOR WINDOWS 3.X

The WMFs files will accumulate in the SPOOL subdirectory of POLYMAT4 when the MFP16 program is not running, These WMF files, designated by TEMP00X.WMF, can be copied and inserted as files within word processing and desktop publishing software. MS Word, for example,

will conveniently give a small preview of each selected file so that the content will be known prior to insertion. Execution of MFP16.exe will allow you to print all or delete all remaining files in SPOOL. Thus POLYMATH output can be selectively inserted into documents or printed or both.

Windows 95, 98, and NT Installation
1. Put the installation disk in your floppy drive, typically Drive A.
2. Minimize all Windows until Desktop appears.
3. Double click on the My Computer icon.
4. Double click on the 3 1/2 Floppy (A:) icon.
5. Double click on the Install icon.
6. Follow the directions on the screen.
7. When installation is complete, press Enter.
8. Close the DOS window.

Windows 95, 98, and NT Execution*
       This 4.1 version of POLYMATH is a DOS program, but it creates Windows Meta files (WMFs) that can be printed or entered into documents. A special MetaFile Print program for Windows 95, 98, and NT (MFP32) prints only POLYMATH WMF files that are generated upon printing requests from within POLYMATH. These generated WMFs are normally placed in the SPOOL subdirectory under the POLYMAT4 directory. When the user executes the POLYMATH.bat file, the MFP32.exeWindows program is also launched. POLYMATH runs in its own Window by the MFP32.exe program only produces a small blue printer icon on the bottom right of the desktop. A right mouse click on this icon gives the options which can be executed by a left mouse click.
       Program execution is accomplished by the following steps:
1. Click on the Start button.
2. Click on the Run icon.
3. Start POLYMATH by entering the storage location for POLYMATH and specify the program as "polymath.bat" such as "c:\polymat4\polymath.bat".

4. The POLYMATH program will initiate both the POLYMATH software and the MFP32.exe program as discussed previously. If the MFP32.exe was not active at POLYMATH startup, then you may need to click on the POLYMATH window to continue with POLYMATH.

* Icons for both the Printer Utility and POLYMATH can be placed on the desktop by using Windows Explorer to find both the Mfp32.exe and Polymath.bat files in the POLYMATH directory. A right mouse click on each of these files followed by a left mouse click on "Create Shortcut" can create a "Shortcut to ..." which can be dragged to the desktop.

WINDOWS 95, 98, AND NT SHUTDOWN

1. POLYMATH can be terminated at any time by pressing Shift-F10 to return to the Program Selection Menu and then by pressing F8 to exit.
2. The MFP32.exe program can be terminated by a right click with the mouse on the small blue printer icon followed by a left mouse click on "terminate."

USING PRINT METAFILES IN DOCUMENTS FOR WINDOWS 95, 98, AND NT

The WMFs files will accumulate in the SPOOL subdirectory of POLYMAT4 when the MFP32.exe program is not running, These WMF files, designated by TEMP00X.WMF, can be copied to word processing and desktop publishing software and inserted as files. MS Word will give a small preview of each selected file so that the content will be known. Execution of MFP32.exe will allow you to print all or delete all remaining files in SPOOL. Thus POLYMATH output can be selectively inserted into documents or printed or both.

INSTALLATION QUESTIONS (DETAILS)

1. Enter drive and directory for POLYMATH [C:\POLYMAT4]:
   ==>
   The default response is indicated by the contents of the brackets [...] which is given by pressing Enter key. The full path (drive and directory) where you wish the POLYMATH program files to be stored must be provided here. If the directory does not exist, then the installation procedure will automatically create it.

NOTE: Network clients will need <u>read</u> and <u>execute</u> permission for this directory and its <u>subdirectories</u>. This procedure does not provide the needed permissions.

2. Is this a network installation? [N]

   If you are installing POLYMATH on a stand-alone computer, take the default or enter "N" for no and **GO TO 5. on this list.** If you are installing on any kind of network server, answer "Y" and continue with the installation.

3. What will network clients call <POLYdir> [POLYdir]?
   ===> _
   This question will only appear if you answered "Y" to question 2 to indicate a Network installation. Here "POLYdir" is what was provided in question 1. On some networks, the clients "see" server directories under a different name, or as a different disk, than the way the server sees them. This question enables POLYMATH to print by indicating where the printer-driver files are located. They are always placed in subdirectory BGI of the POLYMATH directory by the installation procedure. During run time, they must be accessed by the client machines, thus POLYMATH must know what the client's name is for the directory.

4. Enter drive and directory for temporary print files [C:\TMP]:
   ===> _
   This question will only appear if you answered "Y" to question 2 to indicate a Network installation. Depending on the amount of extended memory available, and the type of printer is use, POLYMATH may need disk workspace in order to print. Since client machines are not normally permitted to write on the server disk, you are requested to enter a directory where files may be written. The temporary print files are automatically deleted when a print is completed or cancelled.

5.   POLYMATH INSTALLATION
       Which version of MS Windows are you using [2]:
                1. Windows 3.X
                2. Windows 95
                3. Windows 98
                4. Windows NT
   ===> _

6. The POLYMATH installation program now copies all of the needed files according to your previous instructions. This may take some time as the needed files are compressed on the installation diskette.

Additional Network Installation Needs:
1. POLYMATH requires the creation of the directory C:\TMP\SPOOL.
2. There must be an MFP.INI file on each computer (including the server) connected to the network that is going to run POLYMATH. In this file, a spool directory on the local disk should be specified. This directory has to exist. Any Windows Meta File (*.wmf) that is placed into this directory by the Print Utility (either MFP16.exe or MFP32.exe) will get printed and deleted, so it should not be in a directory in general use.
    A sample MFP.INI file follows:

 [location]
SpoolPath=C:\TMP\SPOOL

TROUBLESHOOTING
    Please look for the most recent troubleshooting hints at

www.polymath-software.com

(a) If you are attempting to print on Windows 3.X and you get the message "abnormal program termination", then try running POLYMATH again. Additional messages such as "out of memory" or "missing batch file" indicates that you must remove some RAM resident programs. If all else fails, then use the DOS printing version 4.02 of POLYMATH.

(b) When POLYMATH says "Could not begin printing: I/O port error", the SPOOL subdirectory does not exist. Please make sure it exists. See the following part (c).

(c) If POLYMATH indicates "print successful" and nothing comes out of the printer then...
- Use Print Manager to check to see that there is no problem with the printer. If there is a job in the queue, this means that POLYMATH and MFP did their part, and the problem is in Windows, Print Manager, or the printer itself.

- Check that MFP16.exe is running for Windows 3.X or that MFP32.exe is running for Windows 95, 98, and NT. There should be a little printer icon visible at the bottom right of the desktop. If not, then run the proper program (File->Run ... C:\POLYMAT4\MFP16.exe for Windows 3.X ; File->, Run ... C:\POLYMAT4\MFP32.exe for Windows 95, 98, and NT)

- MFP.INI file doesn't exist or doesn't match the POLYMATH.BAT file. Please check the POLYMATH.BAT file for a line similar to

PM_PRINTER=_WMF,0,FILE:C:\POLYMAT4\SPOOL\TEMP+++.WMF

where the directory specified in the preceding line, "C:\POLYMAT4\SPOOL" should be the same as it appears in the MFP.INI file. If they don't match, the you must change one of the other, shut down MFP, exit POLYMATH, and start both again.

"OUT OF ENVIRONMENT SPACE" MESSAGE
If you receive this message or if you are having difficulty in printing from POLYMATH, then follow **ONE** of the following instruction sets for your particular operating system.

Window 95, Windows 98, or Windows NT 4.0
1. Open a DOS prompt window (if yours opens full-screen, hit Alt+Enter to get a window).
2. Click on the "Properties" button at the top.
3. At the end of the Cmd line, add the text "/e:2048" (if you already have this, then change the existing number to a higher number in increments of 1024).

Windows 3.x and Windows 95
1. Open a DOS prompt window.
2. At the C:\ prompt type "CD/WINDOWS, and press Enter.
3. Type "EDIT SYSTEM.INI" and press Enter.
4. Locate a line that reads "[NonWindows App]".
5. Make sure that this section contains the following entry:
        "CommandEnvSize=2048".
6. Save the modified file.
7. Reboot your computer.
8. Adjust the size upwards in increments of 1024 as necessary.

DOS or Windows 3.1
1. Open a DOS prompt window.
2. Type "SET" at the prompt.
3. Look for the line that displays the value of the COMSPEC environment variable.
 If COMSPEC is set to C:\COMMAND.COM then add the following line to the CONFIG.SYS file:

   SHELL=C:\COMMAND.COM C:\ /E:2048 /P

If COMSPEC is set to C:\DOS\COMMAND.COM then add this line to the CONFIG.SYS file:

   SHELL=C:\DOS\COMMAND.COM C:\DOS /E:2048 /P

4. Reboot your computer.
5. Adjust the size of E: in Step 3 upwards in increments of 1024 as necessary.