BASIC PROGRAMS FOR CHEMICAL ENGINEERS

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PREFACE

The microcomputer has put a vast amount of computational power in the hands of the practicing chemical engineer. However, a microcomputer is of little use unless there are programs available to solve chemical engineering problems. In this book, I have put together a collection of BASIC programs that will help the practicing engineer be more productive and able to solve complex problems that are normally handled on mainframe computers.

The plant engineer will find the book particularly useful. The plant engineer is called upon to investigate problems that range from simple trouble shooting to the detailed design of complex chemical plants. The larger projects are usually add-on jobs to the regular duties of keeping a chemical plant running. In today's business climate, answers to problems must be obtained quickly and accurately. The computer is capable of testing hypothesis, thereby allowing engineers to evaluate alternative solutions to problems quickly and provide answers to management's questions that invariably shift like the sands in a desert.

The programs do much more than a programmable calculator such as TI-59 or HP 97/67. Many of the programs contain large amounts of primary data allowing engineers to concentrate on solving problems instead of trying to find obscure data in some handbook and then entering them into numerous calculator memory registers. The programs ask for needed data in common engineering units or in units that are popular in handbooks such as the *CRC Manual* and Lang's *Handbook of Chemistry*. The programs' outputs provide clear documentation of the conditions that the calculated results are based on, which is something that programmable calculators cannot do. The programs self-documenting. Programs that request data from user-entered data statements are clearly illustrated by examples.

The programs are written in a simple version of TRS-80 Model III BASIC. I have used commands that are common to most, if not all, popular ver-

sions of Microsoft BASIC. Each program requires less than 16K of memory, and all calculations are done in single precision (7 decimals).

You should not find it difficult to adapt the TRS-80 syntax to your particular version of BASIC. The symbol for exponentiation "[" used by the TRS-80 can be replaced with "^" when the Programs are intended to be run on the IBM PC or the Apple II computers. The Programs employing "PRINT USING" statements are compatible with IBM PC BASIC, but are not compatible with the Apple II because Apple does not have an equivalent statement.

Finally, I urge the user to use your imagination when it comes to applying the programs to particular problems. Don't be afraid to make changes in program logic that will customize the program to a local situation. I hope that you will find the programs as useful as they have been for me.

DENNIS WRIGHT

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I deeply wish to thank the people who helped me put this book together. I particularly want to thank my wife Jane, my friend Jane, my secretary Billi, and Connie who typed most of the manuscript.

CONTENTS

1
MATHEMATICS

DATA REDUCTION

Engineering data reduction can be a time-consuming task. It is essential that the practicing engineer have available quick and easy methods for data reduction. Regression techniques and data plotting are indispensable tools. REGRESS is a program package that allows you to analyze data with reciprocal, linear, exponential, log linear, parabolic, or geometric regressions. Data can be entered through the key board, from data files on tape, or as data statements starting at line 3200. When using data statements, enter the X value first, Y value next. For example,

3200 DATA X1,Y1,X2,Y2, . . .

The program allows you to change regression formula and add, delete, or change data. After you are through manipulating the data, data can be plotted or saved to tape.

EXAMPLE

READY

RUN

1. ENTER DATA FROM KEYBOARD

2. ENTER DATA FROM DATA STATEMENTS

Arkin, H., Colton, R., *Statistical Methods,* 5th Ed, Barnes and Noble, 1970, New York, N.Y.
Poole, L., Borchers, M., *Some Common Basic Programs,* 3rd Ed, Osborne McGraw-Hill, 1979, Berkeley, Cali.

3. ENTER DATA FROM TAPE

4. LIST DATA

5. CHANGE DATA

6. ADD DATA

7. DELETE DATA

8. RUN REGRESSIONS AND PLOT

9. SAVE DATA TO TAPE

ENTER CHOICE(0-9, ENTER 0 TO END):? **2** [ENTERED DATA ARE SHOWN IN **BOLD**.]

HOW MANY DATA PAIRS:? **5**

1. ENTER DATA FROM KEYBOARD

2. ENTER DATA FROM DATA STATEMENTS

3. ENTER DATA FROM TAPE

4. LIST DATA

5. CHANGE DATA

6. ADD DATA

7. DELETE DATA

8. RUN REGRESSIONS AND PLOT

9. SAVE DATA TO TAPE

ENTER CHOICE(0-9, ENTER 0 TO END):? **4**

LIST DATA TO LINE PRINTER (Y/N):? **N**

LIST DATA TO SCREEN (Y/N):? **Y**

NO.	X-VALUE	Y-VALUE
1	.1	.25
2	.4	.55
3	.6	.65
4	.9	.99

NO.	X-VALUE	Y-VALUE
5	.25	.35
6	0	0
7	0	0
8	0	0
9	0	0
10	0	0
11	0	0
12	0	0
13	0	0

1. ENTER DATA FROM KEYBOARD
2. ENTER DATA FROM DATA STATEMENTS
3. ENTER DATA FROM TAPE
4. LIST DATA
5. CHANGE DATA
6. ADD DATA
7. DELETE DATA
8. RUN REGRESSIONS AND PLOT
9. SAVE DATA TO TAPE

ENTER CHOICE(0-9, ENTER 0 TO END):? **8**

1. LINEAR REGRESSION
2. EXPONENTIAL REGRESSION
3. GEOMETRIC REGRESSION
4. RECIPROCAL REGRESSION
5. PARABOLIC REGRESSION
6. LOG-LINEAR REGRESSION
7. PLOT DATA

```
ENTER CHOICE(0-7, ENTER 0 TO RETURN TO MENU)?  1

LINEAR REGRESSION
Y=.144923+.917949X
COEFFICIENT OF DETERMINATION (R**2)=.986036
COEFFICIENT OF CORRELATION=          .992994
STANDARD ERROR OF ESTIMATE=          .0393862
INTERPOLATE-(Y/N)?  N

1. LINEAR REGRESSION
2. EXPONENTIAL REGRESSION
3. GEOMETRIC REGRESSION
4. RECIPROCAL REGRESSION
5. PARABOLIC REGRESSION
6. LOG-LINEAR REGRESSION
7. PLOT
ENTER CHOICE(0-7, ENTER 0 TO RETURN TO MENU)?  7

PLOTTING ROUTINE
X-AXIS:LEFT END POINT, RIGHT ENDPOINT, INCREMENT
?  0,1,.05
Y-AXIS:LOWER ENDPOINT, UPPER END POINT, INCREMENT
?  0,1,.025
```

```
INTERSECTION OF AXES AT ( 0 , 0 )
X-AXIS RANGE= 0 - 1   INCREMENT= .05
Y-AXIS RANGE= 0 - 1   INCREMENT= .025

++++++++++++++++++++++++++++++++++++++++++Y-AXIS
+
+           *
+
+
+                *
+
+
+                          *
+
+
+
+                                 *
+
+
+
+
+
+                                                  *
+
+
X-AXIS
```

1. LINEAR REGRESSION
2. EXPONENTIAL REGRESSION
3. GEOMETRIC REGRESSION
4. RECIPROCAL REGRESSION
5. PARABOLIC REGRESSION
6. LOG-LINEAR REGRESSION
7. PLOT DATA

ENTER CHOICE(0-7, ENTER 0 TO RETURN TO MENU)? **0**

1. ENTER DATA FROM KEYBOARD
2. ENTER DATA FROM DATA STATEMENTS

```
3. ENTER DATA FROM TAPE
4. LIST DATA
5. CHANGE DATA
6. ADD DATA
7. DELETE DATA
8. RUN REGRESSIONS AND PLOT
9. SAVE DATA TO TAPE
ENTER CHOICE(0-9, ENTER 0 TO END):?  0

PROGRAM EXECUTION TERMINATED
READY
   LISTING FOR BASIC PROGRAM "REGRESS"

 10 CLS:DIM X(50),Y(50),X1(50),Y1(50)
 20 PRINT"REGRESSION AND PLOTTING ROUTINE"
 30 PRINT"1. ENTER DATA FROM KEYBOARD"
 40 PRINT"2. ENTER DATA FROM DATA STATEMENTS"
 50 PRINT"3. ENTER DATA FROM TAPE"
 60 PRINT"4. LIST DATA"
 70 PRINT"5. CHANGE DATA"
 80 PRINT"6. ADD DATA"
 90 PRINT"7. DELETE DATA"
100 PRINT"8. RUN REGRESSIONS AND PLOT"
110 PRINT"9. SAVE DATA TO TAPE"
120 PRINT
130 INPUT"ENTER CHOICE(0-9, ENTER 0 TO END):";Z
140 IF Z=0 THEN 170
150 ON Z GOSUB 2020 ,2120 ,2180 ,2260 ,2490 ,2630 ,2740 ,2980 ,3110
160 CLS:GOTO 30
170 CLS:PRINT"PROGRAM EXECUTION TERMINATED"
```

```
180 END
190 SX=0:SY=0:X2=0:Y2=0:XY=0
200 FOR I=1 TO N
210 IF C=1 THEN GOTO 280
220 IF C=2 THEN GOSUB 820  :GOTO 290
230 IF C=3 THEN GOSUB 840  :GOTO 290
240 IF C=4 THEN GOSUB 860  :GOTO 290
250 IF C=5 THEN GOSUB 880  :GOTO 290
260 IF C=6 THEN GOSUB 900  :GOTO 290
270 IF C=7 THEN 1050
280 X=X1(I):Y=Y1(I)
290 SX=SX+X
300 SY=SY+Y
310 X2=X2+X[2
320 Y2=Y2+Y[2
330 XY=XY+X*Y
340 NEXT I
350 B1=(N*XY-SY*SX)/(N*X2-SX[2)
360 A1=(SY-B1*SX)/N
370 LPRINT:LPRINT:LPRINT
380 ON C GOSUB 600  ,630  ,660  ,700  ,740  ,780
390 Z1=(N*XY-SX*SY)[2
400 Z2=(N*X2-SX[2)*(N*Y2-SY[2)
410 R2=Z1/Z2
420 LPRINT:LPRINT
430 Z3=(Y2-SY[2/N)*(1-R2)
440 LPRINT"COEFFICENT OF DETERMINATION (R**2)=";R2
```

Adapted from Poole, L., Borchers, M. *Some Common Basic Programs,* 3rd Ed., Osborne McGraw-Hill. With permission of Osborne McGraw-Hill, 1979.

```
450 LPRINT"COEFFICENT OF CORRELATION=          ";SQR(R2)
460 LPRINT"STANDARD ERROR OF ESTIMATE=         ";SQR(Z3/(N-2))
470 CLS
480 INPUT"INTERPOLATE-(Y/N)";A$
490 IF A$="N" THEN 590
500 LPRINT:LPRINT
510 LPRINT"INTERPOLATION"
520 LPRINT"X",,"Y"
530 LPRINT"--------------------------------------------------"
540 PRINT"INTERPOLATION"
550 INPUT"X-VALUE.......9999 TO END";X
560 IF X=9999 THEN 590
570 ON C GOSUB 920  ,940  ,960  ,980  ,1000 ,1020
580 GOTO 550
590 RETURN
600 LPRINT"LINEAR REGRESSION"
610 LPRINT"Y=";A1;"+";B1;"X"
620 RETURN
630 LPRINT"EXPONENTIAL REGRESSION"
640 LPRINT"A=";EXP(A1);"   ";"B=";B1
650 RETURN
660 LPRINT"GEOMETRIC REGRESSION"
670 LPRINT"Y=A*X**B"
680 LPRINT"A=";EXP(A1);"   ";"B=";B1
690 RETURN
700 LPRINT"RECIPORCAL REGRESSION"
710 LPRINT"Y=A+B*1/X"
720 LPRINT"A=";A1;"    ";"B=";B1
```

```
 730 RETURN
 740 LPRINT"PARABOLIC REGRESSION"
 750 LPRINT"Y=A+B*X**2"
 760 LPRINT"A=";A1;"     ";"B=";B1
 770 RETURN
 780 LPRINT"LOG-LINEAR REGRESSION"
 790 LPRINT"Y=A+B*LN(X)"
 800 LPRINT"A=";A1;"     ";"B=";B1
 810 RETURN
 820 Y=LOG(Y1(I)):X=X1(I)
 830 RETURN
 840 X=LOG(X1(I)):Y=LOG(Y1(I))
 850 RETURN
 860 X=1/X1(I):Y=Y1(I)
 870 RETURN
 880 X=X1(I)[2:Y=Y1(I)
 890 RETURN
 900 X=LOG(X1(I)):Y=Y1(I)
 910 RETURN
 920 LPRINT X,,A1+B1*X
 930 RETURN
 940 LPRINT X,,EXP(A1)*EXP(X*B1)
 950 RETURN
 960 LPRINT X,,EXP(A1)*X[B1
 970 RETURN
 980 LPRINT X,,A1+B1*1/X
 990 RETURN
1000 LPRINT X,,A1+B1*X[2
```

```
1010 RETURN

1020 LPRINT X,,A1+B1*LOG(X)

1030 RETURN

1040 REM-PLOTTING ROUTINE FROM "SOME COMMON BASIC PROGRAMS-3RD EDTION",
       LON POOLE, MARY BORCHERS, WITH PERMISSION OSBORNE-MC GRAW HILL
      BOOKS @1979

1050 CLS:PRINT"PLOTTING ROUTINE"

1060 PRINT"X-AXIS:LEFT END POINT,RIGHT ENDPOINT,INCREMENT"

1070 INPUT A1,A2,A3

1080 PRINT"Y-AXIS:LOWER ENDPOINT,UPPER END POINT,INCREMENT"

1090 INPUT B1,B2,B3

1095 LPRINT:LPRINT:LPRINT

1100 LPRINT"INTERSECTION OF AXES AT (";A1;",";B1;")"

1110 LPRINT"X-AXIS RANGE=";A1;"-";A2;" INCREMENT=";A3

1120 LPRINT"Y-AXIS RANGE=";B1;"-";B2;" INCREMENT=";B3

1130 B2=(B2-B1)/B3

1140 IF B2<=80 THEN 1170

1150 PRINT"Y RANGE TOO LARGE"

1160 GOTO 1080

1170 FOR I=1 TO N

1180 X(I)=INT((X1(I)-A1)/A3+.5)

1190 Y(I)=INT((Y1(I)-B1)/B3+.5)

1200 NEXT I

1210 Y(N+1)=INT(B2+.5)+1

1220 X(N+1)=INT((A2-A1)/A3+.5)+1

1230 LPRINT:LPRINT

1240 FOR J=1 TO N

1250 FOR I=1 TO N-J

1260 A=X(I)
```