MIMIC - A STUDY OF THE TECHNIQUE
AND APPLICATION TO MODELING
OF AN EXTRACTION COLUMN

MIMIC - A STUDY OF THE TECHNIQUE AND APPLICATION TO MODELING OF AN EXTRACTION COLUMN

by

THOMAS HARRY NORTHCOTT, B.Eng.

A Major Study Report
Submitted to the Faculty of Graduate Studies
in Partial Fulfilment of the Requirements
for the Degree
Master of Engineering

McMaster University,
October, 1967

MASTER OF ENGINEERING (1967)
(Chemical Engineering)

McMASTER UNIVERSITY
Hamilton, Ontario.

TITLE : MIMIC - A Study of the Technique and Application to Modeling of an Extraction Column

AUTHOR : Thomas Harry Northcott, B.Eng. (McMaster University)

SUPERVISOR : Professor A.I. Johnson

NUMBER OF PAGES : (viii), 182

SCOPE AND CONTENTS :

MIMIC, a digital analog simulator language is reviewed in some detail. Part A of the report, which was written as a preliminary handbook for the Chemical Engineering Department at McMaster University, deals with a description and use of MIMIC, and several example problems are given. Part B provides an example of the application of MIMIC to a simulation problem which is, in this case, the transient response of a liquid-liquid extraction column to step inputs in feed concentration. An overall evaluation of MIMIC is made, and some of the shortcomings and some of the features are outlined. For certain types of simulation problems faced by the chemical engineer, MIMIC is a solution technique which should be considered.

TABLE OF CONTENTS

STUDY AND APPLICATION OF MIMIC
- A DIGITAL ANALOG SIMULATOR

PAGE

B. Application of MIMIC to Modeling

LIST OF FIGURES

LIST OF TABLES

PART A

DESCRIPTION AND USE OF MIMIC

INTRODUCTION

The past several years have witnessed the birth of several digital analog simulator programs(A.11.2, A.11.3, A.11.4, A.11.5), of which MIMIC(A.11.12, A.11.13, A.11.14) is one.

Although the use of such programs is becoming more widespread, there seems to be litle interest in them by the chemical process industries and by university chemical engineering departments. Before this study began, both MIDAS and a version of MIMIC were available at McMaster, but few students or faculty were using these techniques to solve problems.

Information obtained from available manuals(A.11.12, A.11.13) indicated that MIMIC had possible applications in the field of chemical engineering. To explore these possibilities, a major study project was initiated with the following purposes: to examine MIMIC in detail; to test the MIMIC functions; to amplify existing MIMIC operating manuals; to use the technique in a given simulation study and then to evaluate its usefulness for simulation operations. The particular simulation study to be undertaken was that of the transient response of a liquid-liquid extraction column to step inputs in feed concentration.

The report on this work is given in two completely separate sections.

Part A deals with MIMIC, its development, its functions and its application. Special discussion is given to certain operations, and several solved example problems are included. Part A is intended to be a preliminary MIMIC working manual for the department of Chemical Engineering at McMaster. It is written in an open-ended manner so that further sections or example problems may be added as required.

Part B considers the application of MIMIC to modeling, in this case, a countercurrent liquid-liquid extraction column. A previous model by Pollock$^{(B.6.3)}$ is extended to include a concentration - dependent mass transfer coefficient by using a modification of a relationship given by Karr and Scheibel$^{(B.6.4)}$. The major incentive for this work was to extend Pollock's model such that both the transient raffinate and extract concentrations could be accurately predicted at the same time. This has not been reported previously.

A.1. INTRODUCTION

Chemical engineers often encounter problems, especially in simulation, which can be described in terms of ordinary differential equations, partial differential equations, and non-linear algebraic equations. Several paths are open to the engineer who wishes to solve such problems, but the two most common means are access to an analog or digital computer.

Certain features of the analog make it very useful for the solution of some of these problems(A.11.1, A.11.14):

1. The analog is ideally suited for solving systems of ordinary differential equations.
2. The engineer-computer relationship is very close, and the engineer can easily change initial conditions. Execution may be halted at any point, conditions reset, and the problem rerun easily.
3. The user is not concerned a great deal with the order in which the program is arranged, since solution of all equations occurs simultaneously.

On the other hand, the conventional analog has several drawbacks, some of which have been overcome in modern hybrid computer facilities:

1. The foremost of these faults is the problem of amplitude and time scaling. This operation is frustrating, tedious and difficult, especially for the novice programmer.

2. Accuracy is limited to the accuracy of potentiometer settings and of the elements in the computer.
3. Only a limited supply of computing elements may be available.
4. Relatively few logic operations are possible.

Digital machines have several advantages which make them particularly useful.

a. Accuracy and reproducibility are far greater than for the analog
b. Memory and logic capabilities enable a wider range of operation.
c. A subroutine library allows many operations to be carried out without much programming.

However, the digital machine too has certain drawbacks:

1. The writing of digital programs requires knowledge of a compiler language such as FORTRAN or a machine language such as MAP.
2. Many operations cannot be programmed unless the user has a firm background in numerical techniques. For instance, integration must be done by some programmed numerical method.
3. The sequential order of calculation requires that strict attention be given to the order in which relationships and instructions are defined in the program.

Thus it was advantageous to develop digital programs combining the advantages of both digital and analog machines, and having some unique characteristics. During the past few years, many such programs have appeared, among them MIDAS$^{(A.11.6, A.11.7, A.11.8)}$, DYSAC $^{(A.11.9)}$, DSL/90$^{(A.11.10, A.11.11)}$, SLASH$^{(A.11.15)}$, and MIMIC$^{(A.11.12, A.11.13, A.11.14)}$.

This handbook will deal only with MIMIC and will outline its development, functions and applications.

A.2 MIMIC

MIMIC was developed at the Wright-Patterson Air Force Base for use on the IBM 7090/7094. The version now at McMaster was subsequently modified for the 7040/44 at the University of Alberta, and certain changes were also made at the University of Waterloo. These modifications have not been perfect and errors have been discovered in the system. A considerable amount of corrective work has been done on the 7040/44 version at McMaster. However, it is thought that errors still exist, and the user is encouraged to report any suspicious behaviour to Dr. Kenworthy at the McMaster Computation Centre.

MIMIC may be described as a language which allows the simulation of an analog operation on the digital machine. MIMIC consists of a number of subprograms written in MAP and FORTRAN which compile, sort, assemble and execute programs written according to specified rules. In writing the program,little attention has to be given to the logical sequence of operations since the sorting and assembling subprograms arrange all operations into an order of calculation, which is done sequentially although it appears to be done simultaneously.

MIMIC is an equation-oriented language which is easily learned and retained by novice programmers. It allows solutions of complicated systems of differential equations to be obtained without the user being mired in numerical techniques. The rules specified for writing MIMIC programs are simple, and will be outlined in later sections.

MIMIC programming is fast and efficient, and the large array of MIMIC functions available allows most operations, including integration, to be carried out with ease. For extraordinary operations, MIMIC allows the inclusion of user-written subroutines.

These features should make MIMIC useful for solving many of the types of problems faced by chemical engineers.

A.3 NOMENCLATURE

At this time, several definitions have to be made to provide a basis for future discussion.

A.3.1 MIMIC Program

The program written by the user in the MIMIC format to describe his problem.

A.3.2 MIMIC Processor

The collection of subroutines which assembles and executes the MIMIC program. A brief description of the MIMIC processor is found in Section A.12.2.

A.3.3 Variable Name

A group of from one to size alphameric characters, of which at least one must be alphabetic. Six names are reserved, and their definitions cannot be changed. These are the following:

1. T : The independent variable
2. DT : The amount T changes between printouts. If not specified, DT = 0.1.
3. DTMAX : The maximum integration step size allowed. If not specified, DTMAX = DT.
4. DTMIN : The minimum integration step size allowed. If not specified, DTMIN = 0.0.
5. TRUE : A logical constant which always has the value "true".
6. FALSE : A logical constant which always has the value "false".

It should be noted that there are no integer variable names in MIMIC. Variable names may begin with any of the alphabetic letters or a numeral.

Variables may be either numeric variables or logical variables. A numeric variable cannot exceed $|1.7| \times 10^{38}$.

Some valid MIMIC variables are the following

N3MAX, 12345M, SPEED, TIME, A1, 2DERIV, MAYBE

A.3.4 Literal

(a) A numeric constant which must have the following characteristics:

1. A decimal point.
2. At least one digit.
3. At most, six characters, including the decimal point, but not including a plus sign or minus sign which may accompany the numerical constant.

If the numeric constant should be given more than the allowed six characters, the characters after the sixth one are neglected by the processor.

(b) logical constants TRUE, FALSE.

A.3.5 Arithmetic Operators

Symbols denoting some arithmetic operation. The arithmetic operators which may be used to denote addition, subtraction, multiplication, and division are +, -, *, and / repsectively. It should be noted that exponentiation as denoted by the usual FORTRAN symbol ** is not allowed.

A.3.6 MIMIC Function

A three-letter code word followed by up to six arguments (i.e.

inputs) enclosed in parentheses and separated by commas. For example,

```
ADD (A, B, C, D. E, F)
```

Arguments may be literals, variables, or expressions. Over fifty MIMIC functions covering a wide range of operations are available. These will be outlined in a later section.

A.3.7 Expression

A sequence of literals, variables, and functions, separated by arithmetic operators, commas and parentheses.

Some examples of valid MIMIC expressions are the following

```
INT (A* (X1 - X2) - C* (Y2STAR - Y2), X200)

AAA* FACT1 * EXP (-13700./TEMP)

SQR (W*INT (X, X1))

1.7638

VAR1 + 2.03
```

A.4 MIMIC FORMAT

A.4.1 Control Cards

Only three control cards are necessary.

1. The first card in the program has $JOB in columns 1-4, the user's account number in columns 16-21, and the user's name in columns 22-33. The format must be exactly the same as that on the card issued by the Computation Centre to the user.
2. The second card in the program has $EXECUTE in columns 1-8 and MIMIC in the columns 16-20.
3. The last card in the program (immediately after the data) is a $IBSYS control card.

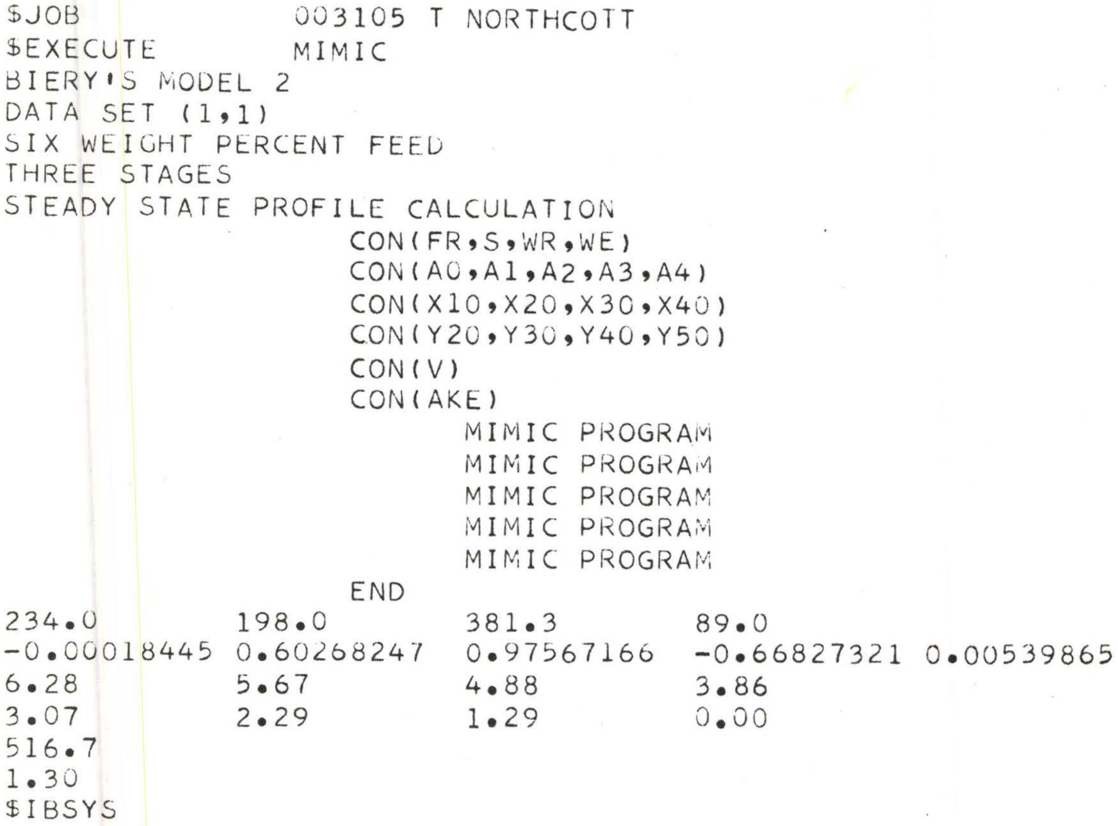
Figure 1 displays a typical program with appropriate control cards.

A.4.2 General Card Format

A card in a MIMIC program contains three main fields into which variables or expressions are placed.

FIELD 1 (Columns 2-7) may contain a logical control variable (LCV) which has the value either TRUE or FALSE. This variable may be generated by one of the MIMIC logical functions. The statement on the card is executed only if the LCV has the value TRUE. If no LCV is used on the card, the statement is automatically executed.

FIELD 2 (Columns 10-15) contains the name of a variable given to the result of the operation carried out in field 3. Certain MIMIC functions do not require a result name. These are CON, PAR, RSP, HDR, OUT, FIN, and END.



```
$JOB             003105 T NORTHCOTT
$EXECUTE         MIMIC
BIERY'S MODEL 2
DATA SET (1,1)
SIX WEIGHT PERCENT FEED
THREE STAGES
STEADY STATE PROFILE CALCULATION
                       CON(FR,S,WR,WE)
                       CON(A0,A1,A2,A3,A4)
                       CON(X10,X20,X30,X40)
                       CON(Y20,Y30,Y40,Y50)
                       CON(V)
                       CON(AKE)
                                 MIMIC PROGRAM
                                 MIMIC PROGRAM
                                 MIMIC PROGRAM
                                 MIMIC PROGRAM
                                 MIMIC PROGRAM
                       END
234.0        198.0        381.3        89.0
-0.00018445  0.60268247   0.97567166   -0.66827321 0.00539865
6.28         5.67         4.88         3.86
3.07         2.29         1.29         0.00
516.7
1.30
$IBSYS
```

FIGURE 1

```
LCV     RESULT   EXPRESSION
CV BEGINS IN COLUMN 2, RESULT IN COLUMN 10, AND EXPRESSION IN COLUMN 19

TZERO   X2       EQL(X200)
        X2       INT(A*(X1-X2)-C*(Y2STAR-YI),X200)
```

FIGURE 2

```
ATA ARE ENTERED IN 12-POINT FIELDS.
HERE ARE 6 DATA FIELDS PER CARD.
UMBERS WRITTEN IN E-NOTATION MUST BE RIGHT-JUSTIFIED.

.0079        1.862E+08   1.0016E-3   2.00          4.73E44.3329
.00018445 0.60268247  0.97567166  -0.66827321 0.00539865
```

FIGURE 3

```
 STATEMENT BEGINNING IN COLUMN 1 IS TREATED AS A COMMENT CARD.

ANSIENT RESPONSE TO A STEP INPUT OF 17.83 WEIGHT PERCENT
TA SET (1,1)
E MASS TRANSFER COEFFICIENT IS A FUNCTION OF CONCENTRATION.
```

FIGURE 4

```
LUMNS 73-80 MAY BE USED FOR IDENTIFICATION OR COMMENTS.

       DT       EQL(0.50)                                            MINUTES
       X4       INT(A*(X3-X4)-C*(Y3STAR-Y4),X400)                    OUT RAF
                FIN(T,30.0)                                           00064
```

FIGURE 5

FIELD 3 (Columns 19-72) contains a MIMIC expression which defines some arithmetic or logical operation.

Example of the use of these fields can be seen in Figure 1 and Figure 2.

A.4.3 Data Cards

Data are entered into 12-column fields with up to 6 fields per card. Either F- or E- notation is used. It should be noted that with E- notation, the number must be right-justified i.e. end exactly in the last right-hand space in the field. An example is shown in the third number of Figure 3.

No integer numbers exist in MIMIC i.e., every number must be given a decimal point.

Cards in Figure 1 and Figure 3 show typical data entries.

A.4.4 Comment Cards

Any card having a statement beginning in column 1 is treated as a comment card. (Figure 1, Figure 4).

A.4.5 Identification and Comments

In the same manner as FORTRAN statements, columns 73-80 may be used for card identification or comments. Typical examples are shown in Figure 5.

A.5 MIMIC FUNCTIONS

MIMIC functions, represented by three-letter code words, define a wide range of algebraic and logical operations. In the following section, the functions are organized into 8 main groups.

1. Arithmetic functions.
2. Elementary transcendentals
3. Logical functions.
4. Input/Output functions
5. Subprogram functions
6. Special functions
7. Hybrid functions
8. Control functions.

To provide some order to this section, the letter R is used as a result name, and the letters A to F are used as arguments (i.e. inputs) of the MIMIC functions.

The final column of each table gives the location of an example of the application of the function.

A.5.1 ARITHMETIC FUNCTIONS

FUNCTION	CODE	INPUT	RESULT VALUE	COMMENTS	LOCATION OF EXAMPLE
Addition	ADD SUM	A,B,C,D,E,F	R=A+B+C+D+E+F	The arguments C,D,E, and F do not have to be specified	
Subtraction	SUB	A,B	R=A-B		
Multiplication	MPY	A,B,C,D,E,F	R=A*B*C*D*E*F	The arguments C,D,E, and F do not have to be specified	Figure 24.1
Divide	DIV	A,B	R=A/B		
Multiply & Add	MAD	A,B,C,D,E,F	R=A*B+C*D+E*F	The arguments D,E, and F do not have to be specified	Figure 24.1
Negation	NEG	A	R=-A		
Absolute Value	ABS	A	R=|A|	Instead of using this function, the argument may be written beginning in column 19	Figure 24.1
Equality	EQL	A	R=A		

For the arithmetic functions, the arguments A,B,C,D,E and F may themselves be expressions.

A.5.2 ELEMENTARY TRANSCENDENTALS

Square Root	SQR	A	$R = \sqrt{A}$	A is greater than zero	
Sine	SIN	A	$R = \sin(A)$	A is in radians	
Cosine	COS	A	$R = \cos(A)$	A is in radians	
Arctangent	ATN	A,B	$R = \tan^{-1}(A/B)$	If B is not specified, it is assumed to be + 1.0.	
Exponential	EXP	A,B	$R = B^{A}$	If B is not specified, B = e is assumed. B > 0	Figures 22.1, 27.1
Logarithm	LOG	A,B	$R = \log_{B}{}^{A}$	If B is not specified, B = e is assumed.	

For the elementary transcendental functions, the arguments, A,B,C,D,E,F may also themselves be expressions.

A.5.3 LOGICAL FUNCTIONS

Function Switch	FSW	A,B,C,D	R=B if A<0 R=C if A=0 R=D if A>0	B,C,D must be logical-valued expressions	Figure 24.1,25,27.1
Logical switch	LSW	A,B,C	R=B if A=TRUE R=C if A=FALSE	B and C are any logical valued expressions	Figure 19.1
And	AND	A,B,C,D,E,F	R=TRUE if A and B and C and D and E and F are true R=FALSE otherwise	C,D,E, and F do not need to be specified	Figure 27.1
Exclusive or	EOR	A,B	R=TRUE if A and B are different. R=FALSE if A and B are the same		Figure 19.1
Inclusive or	IOR	A,B,C,D,E,F	R=TRUE if A or B or C or D or E or F is TRUE R=FALSE otherwise		Figure 27.1
Complement	COM NOT	A	R=FALSE if A=TRUE R=TRUE if A=FALSE		Figure 27.1

A.5.4 INPUT/OUTPUT FUNCTIONS

Name constants	CON	A,B,C,D,E,F	B,C,D,E, and F do not have to be specified. Names of constants are recorded	Figures 22.1,23.1,24.1 etc.
Name parameters	PAR	A,B,C,D,E,F	B,C,D,E, and F do not have to be specified. Parameter names are recorded	Figure 18.1, 25
Name function (constant)	CFN	A		Figure 6.1
Name function (parameter)	PFN	A	A must be a whole number. It represents the number of data points defining the function. The name of the function is entered in the result field	Figure 6.1
Print titles	HDR HEA	A,B,C,D,E,F	B,C,D,E and F do not have to be specified. Arguments are title names of up to six alphabetic or numerical characters.	Figure 9.1,10, 14.1 etc.
Print output	OUT PRI	A,B,C,D,E,F	Print A,B,C,D,E, and F every DT units of T. A,B,C,D,E and F are values of variables. OUT follows HDR in the MIMIC program	Figures 11, 12, 14.1 etc.
Plot	PLO	A,B,C,D,E,F	Supply A,B,C,D,E,F to the subroutine PLO every DT units of T. This function is not in operating order for the McMaster version of MIMIC	

A.5.5 SUBPROGRAM FUNCTIONS

Begin subprogram	BSP	A,B,C,D,E,F	R = subprogram name	The arguments B→F need not be specified. Both BSP and ESP functions are used to define a subprogram, which consists of operations defined in statements on cards between a card containing a BSP statement and a card containing a ESP statement. The arguments of BSP are dummy variables representing the input variables to the subprogram. Similarly, the arguments of ESP are dummy variables representing the output variables from the subprogram. Statements in the body of the subprogram define the relationships between input and output variables in terms of these dummy variables.	Figure 27.1
End subprogram	ESP	A,B,C,D,E,F	R = subprogram name		Figure 27.1
Call subprogram	CSP	A,B,C,D,E,F		The arguments B→F need not be specified. The arguments of CSP are variable names or constants representing numerical inputs to the subprogram. The order of arguments is the same as that of the corresponding dummy arguments of BSP. The arguments of RSP are variable names representing the numerical outputs from the subprogram. Similarly, the order of the arguments is that of the corresponding dummy arguments of ESP. NOTE : a CSP statement must be followed immediately by an RSP statement.	Figure 27.1
Return subprogram	RSP	A,B,C,D,E,F			Figure 27.1

Further discussion and an example of subprogram used will be given in a later section.

A.5.6 SPECIAL FUNCTIONS

Integration	INT	A,B,C,D.	$R = B + \int Adt$	C,D must be logical valued but do not have to be specified C and D control the mode of the integration routine i.e., OPERATE HOLD, Or RESET. Further discussion on the integration routine will be given in a special section.	Figure 23.1
Limit integrators	LIN	A,B,C,D	$R = 0$ if $B<C$ $R = A$ if $C<B<D$ $R = 0$ if $B<D$		Figures 14,1, 15
First order transfer function	FTR	A,B	$R = \mathcal{L}^{-1}$ $[A(S)/(BS+1)]$	A is the variable operated on by $1/[BS+1]$	
Limiter	LIM	A,B,C	$R = B$ if $A<B$ $R = A$ if $B<A<C$ $R=C$ if $A>C$		Figures 14.1, 20
Dead space	DSP	A,B,C	$R = (A-B)$ if $A<B$ $= 0$ if $B<A<C$ $= (A-C)$ if $A>C$		Figure 20
Time delay	TDL	A,B,C	$R = \left. A \right\vert_{(T-B)}$	B is the length of the time delay. C is the number of points of A to be stored and must be a literal or a constant. If C is not specified, C is 100. B may be variable If $T< B$, $R = \left. A \right\vert_{T = 0}$	

Function	FUN	A,B.	R = A(B)	A is the name of the function B is the value of the independent variable at which the value of the dependent variable is desired.	Figure 6.2
Implicit Function	IMP	A,B	R=A where $\lvert A-B(A)\rvert < 5 \times 10^{-6}\lvert A\rvert$	Further discussion will be presented later	Figure 16
Maximum	MAX	A,B,C,D,E,F	R = maximum of the arguments	For both MAX and MIN, C,D,E, or F need not be specified.	
Minimum	MIN	A,B,C,D,E,F	R = minimum of the arguments	"	
Random number generator	RNG	A,B,C		R is a random sample from a Gaussian distribution with mean A and standard deviation B. C is a starting number.	
Random number generator	RNU	A,B,C		R is a random sample from a uniform distribution with lower limit A and upper limit B. C is a starting number. For both RNG and RNU, different starting numbers will produce independent sequences. One value in the sequence may be printed out every DT units.	Figure 21
Derivative	DER	A,B,C	R = dA/dB R= C at T = 0	This routine calculates the derivative using a simple backward difference technique	Figures 17, 18.1

A.5.7 HYBRID FUNCTIONS

Monostable multivibrator	MMV	A,B	R set TRUE when A is TRUE, and stays TRUE for B units of T after A goes FALSE. R=A at T=0	This function is particularly useful for controlling the integration logical variables DTMAX must equal DTMIN	Figure 27.1
Track & store	TAS	A,B,C	R=A when B is TRUE R = previous R when B is FALSE	TAS is useful when the operation is an iteration and some initial condition etc. is being changed. DTMAX must equal DTMIN	Figure 27.2
Flip-flop	FLF	A,B,C	R=TRUE if A is TRUE R=TRUE if B is FALSE and previous R is TRUE R is FALSE otherwise R=C at T=0	DTMAX must equal DTMIN	Figure 19.1
Zero order hold	ZOH	A,B	A is sampled every B units of T. R = held sample value R = A at T=0	DTMAX must equal DTMIN	Figures 25, 26.1

A.5.8 CONTROL FUNCTIONS

Go to the next case	FIN	A,B	Go to the next case when A>B	A and/or B may be MIMIC expressions	
End of Program	END			signifies end of MIMIC program and beginning of MIMIC data	

A.6 INFORMATION INPUT

A.6.1 Constants

A constant may be defined in any of the following three ways:

1. It may be defined directly in the MIMIC program.
2. It may be defined by means of a CON statement.
3. If it varies between successive runs of the same program, it may be defined by means of a PAR statement.

A.6.1.1 CON

There are two pieces of information which must be known about a constant - its name and its value. The name of a constant may be defined by using the MIMIC function CON. Up to six names may be defined with one CON statement, and as many CON statements as necessary may be used.

The statement in FIGURE 6.1

```
CON (A,B,C)
```

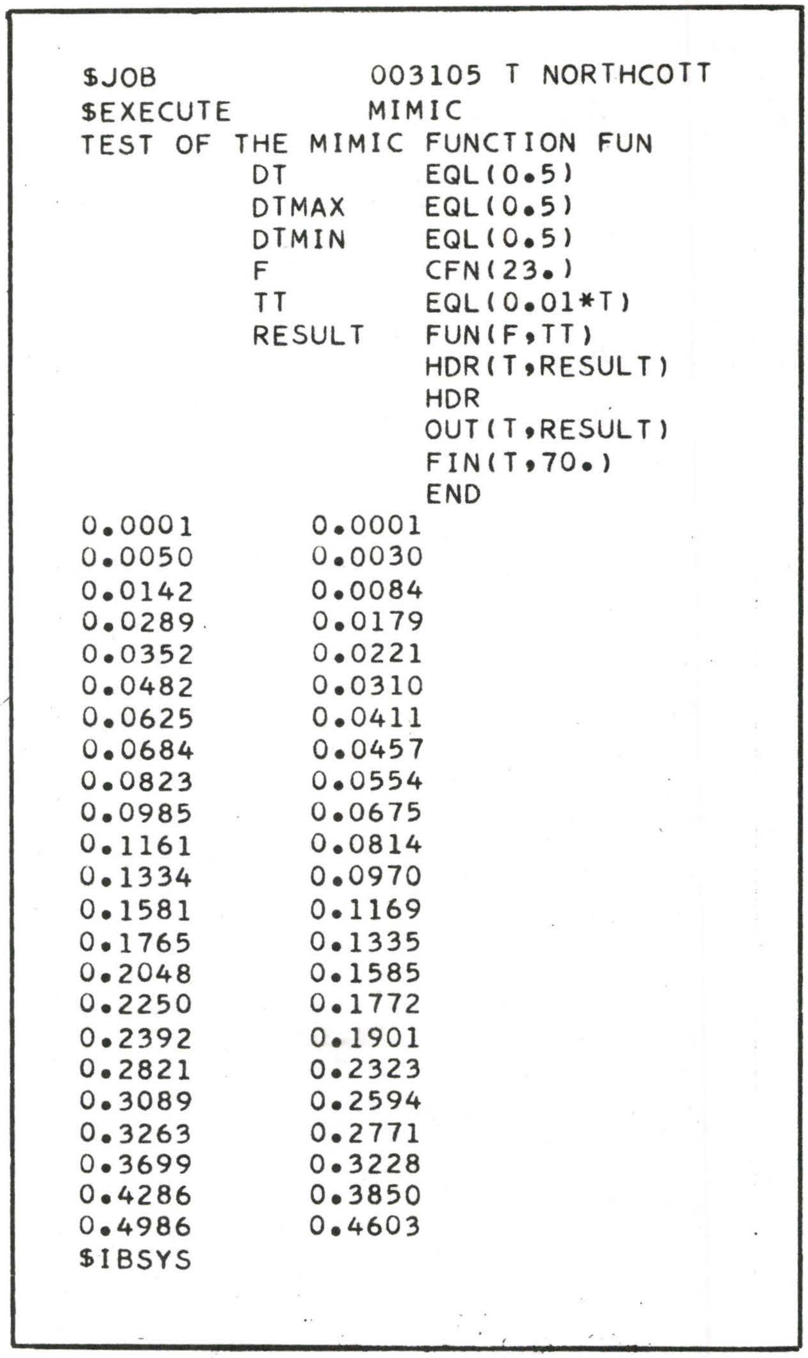
records A,B, and C as the names of constants, and alerts the processor to expect a data card with numerical values for these constants in the same order as defined in the CON statement. CON statements are placed at the beginning of the MIMIC program, immediately after the control cards.

A.6.1.2 PAR

PAR statements are used to define names of constants which vary between consecutive runs. A procedure identical to that used with CON

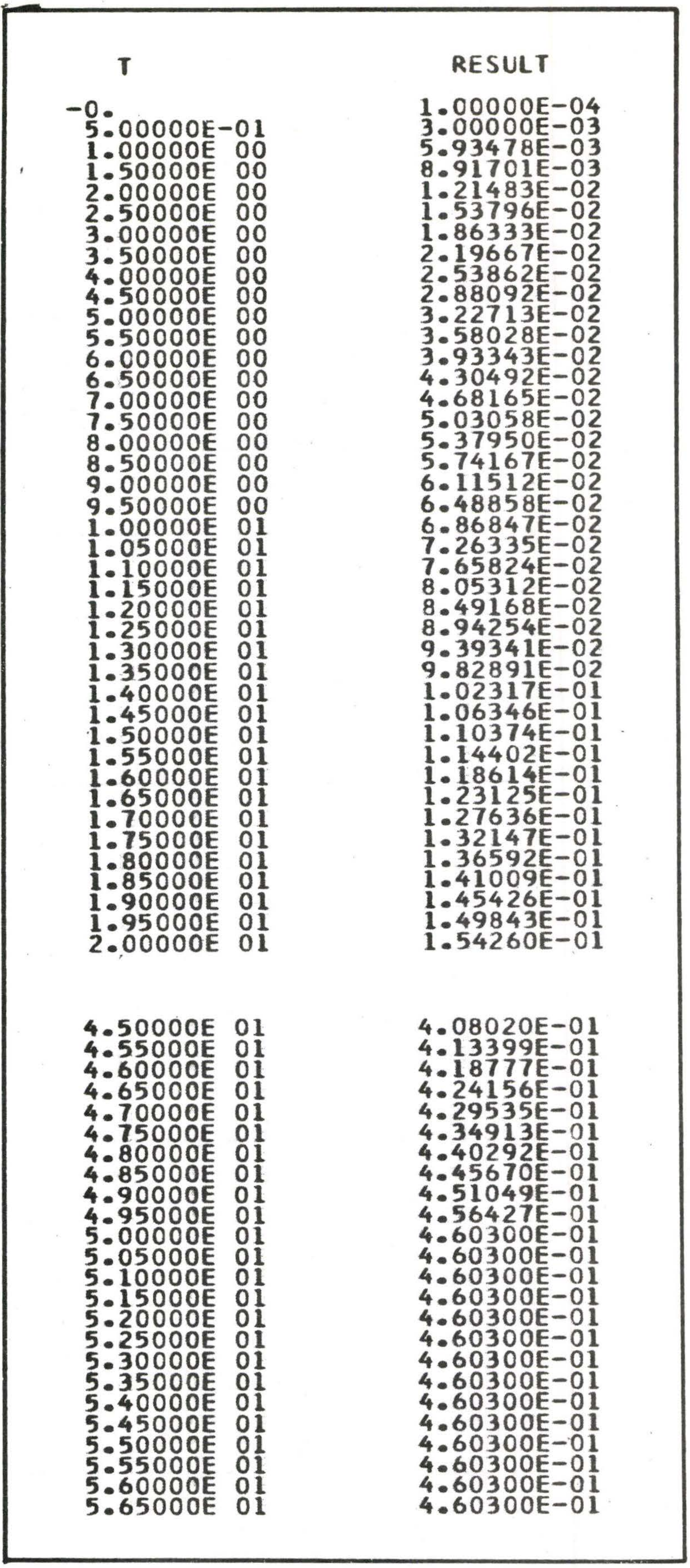
```
$JOB         003105 T NORTHCOTT
$EXECUTE     MIMIC
        F1      CON(A,B,C)
                CFN(10.)
        F2      PAR(D,E,F)
                PPN(5.)
                     MIMIC PROGRAM
                     MIMIC PROGRAM
                     MIMIC PROGRAM
                     MIMIC PROGRAM
                     MIMIC PROGRAM
                END
1.0       2.0        3.0
0.0       0.0
1.0       1.0
2.0       4.0
3.0       9.0
4.0       16.0
5.0       25.0
6.0       36.0
7.0       49.0
8.0       64.0
9.0       81.0
1.0       2.0        3.0
0.0       0.0
1.0       1.0
2.0       2.5
3.0       6.5
4.0       10.5
4.0       5.0        6.0
0.0       1.5
1.0       3.5
2.0       5.5
3.0       7.5
4.0       9.5
7.0       8.0        9.0
0.0       5.0
2.0       7.5
4.0       10.5
6.0       14.5
8.0       19.0
$IBSYS
```

FIGURE 6.1



```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
TEST OF THE MIMIC FUNCTION FUN
         DT        EQL(0.5)
         DTMAX     EQL(0.5)
         DTMIN     EQL(0.5)
         F         CFN(23.)
         TT        EQL(0.01*T)
         RESULT    FUN(F,TT)
                  HDR(T,RESULT)
                  HDR
                  OUT(T,RESULT)
                  FIN(T,70.)
                  END
0.0001      0.0001
0.0050      0.0030
0.0142      0.0084
0.0289      0.0179
0.0352      0.0221
0.0482      0.0310
0.0625      0.0411
0.0684      0.0457
0.0823      0.0554
0.0985      0.0675
0.1161      0.0814
0.1334      0.0970
0.1581      0.1169
0.1765      0.1335
0.2048      0.1585
0.2250      0.1772
0.2392      0.1901
0.2821      0.2323
0.3089      0.2594
0.3263      0.2771
0.3699      0.3228
0.4286      0.3850
0.4986      0.4603
$IBSYS
```

FIGURE 6.2



```
       T                            RESULT

  -0.                             1.00000E-04
   5.00000E-01                    3.00000E-03
   1.00000E 00                    5.93478E-03
   1.50000E 00                    8.91701E-03
   2.00000E 00                    1.21483E-02
   2.50000E 00                    1.53796E-02
   3.00000E 00                    1.86333E-02
   3.50000E 00                    2.19667E-02
   4.00000E 00                    2.53862E-02
   4.50000E 00                    2.88092E-02
   5.00000E 00                    3.22713E-02
   5.50000E 00                    3.58028E-02
   6.00000E 00                    3.93343E-02
   6.50000E 00                    4.30492E-02
   7.00000E 00                    4.68165E-02
   7.50000E 00                    5.03058E-02
   8.00000E 00                    5.37950E-02
   8.50000E 00                    5.74167E-02
   9.00000E 00                    6.11512E-02
   9.50000E 00                    6.48858E-02
   1.00000E 01                    6.86847E-02
   1.05000E 01                    7.26335E-02
   1.10000E 01                    7.65824E-02
   1.15000E 01                    8.05312E-02
   1.20000E 01                    8.49168E-02
   1.25000E 01                    8.94254E-02
   1.30000E 01                    9.39341E-02
   1.35000E 01                    9.82891E-02
   1.40000E 01                    1.02317E-01
   1.45000E 01                    1.06346E-01
   1.50000E 01                    1.10374E-01
   1.55000E 01                    1.14402E-01
   1.60000E 01                    1.18614E-01
   1.65000E 01                    1.23125E-01
   1.70000E 01                    1.27636E-01
   1.75000E 01                    1.32147E-01
   1.80000E 01                    1.36592E-01
   1.85000E 01                    1.41009E-01
   1.90000E 01                    1.45426E-01
   1.95000E 01                    1.49843E-01
   2.00000E 01                    1.54260E-01


   4.50000E 01                    4.08020E-01
   4.55000E 01                    4.13399E-01
   4.60000E 01                    4.18777E-01
   4.65000E 01                    4.24156E-01
   4.70000E 01                    4.29535E-01
   4.75000E 01                    4.34913E-01
   4.80000E 01                    4.40292E-01
   4.85000E 01                    4.45670E-01
   4.90000E 01                    4.51049E-01
   4.95000E 01                    4.56427E-01
   5.00000E 01                    4.60300E-01
   5.05000E 01                    4.60300E-01
   5.10000E 01                    4.60300E-01
   5.15000E 01                    4.60300E-01
   5.20000E 01                    4.60300E-01
   5.25000E 01                    4.60300E-01
   5.30000E 01                    4.60300E-01
   5.35000E 01                    4.60300E-01
   5.40000E 01                    4.60300E-01
   5.45000E 01                    4.60300E-01
   5.50000E 01                    4.60300E-01
   5.55000E 01                    4.60300E-01
   5.60000E 01                    4.60300E-01
   5.65000E 01                    4.60300E-01
```

FIGURE 6.3

statements is followed.

PAR statements follow immediately after CON and CFN statements. Examples are shown in Figure 6.1

A.6.2 Arbitrary Functions

MIMIC allows functions of one or two independent variables to be generated from tabulated data. Two types of functions exist - constant functions whose data do not change from run to run, and parameter functions whose data do change from run to run. Linear interpolation is used in all arbitrary functions for values of the independent variables between the tabulated points, and the derivative of the function outside the range of tabulated points is zero.

A.6.2.1 CFN

If the data are constant from run to run, tabulated data are entered by using the MIMIC function CFN. The name of the data array is recorded in the result column (column 10), and the number of sets of tabulated points is used as the argument of the CFN function.

For example,

```
F1            CFN(10.)
```

defines a function F1 which is described by 10 sets of tabulated points (x, y). A description of how data for functions are entered is found in Section A.7.3.2 (see also Figure 6.1).

Functions are used by employing a FUN statement. The result name is entered in the field starting at column 10. The function name and the values of the independent variables are used as the arguments of the FUN operator. If there is only one independent variable, then the arguments are the function name and the value of the independent variable.

For example

```
RESULT              FUN (F,TT)
```

defines RESULT, the value of the function F at which the independent variable has a value of TT. TT may be a constant which has been read in or stated, or has been calculated as the result of an expression.

In Figure 6.2 and Figure 6.3, the listing and some of the results of a test program are shown. It should be noted that when the independent variable used as an argument to FUN is larger than the largest tabulated value of the independent variable, the derivative is set equal to zero. The value of the function F is then the value of the tabulated dependent variable for the largest tabulated independent variable.

The number of data points as well as the number of arbitrary functions per program is limited only by the storage space available in the computer.

A.6.2.2 PFN

PFN is used in exactly the same manner as CFN. For PFN the points defining the function change for succeeding runs. This is further explained in A.6.2.3.

A.6.2.3 Card Order

It should be noted that the order of these functions (i.e. CON CFN, PAR, PFN) in the program is important. These functions should be used at the beginning of the program immediately after the control cards. The following order must be used: CON, CFN, PAR, PFN. An example is shown in Figure 6.1.

When PAR and/or PFN statements are used, successive runs are made until all the data are used. For instance, the example in Figure 6.1 would solve the problem described in the MIMIC program three times. For each solution, a different value of D, E, and F, and a different set of data points describing the function F2 would be used.

A.6.3 DATA

A.6.3.1 CON and PAR data

CON and PAR data are defined in 12-column fields with as many as six fields per card. Data are punched on the cards in the same field as the number of the corresponding argument on the CON or PAR statement, and the data cards are arranged in the same order as the CON or PAR statements defining the data.

The following rules are to be followed.

1. Either F- or E- notation may be used.
2. E- type numbers must be right-justified in the field.
3. E- type numbers may have any of the following exponent forms : E±dd, E±d , Edd, Ed, where d is an integer digit.
4. No more than 12 characters per number are allowed.
5. Decimal points must be included in all numbers, except the exponent in E-notation numbers.

A.6.3.2 CFN and PFN Data

a. One Independent Variable

One set of tabulated points (x,y) is recorded on each card, the independent variable in columns 1-12 and the dependent variable in in columns 13-24. The cards are arranged in algebraically increasing values of the independent variable (Figure 7).

b. Two Independent Variables

Data is recorded in 12-point fields, one set of points per card. The first independent variable is placed in columns 1-12, the second independent variable in columns 13-24, and the dependent variable in columns 25-36.

At least two values of the second independent variable and the corresponding dependent variable must be supplied for each given value of the first independent variable. Points both less than and greater than the expected values of both independent variables must be included.

Cards are arranged such that the following conditions are met:

1. The values of the first independent variable form a non-decreasing sequence.
2. At each given value of the first independent variable, the values of the second independent variable must form an algebraically increasing sequence.

For example, the data in Figure 8 are correctly arranged for the function Z = f(x,y) where x is the first independent variable and y is the second independent variable.

X	Y
0.0	0.0
3.0	-2.0
4.0	-1.0
5.0	1.0
7.0	5.0
10.0	8.0
12.0	7.5
15.0	5.0

FIGURE 7

X	Y	Z
-2.0	1.0	3.0
-2.0	2.0	3.3
-2.0	2.5	2.6
0.00	-4.0	5.0
0.00	2.0	3.0
0.00	3.0	2.0
3.00	1.5	-2.0
3.00	2.3	-3.0
4.00	1.0	-1.0
4.00	2.5	2.5
4.00	4.5	3.3

FIGURE 8

A.7 INFORMATION OUTPUT

Several types of output may be given in a MIMIC program.

A.7.1 Automatic Output

This includes printout of the following:

1. The MIMIC source program listing
2. A listing of the internally generated "circuit diagram"
3. Diagnostics, if any (Appendix I)
4. Input constant, parameter and function names and their corresponding values.

For an example, refer to Figures 9.1, 9.2, and 9.3.

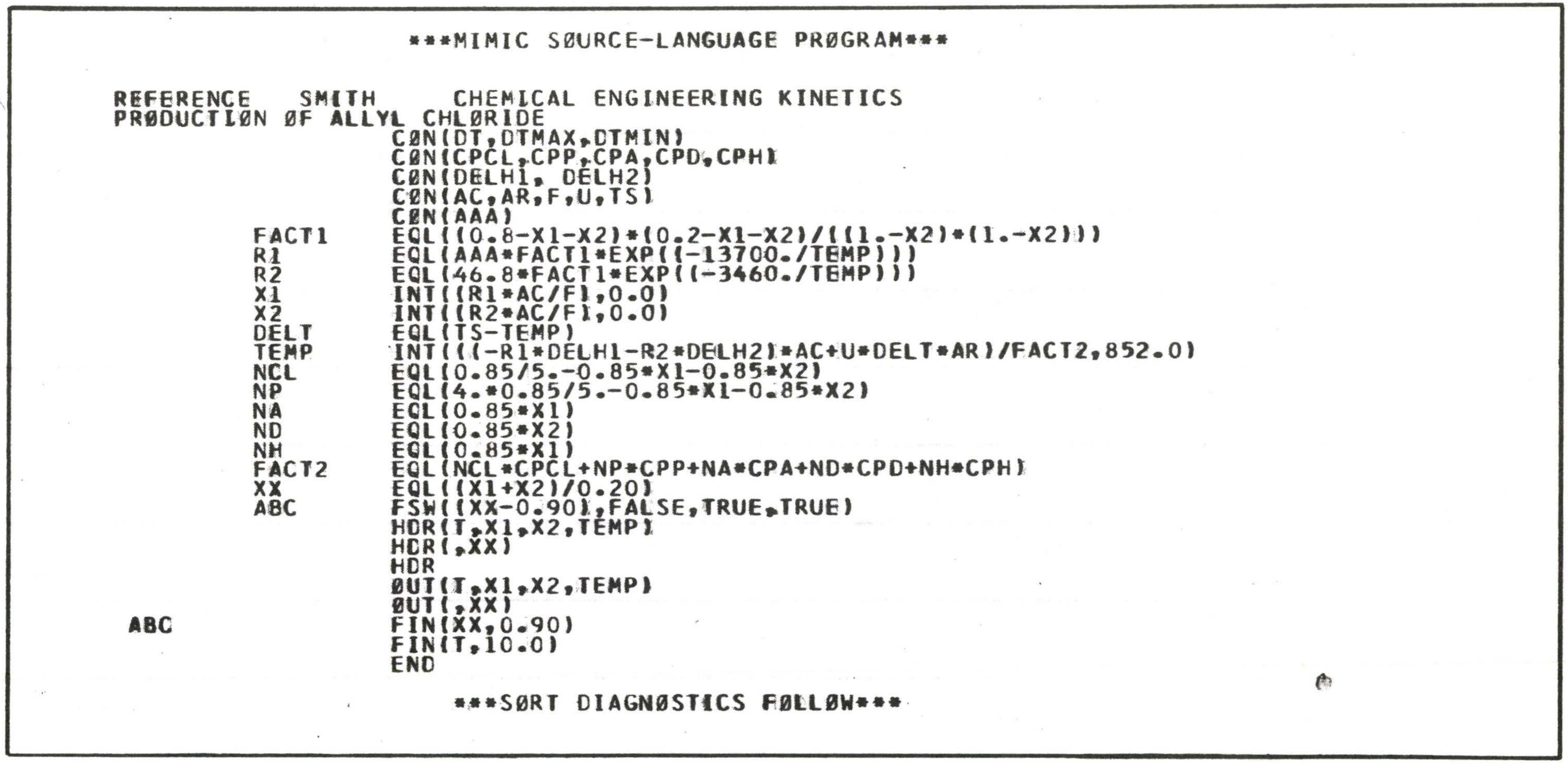
If parameters or parameter functions are being used, only the new values for the parameters or the parameter functions are printed out for the second and succeeding runs.

A.7.2 Controlled Output

This includes output titles and output of any desired variable Six evenly-spaced fields are reserved for output, and variables are printed out in the format ±x·xxxxxE±xx.

A.7.2.1 Output Titles

Title headings for output are defined by the HDR (or equivalently, the HEA) function. A title may have up to six alphameric characters, but no arithmetic operator (+, -, *, /) is allowed. The desired titles are supplied as arguments of the HDR function. If a blank line is desired between titles and numerical output, a HDR statement with no arguments is used. If a blank column in the title listing is desired, a comma with no corresponding argument is used in the HDR statement.



```
                   ***MIMIC SØURCE-LANGUAGE PRØGRAM***


REFERENCE   SMITH     CHEMICAL ENGINEERING KINETICS
PRØDUCTIØN ØF ALLYL CHLØRIDE
                  CØN(DT,DTMAX,DTMIN)
                  CØN(CPCL,CPP,CPA,CPD,CPH)
                  CØN(DELH1, DELH2)
                  CØN(AC,AR,F,U,TS)
                  CØN(AAA)
         FACT1    EQL((0.8-X1-X2)*(0.2-X1-X2)/((1.-X2)*(1.-X2)))
         R1       EQL(AAA*FACT1*EXP((-13700./TEMP)))
         R2       EQL(46.8*FACT1*EXP((-3460./TEMP)))
         X1       INT((R1*AC/F),0.0)
         X2       INT((R2*AC/F),0.0)
         DELT     EQL(TS-TEMP)
         TEMP     INT(((-R1*DELH1-R2*DELH2)*AC+U*DELT*AR)/FACT2,852.0)
         NCL      EQL(0.85/5.-0.85*X1-0.85*X2)
         NP       EQL(4.*0.85/5.-0.85*X1-0.85*X2)
         NA       EQL(0.85*X1)
         ND       EQL(0.85*X2)
         NH       EQL(0.85*X1)
         FACT2    EQL(NCL*CPCL+NP*CPP+NA*CPA+ND*CPD+NH*CPH)
         XX       EQL((X1+X2)/0.20)
         ABC      FSW((XX-0.90),FALSE,TRUE,TRUE)
                  HDR(T,X1,X2,TEMP)
                  HDR(,XX)
                  HDR
                  ØUT(T,X1,X2,TEMP)
                  ØUT(,XX)
 ABC              FIN(XX,0.90)
                  FIN(T,10.0)
                  END

                      ***SØRT DIAGNØSTICS FØLLØW***
```

FIGURE 9.1

```
                  ***FUNCTIØN-LANGUAGE PRØGRAM GENERATED***

IFN   LCV       RESULT  FTN   A     B     C     D     E       F

 1              CØN     DT    DTMAX DTMIN
 2              CØN     CPCL  CPP   CPA   CPD   CPH
 3              CØN     DELH1 DELH2
 4              CØN     AC    AR    F     U     TS
 5              CØN     AAA
 6              105     SUB  1.    X2
 7              106     SUB  1.    X2
 8              107     MPY  106   105
 9              108     SUB  0.2   X1
10              109     SUB  108   X2
11              110     SUB  0.8   X1
12              111     SUB  110   X2
13              112     MPY  111   109
14              113     DIV  112   107
15              FACT1   EQL  113
16              115     DIV  13700. TEMP
17              00      NEG  115
18              116     EXP  00
19              118     MPY  AAA   FACT1 116
20              R1      EQL  118
21              120     DIV  3460. TEMP
22              01      NEG  120
23              121     EXP  01
24              123     MPY  46.8  FACT1 121
25              R2      EQL  123
26              125     MPY  R1    AC
27              126     DIV  125   F
28              X1      INT  126   0.0
29              128     MPY  R2    AC
30              129     DIV  128   F
31              X2      INT  129   0.0
32              131     SUB  TS    TEMP
33              DELT    EQL  131
34              133     MPY  R1    DELH1
35              134     MPY  R2    DELH2
36              02      NEG  133
37              135     SUB  02    134
38              136     MPY  135   AC
39              138     MPY  U     DELT  AR
40              139     ADD  136   138
41              142     DIV  0.85  5.
42              143     MPY  0.85  X1
43              144     MPY  0.85  X2
44              145     SUB  142   143
45              146     SUB  145   144
46              NCL     EQL  146
47              148     MPY  4.    0.85
48              149     DIV  148   5.
49              150     MPY  0.85  X1
50              151     MPY  0.85  X2
51              152     SUB  149   150
52              153     SUB  152   151
53              NP      EQL  153
54              155     MPY  0.85  X1
```

FIGURE 9.2

```
        NA      EQL  155
        157     MPY  0.85  X2
        ND      EQL  157
        159     MPY  0.85  X1
        NH      EQL  159
        161     MPY  NCL   CPCL
        162     MPY  NP    CPP
        163     MPY  NA    CPA
        164     MPY  ND    CPD
        165     MPY  NH    CPH
        166     ADD  161   162
        167     ADD  166   163
        168     ADD  167   164
        169     ADD  168   165
        FACT2   EQL  169
        171     ADD  X1    X2
        172     DIV  171   0.20
        XX      EQL  172
        174     SUB  XX    0.90
        ABC     FSW  174   FALSE  TRUE  TRUE
ABC             FIN  XX    0.90
                FIN  T     10.0
        140     DIV  139   FACT2
        TEMP    INT  140   852.0
                HDR  T     X1     X2    TEMP
                HDR        XX
                HDR
                ØUT  T     X1     X2    TEMP
                ØUT        XX
                END

             ***FURTHER DIAGNØSTICS AND EXECUTIØN FØLLØW***

   DT                DTMAX             DTMIN
1.00000E 00       1.00000E-01       1.00000E-01

   CPCL              CPP               CPA               CPD               CPH
8.60000E 00       2.53000E 01       2.80000E 01       3.07000E 01       7.20000E 00

   DELH1             DELH2
-4.80000E 04     -7.92000E 04

   AC                AR                F                 U                 TS
2.18000E-02       5.24000E-01       8.50000E-01       5.00000E 00       8.52000E 02

   AAA
8.24000E 05
```

FIGURE 9.3

The example in Figure 10 will cause T, x1, x2, x3, x4, x5 to be printed out as titles of the six output fields. In this example, a blank line will be left between titles and the beginning of the numerical output.

A.7.2.2 Numerical Output

Desired numerical outputs can be obtained every DT units of the independent variable T by defining the desired output variables as arguments of an OUT function. The same rules that were outlined for the HDR statement apply.

It should be noted that HDR statements preceed OUT statements in the MIMIC program.

The example in Figure 11 will cause the numerical values of T, x1, x2, x3, x4, x5 to be printed out every DT units.

DT is defined by a CON or PAR statement, or by an operation in the MIMIC program. If DT is not specified, a value of 0.1 is assumed.

A.7.2.3 Logical Control of Output

Logical control variables may be easily used to control output to within certain values of the independent variable. For instance, if output for the previous example was desired only for values of T greater than 5, say, then the type of statements in Figure 12 could be used. The LCV T5 is true only if T is equal to or greater than 5, and therefore the OUT statements are executed only if this condition holds.

The length of execution may be controlled by the FIN statement. This statement is of the form

```
FIN (A, B)
```

where A and B are expressions or constants. The program will stop when A is equal to or greater than B. If, for instance, it were desired to

FORMAT OF A HDR STATEMENT.

```
                  19
                   HDR(T,X1,X2,X3,X4,X5)
                   HDR(,Y1,Y2,Y3,Y4,Y5)
                   HDR
```

FIGURE 10

FORMAT OF AN OUT STATEMENT.

```
                  19
                   OUT(T,X1OUT,X2OUT,X3OUT,X4OUT,X5OUT)
                   OUT(,Y1OUT,Y2OUT,Y3OUT,Y4OUT,Y5OUT)
```

FIGURE 11

LOGICAL CONTROL OF OUTPUT.

```
 2       10       19
          T5       FSW((T-5.0),FALSE,TRUE,TRUE)
 T5                OUT(T,X1OUT,X2OUT,X3OUT,X4OUT,X5OUT)
 T5                OUT(Y1OUT,Y2OUT,Y3OUT,Y4OUT,Y5OUT)
```

FIGURE 12

halt calculation at T = 100.,

```
FIN (T, 100.)
```

would be used. Similarly, if it were desired to halt calculations if ERROR were equal to or smaller than 0.0001, then

```
FIN (0.0001,ERROR)
```

would be appropriate.

Several FIN statements may be used in the same program, and combinations of FIN statements with logical control variables are also possible.

A.8 DETAILED EXAMINATION OF SELECTED MIMIC OPERATIONS

This section deals with functions which may need a more detailed description than that given in the section dealing with the MIMIC functions. An attempt will be made to provide examples where necessary, and to point out areas in which the programmer may experience some difficulty.

A.8.1 Integration

Integration in MIMIC is carried out using the MIMIC function INT which uses a fourth-order Runge Kutta technique.

The integration step size varies between DTMAX and DTMIN. If these values are not specified, then DTMAX = DT and DTMIN = 0.0.

The integration begins with a trial step size of DTMAX. The value of the dependent variable is calculated at the end of a step using the fourth-order Runge Kutta method. At the same time, another value of the dependent variable is calculated at the end of the same total step length by using a step size half as large. If the relative error is larger than 0.000005, the step size is halved; if the relative error is smaller than 0.0000005, the step size is doubled. The process is repeated until the criterion is met or until the step size is equal to or smaller than DTMIN.

It is interesting to note that for certain cases where DTMAX = DTMIN, the step size may actually be larger than DTMAX. This occurs in the following example.

Let DX = 5.0 and DXMAX = 1.5.

Then the number of integration steps is calculated by

```
KF = IFIX/DX/DXMAX

   = IFIX(5./1.5) = 3
```

Then the step size is calculated by

```
H = DX/FLOAT (KF)

  = 5.0/3.0 = 1.67
```

Thus H > DXMAX (lines 155 - 156 of MIN 4).

An integration statement is specified in the form

```
R          INT (A,B,C,D)
```

where A is the expression being integrated

B is the value of R at T = 0

and C and D are logical variables having values either TRUE or FALSE.

C and D are used to control the mode of the integrator.

It should be noted that A,B,C, and D are not reserved variables, but merely indicate position in the argument list.

A maximum of 95 integrators is allowed. However, it has been found that for systems with more than, say, 20 integrators, computation time becomes large. It was also pointed out by a spokesman from the University of Waterloo that workers there have experienced difficulty in obtaining accurate results from systems with more than 20 - 25 integrators.

A.8.1.1 Integrator Modes

The three possible states of operation that the integrator may be in are OPERATE, HOLD and RESET.

In the OPERATE mode, the integrator is in actual operation and integration proceeds.

In the HOLD mode, the input to the integrator is removed and the value on the integrator at that time is retained.

In the RESET mode, the output of the integrator is set equal to the initial condition, and no integration occurs.

These modes are the same as the standard modes of operation on the analog computer.

Certain types of calculations, such as iterations, require the integrator to change from one mode to another. These mode changes are controlled by values of the logical variables, in positions C and D as shown in the following table.

TABLE 1

C D	TRUE	FALSE
TRUE	OPERATE	HOLD
FALSE	RESET	OPERATE

Thus C and D must be controlled in such a way that their values produce the desired mode control. This can be done by setting up a "truth table" and using logical functions and certain hybrid functions to produce the desired logical values for C and D.

It should be noted that for most integration operations, only the OPERATE mode is desired. It should be noted also that if a logical control variable is used on statements containing expressions involving INT or FTR, these functions will not be initialized unless the variable is TRUE at T = 0.

A.8.2 LIN

For certain operations it may be desirable to limit the value of a variable produced by an integrator to a certain range. This may be accomplished by the use of the LIN function in conjunction with the INT function. The LIN function sets the derivative of the variable equal to zero whenever the variable is equal to a value at the upper or lower limit of the range to which it is restricted.

The procedure is to define a "limited derivative" from the derivative which is to be integrated. Then, this limited derivative is used as the one to be integrated. The following example is taken from Cress' handbook (A.11.12)

If x is the output of an integrator, but is to be limited such that $L \leq x \leq U$ the MIMIC statements would be of the form

```
                XDOTLM    LIN (XDOT, X, L, U)
                X         INT (XDOTLM, X0)
          or    X         INT (LIN(XDOT,X,L,U), X0)
```

It is assumed that XDOT has been specified previously.

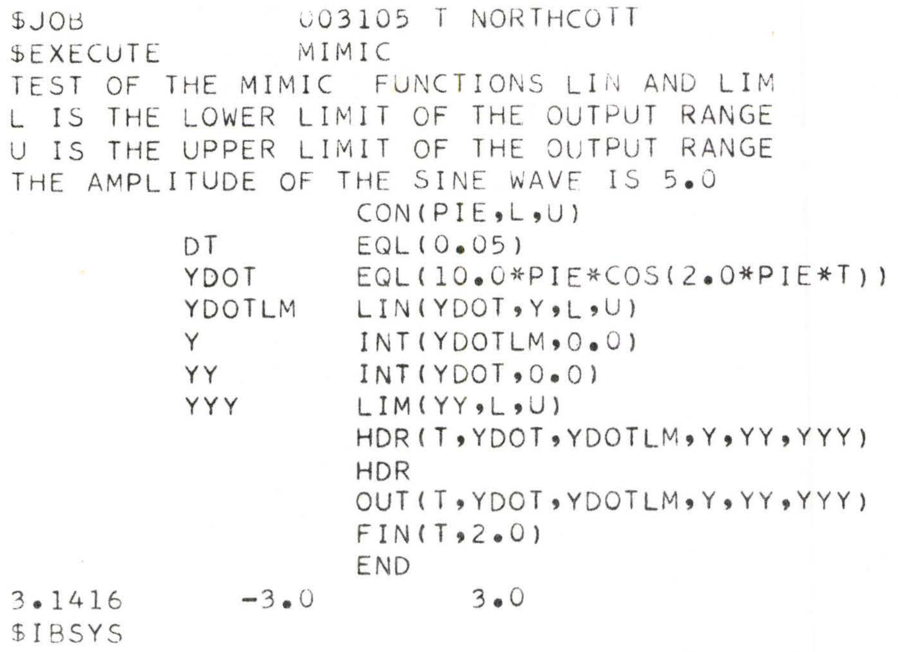
This example for specified XDOT, L, and U is given in Figure 13.

It was noted that the initial condition, x0, must be in the range $L \leq X0 \leq U$.

In a second example, the function $y = 5.0 \sin 2\Pi T$ was considered. The derivative is $\dot{y} = 10\Pi \cos 2\Pi T$. It was arbitrarily decided to limit y to

```
$JOB               003105 T NORTHCOTT
$EXECUTE           MIMIC
TEST OF EXAMPLE IN CRESS' HANDBOOK
PAGE 14  LIN FUNCTION USE
LIN LIMITS THE OUTPUT OF AN INTEGRATOR
                        CON(L,U,     X0)
          XDOT          EQL(2.0)
          XDOTLM        LIN(XDOT,X,L,U)
          X             INT(XDOTLM,X0)
                        HDR(T,X)
                        OUT(T,X)
                        FIN(T,3.0)
                        END
1.0           2.5             1.0
$IBSYS




   T                        X
-0.                      1.00000E 00
 1.00000E-01             1.20000E 00
 2.00000E-01             1.40000E 00
 3.00000E-01             1.60000E 00
 4.00000E-01             1.80000E 00
 5.00000E-01             2.00000E 00
 6.00000E-01             2.20000E 00
 7.00000E-01             2.40000E 00
 8.00000E-01             2.50009E 00
 9.00000E-01             2.50009E 00
 1.00000E 00             2.50009E 00
 1.10000E 00             2.50009E 00
 1.20000E 00             2.50009E 00
 1.30000E 00             2.50009E 00
 1.40000E 00             2.50009E 00
 1.50000E 00             2.50009E 00
 1.60000E 00             2.50009E 00
 1.70000E 00             2.50009E 00
 1.80000E 00             2.50009E 00
 1.90000E 00             2.50009E 00
 2.00000E 00             2.50009E 00
 2.10000E 00             2.50009E 00
 2.20000E 00             2.50009E 00
 2.30000E 00             2.50009E 00
 2.40000E 00             2.50009E 00
 2.50000E 00             2.50009E 00
 2.60000E 00             2.50009E 00
 2.70000E 00             2.50009E 00
 2.80000E 00             2.50009E 00
 2.90000E 00             2.50009E 00
 3.00000E 00             2.50009E 00
 3.10000E 00             2.50009E 00
```

FIGURE 13



```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
TEST OF THE MIMIC  FUNCTIONS LIN AND LIM
L IS THE LOWER LIMIT OF THE OUTPUT RANGE
U IS THE UPPER LIMIT OF THE OUTPUT RANGE
THE AMPLITUDE OF THE SINE WAVE IS 5.0
                  CON(PIE,L,U)
         DT       EQL(0.05)
         YDOT     EQL(10.0*PIE*COS(2.0*PIE*T))
         YDOTLM   LIN(YDOT,Y,L,U)
         Y        INT(YDOTLM,0.0)
         YY       INT(YDOT,0.0)
         YYY      LIM(YY,L,U)
                  HDR(T,YDOT,YDOTLM,Y,YY,YYY)
                  HDR
                  OUT(T,YDOT,YDOTLM,Y,YY,YYY)
                  FIN(T,2.0)
                  END
3.1416      -3.0        3.0
$IBSYS
```

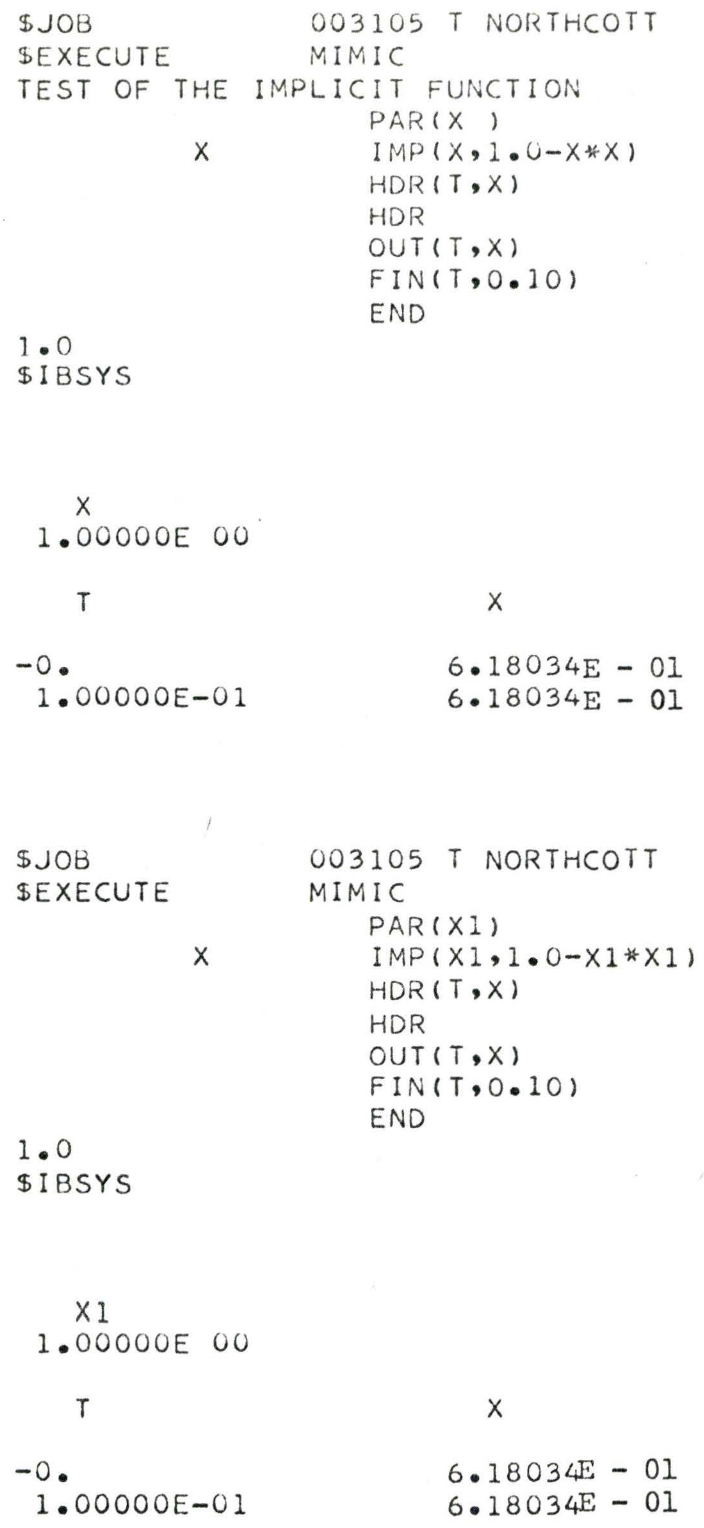
FIGURE 14.1

```
      T               YDØT          YDØTLM            Y               YY              YYY

 -0.             3.14160E 01    3.14160E 01     0.              0.              0.
  5.00000E-02    2.98784E 01    2.98784E 01     1.54509E 00     1.54509E 00     1.54509E 00
  1.00000E-01    2.54161E 01    2.54161E 01     2.93893E 00     2.93893E 00     2.93893E 00
  1.50000E-01    1.84658E 01    0.              3.00001E 00     4.04509E 00     3.00000E 00
  2.00000E-01    9.70799E 00    0.              3.00001E 00     4.75529E 00     3.00000E 00
  2.50000E-01   -1.15598E-04    0.              3.00001E 00     5.00000E 00     3.00000E 00
  3.00000E-01   -9.70821E 00    0.              3.00001E 00     4.75527E 00     3.00000E 00
  3.50000E-01   -1.84660E 01    0.              3.00001E 00     4.04507E 00     3.00000E 00
  4.00000E-01   -2.54162E 01    0.              3.00001E 00     2.93890E 00     2.93890E 00
  4.50000E-01   -2.98785E 01    0.              3.00001E 00     1.54505E 00     1.54505E 00
  5.00000E-01   -3.14160E 01    0.              3.00001E 00    -3.80665E-05    -3.80665E-05
  5.50000E-01   -2.98783E 01    0.              3.00001E 00    -1.54512E 00    -1.54512E 00
  6.00000E-01   -2.54159E 01    0.              3.00001E 00    -2.93896E 00    -2.93896E 00
  6.50000E-01   -1.84656E 01    0.              3.00001E 00    -4.04511E 00    -3.00000E 00
  7.00000E-01   -9.70777E 00    0.              3.00001E 00    -4.75530E 00    -3.00000E 00
  7.50000E-01    3.43050E-04    0.              3.00001E 00    -5.00000E 00    -3.00000E 00
  8.00000E-01    9.70843E 00    0.              3.00001E 00    -4.75526E 00    -3.00000E 00
  8.50000E-01    1.84662E 01    0.              3.00001E 00    -4.04505E 00    -3.00000E 00
  9.00000E-01    2.54163E 01    0.              3.00001E 00    -2.93887E 00    -2.93887E 00
  9.50000E-01    2.98785E 01    0.              3.00001E 00    -1.54502E 00    -1.54502E 00
  1.00000E 00    3.14160E 01    0.              3.00001E 00     7.23531E-05     7.23531E-05
  1.05000E 00    2.98782E 01    0.              3.00001E 00     1.54516E 00     1.54516E 00
  1.10000E 00    2.54158E 01    0.              3.00001E 00     2.93899E 00     2.93899E 00
  1.15000E 00    1.84654E 01    0.              3.00001E 00     4.04513E 00     3.00000E 00
  1.20000E 00    9.70756E 00    0.              3.00001E 00     4.75531E 00     3.00000E 00
  1.25000E 00   -5.68628E-04    0.              3.00001E 00     5.00000E 00     3.00000E 00
  1.30000E 00   -9.70864E 00    0.              3.00001E 00     4.75525E 00     3.00000E 00
  1.35000E 00   -1.84664E 01    0.              3.00001E 00     4.04503E 00     3.00000E 00
  1.40000E 00   -2.54164E 01    0.              3.00001E 00     2.93884E 00     2.93884E 00
  1.45000E 00   -2.98786E 01    0.              3.00001E 00     1.54498E 00     1.54498E 00
  1.50000E 00   -3.14160E 01    0.              3.00001E 00    -1.08943E-04    -1.08943E-04
  1.55000E 00   -2.98782E 01    0.              3.00001E 00    -1.54519E 00    -1.54519E 00
  1.60000E 00   -2.54157E 01    0.              3.00001E 00    -2.93902E 00    -2.93902E 00
  1.65000E 00   -1.84653E 01    0.              3.00001E 00    -4.04516E 00    -3.00000E 00
  1.70000E 00   -9.70735E 00    0.              3.00001E 00    -4.75532E 00    -3.00000E 00
  1.75000E 00    7.92335E-04    0.              3.00001E 00    -5.00000E 00    -3.00000E 00
  1.80000E 00    9.70885E 00    0.              3.00001E 00    -4.75524E 00    -3.00000E 00
  1.85000E 00    1.84665E 01    0.              3.00001E 00    -4.04501E 00    -3.00000E 00
  1.90000E 00    2.54166E 01    0.              3.00001E 00    -2.93882E 00    -2.93882E 00
  1.95000E 00    2.98787E 01    0.              3.00001E 00    -1.54495E 00    -1.54495E 00
  2.00000E 00    3.14160E 01    0.              3.00001E 00     1.43989E-04     1.43989E-04
  2.05000E 00    2.98781E 01    0.              3.00001E 00     1.54523E 00     1.54523E 00
```

FIGURE 14.2

```
$JOB            003105 T NORTHCOTT
$EXECUTE        MIMIC
TEST OF FUNCTION LIN
                     CON(A,B,C)
          RESULT     LIN((A+B*T+C*T*T),T,1.0,2.0)
                     HDR(T,RESULT)
                     HDR
                     OUT(T,RESULT)
                     FIN(T,3.0)
                     END
1.0          2.0          3.0
$IBSYS



   T                          RESULT

-0.                         0.
 1.00000E-01                0.
 2.00000E-01                0.
 3.00000E-01                0.
 4.00000E-01                0.
 5.00000E-01                0.
 6.00000E-01                0.
 7.00000E-01                0.
 8.00000E-01                0.
 9.00000E-01                0.
 1.00000E 00                6.00000E 00
 1.10000E 00                6.83000E 00
 1.20000E 00                7.72000E 00
 1.30000E 00                8.67000E 00
 1.40000E 00                9.68000E 00
 1.50000E 00                1.07500E 00
 1.60000E 00                1.18800E 00
 1.70000E 00                1.30700E 00
 1.80000E 00                1.43200E 00
 1.90000E 00                1.56300E 00
 2.00000E 00                1.70000E 00
 2.10000E 00                0.
 2.20000E 00                0.
 2.30000E 00                0.
 2.40000E 00                0.
 2.50000E 00                0.
 2.60000E 00                0.
 2.70000E 00                0.
 2.80000E 00                0.
 2.90000E 00                0.
 3.00000E 00                0.
 3.10000E 00                0.
```

FIGURE 15

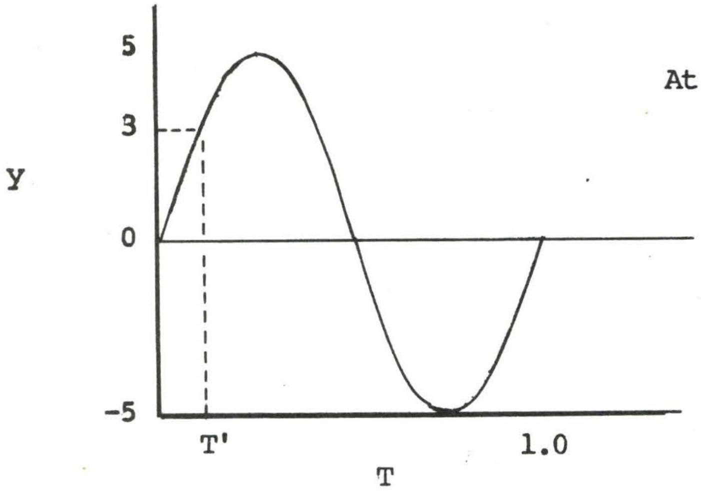


```
$JOB                003105 T NORTHCOTT
$EXECUTE            MIMIC
TEST OF THE IMPLICIT FUNCTION
                            PAR(X )
             X              IMP(X,1.0-X*X)
                            HDR(T,X)
                            HDR
                            OUT(T,X)
                            FIN(T,0.10)
                            END
1.0
$IBSYS



   X
 1.00000E 00

   T                             X

-0.                            6.18034E - 01
 1.00000E-01                   6.18034E - 01



$JOB                003105 T NORTHCOTT
$EXECUTE            MIMIC
                            PAR(X1)
             X              IMP(X1,1.0-X1*X1)
                            HDR(T,X)
                            HDR
                            OUT(T,X)
                            FIN(T,0.10)
                            END
1.0
$IBSYS



   X1
 1.00000E 00

   T                             X

-0.                            6.18034E - 01
 1.00000E-01                   6.18034E - 01
```

FIGURE 16

$$-3.0 \le y \le 3.0$$

The listing and results for this program are given in Figures 14.1 and 14.2. It should be noted that the output value of y remains constant at + 3.0 after it meets this limit. The explanation for this behaviour is that when y becomes equal to 3.0, the limited derivative is set equal to 0.0. Thus, y cannot change.



At T, YDOTLM becomes zero

In the same program, the function LIM is used to produce the output of that part of the sine wave varying from -3.0 to +3.0.

The function LIN can be used to limit the output of some variable to within a specified range. For instance, in the sample program and results shown in Figure 15 the output of $1.0 + 2.0\ T + 3.0\ T^2$ is limited to $1.0 \le T \le 2.0$.

A.8.3 Implicit Functions

Equations of the form $x = f(x)$ are solved automatically through the use of the MIMIC function IMP.

The function uses the following iterative method. An initial guess of the solution, x_o, is supplied to the function. Then,

$$x_n = \left(\frac{f_n - C_n x_n}{1 - C_n}\right)$$

where

$$C_n = \left(\frac{f_n - f_{n-1}}{x_n - x_{n-1}}\right)$$

and f_n is the value of f(x) at the nth iteration.

Iteration proceeds until $|x_n - f_n| \leq 5 \times 10^{-6} \quad |x_n|$

The implicit function is used by specifying the variable x using a PAR statement, or specifying it by means of a previous calculation within the program. Then, x is used as the result name, and x and f(x) are used as the first and second arguments respectively of the IMP function.

A more efficient method according to the Wright-Patterson manual (A.11.12) is to use a dummy variable for x in the PAR statement and in the arguments of IMP.

It should be noted that if the problem has more than one answer, no guarantee can be given as to which answer will be obtained.

The examples which are illustrated in Figure 16 show the solution of

$$\boxed{x = 1.0 - x^2}$$

It should be noted that the solution is obtained at T = 0.0.

A.8.4 Subprograms

Subprograms are useful for defining operations which are not performed by one of the MIMIC functions. The four subprogram functions previously noted (BSP, ESP, CSP, RSP) are used to define and use the subprogram.

A.8.4.1 Defining the Subprogram

A subprogram is defined by using the MIMIC functions BSP and ESP, and by following the rules given below:

1. The name of the subprogram is entered into the result field of both BSP and ESP cards.
2. The arguments of BSP are dummy variables representing inputs to the subprogram, and the arguments of ESP are dummy variables representing outputs from the program. These dummy variables may not be used elsewhere in the program.
3. The main part of the subprogram consists of those expressions between BSP and ESP which describe the relationships between the inputs to the subprogram and the outputs from the subprogram.
4. The subprogram must be written in the order in which operations are to be carried out.
5. The functions INT and FTR may not be used in the subprogram and the name of an array defined by CFN or PFN cannot be used as an input to a subprogram.

A.8.4.2 Using the Subprogram

The functions CSP and RSP control the use of the subprogram. The rules given below are to be followed.

1. The name of the subprogram is entered in the result field of both CSP and RSP cards.
2. The names of the inputs to the subprogram are used as the arguments of CSP and the names of the outputs from the

subprogram are used as arguments of RSP.

3. The CSP card must follow immediately after the RSP card.

Sample problem number 7 illustrates the method of defining and using subprograms.

A.9 SAMPLE PROBLEMS

This section illustrates the use of a wide range of MIMIC functions. Some problems are simple tests of the MIMIC function, but others are more complicated and involve the use of many functions.

A brief description of the problem, a sample listing and a sample output, and a brief discussion are given with each problem.

A.9.1 Sample Problem 1

Subject : Test of the MIMIC function DER

Description : To obtain the derivative of a function at different points along the function.

The functions given are $y = 1.0 + 2T + 3T^2$ and $y = \sqrt{T}$

Program Listing : Figures 17, 18.1

Sample Output : Figures 17, 18.2

Discussion : The derivative function DER uses a simple backward difference technique

$$\boxed{\dot{y} = \frac{y_n - y_{n-1}}{\Delta x}}$$

This is the simplest of all possible approximations and consequently errors are to be expected in the derivative. The derivative obtained using the function will be higher or lower than the actual analytical derivative depending upon the function. For instance, for the function $y = 1.0 + 2.0T + 3.0T^2$, the derivative obtained using DER is always lower than the analytical derivative. For the function $y = \sqrt{T}$, the derivative obtained using DER is larger than the analytical derivative.

It should also be noted from the sample outputs given that the accuracy of the DER derivative increases as the step size decreases. This is to be expected.

Some discussion should be given to the second example $y = \sqrt{T}$

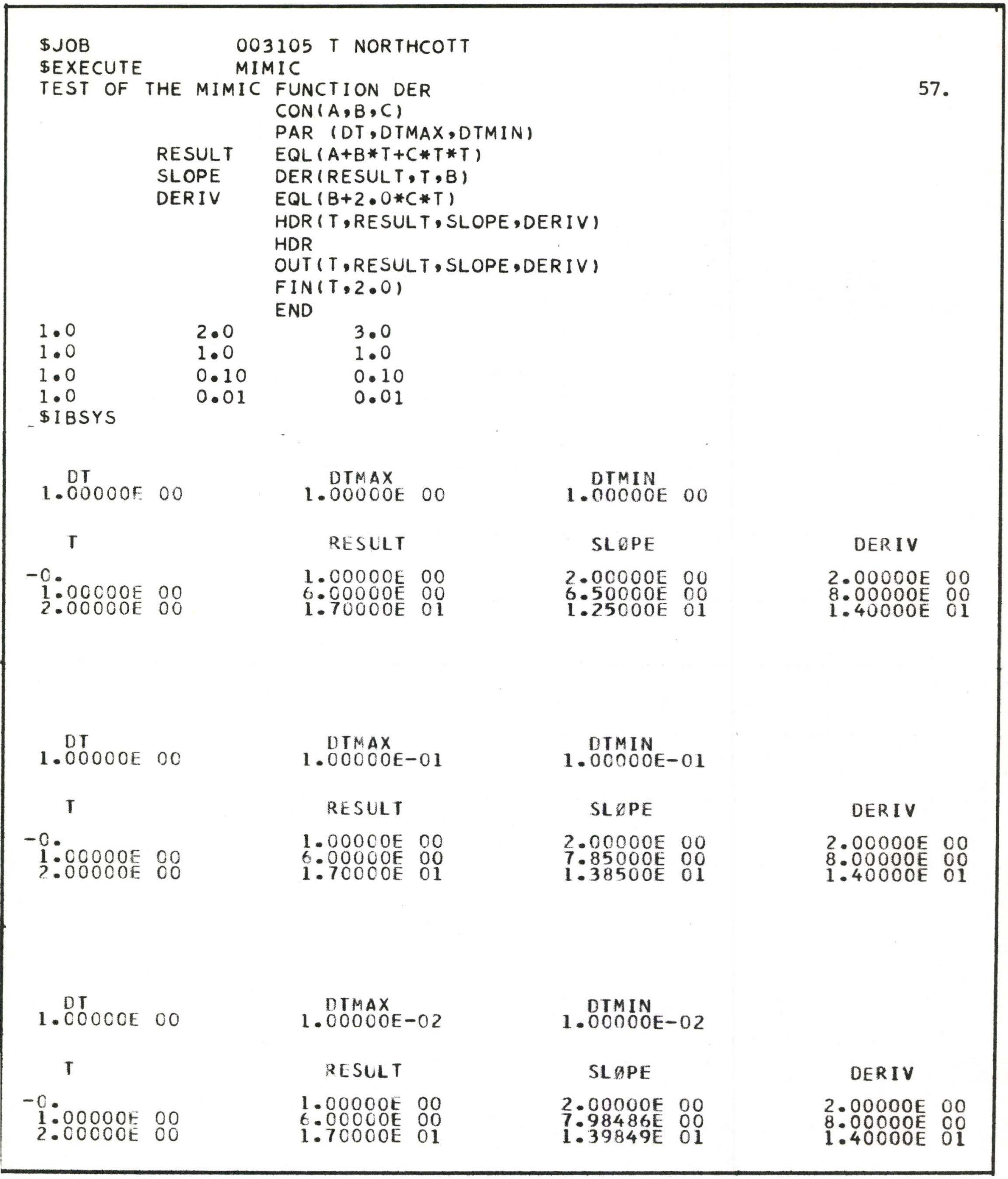
The derivative is

$$\boxed{\dot{y} = \frac{1}{2\sqrt{T}}}$$

At $T = 0$, $\dot{y} = 00$.

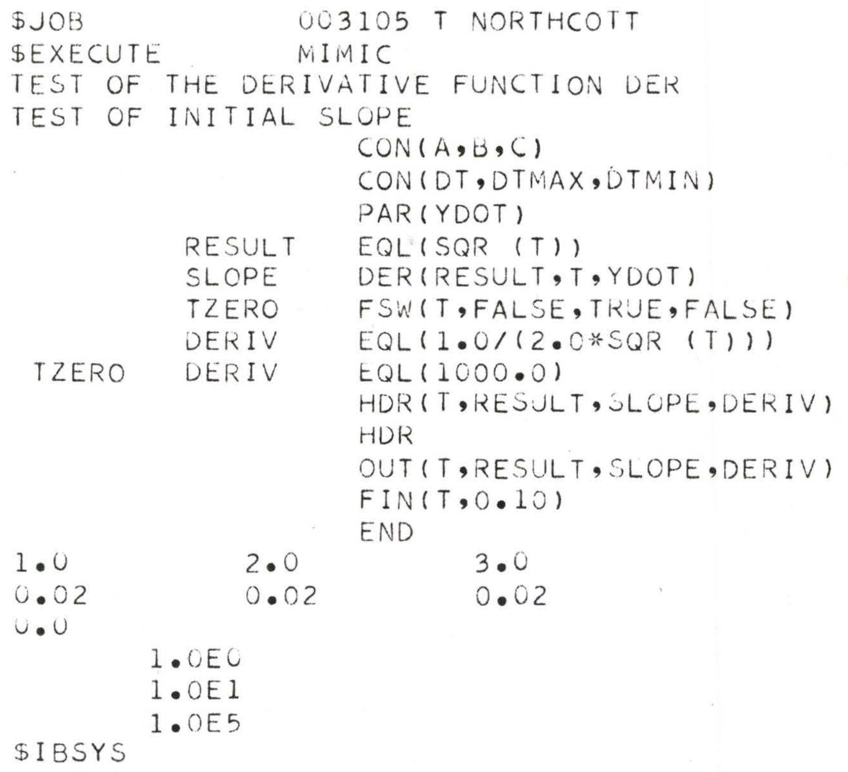
In using the function DER, we must specify $\dot{y}$ at $T = 0$ (the third argument). Several runs were done with different values of the derivative at $T = 0$. The runs are identical except at $T = 0$.

It seems, that when $\dot{y}|_o = 00$, any reasonable value may be used as the third argument of the DER function.



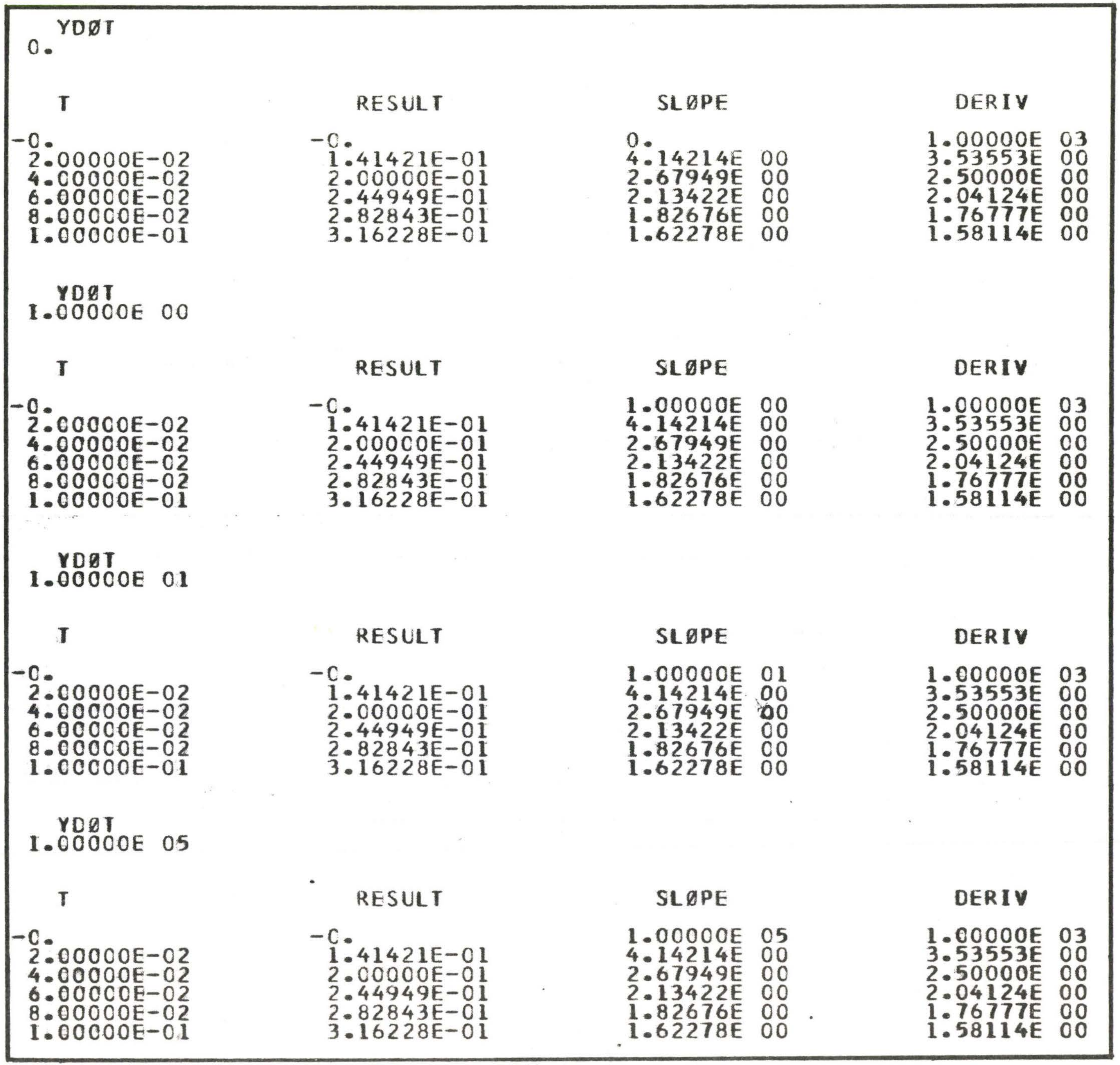
```
$JOB            003105 T NORTHCOTT
$EXECUTE        MIMIC
TEST OF THE MIMIC FUNCTION DER
                     CON(A,B,C)
                     PAR (DT,DTMAX,DTMIN)
         RESULT      EQL(A+B*T+C*T*T)
         SLOPE       DER(RESULT,T,B)
         DERIV       EQL(B+2.0*C*T)
                     HDR(T,RESULT,SLOPE,DERIV)
                     HDR
                     OUT(T,RESULT,SLOPE,DERIV)
                     FIN(T,2.0)
                     END
1.0         2.0         3.0
1.0         1.0         1.0
1.0         0.10        0.10
1.0         0.01        0.01
$IBSYS

    DT                  DTMAX               DTMIN
 1.00000E 00         1.00000E 00         1.00000E 00

    T                   RESULT              SLØPE               DERIV

-0.                  1.00000E 00         2.00000E 00         2.00000E 00
 1.00000E 00         6.00000E 00         6.50000E 00         8.00000E 00
 2.00000E 00         1.70000E 01         1.25000E 01         1.40000E 01



    DT                  DTMAX               DTMIN
 1.00000E 00         1.00000E-01         1.00000E-01

    T                   RESULT              SLØPE               DERIV

-0.                  1.00000E 00         2.00000E 00         2.00000E 00
 1.00000E 00         6.00000E 00         7.85000E 00         8.00000E 00
 2.00000E 00         1.70000E 01         1.38500E 01         1.40000E 01



    DT                  DTMAX               DTMIN
 1.00000E 00         1.00000E-02         1.00000E-02

    T                   RESULT              SLØPE               DERIV

-0.                  1.00000E 00         2.00000E 00         2.00000E 00
 1.00000E 00         6.00000E 00         7.98486E 00         8.00000E 00
 2.00000E 00         1.70000E 01         1.39849E 01         1.40000E 01
```

FIGURE 17



```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
TEST OF THE DERIVATIVE FUNCTION DER
TEST OF INITIAL SLOPE
                  CON(A,B,C)
                  CON(DT,DTMAX,DTMIN)
                  PAR(YDOT)
         RESULT   EQL(SQR (T))
         SLOPE    DER(RESULT,T,YDOT)
         TZERO    FSW(T,FALSE,TRUE,FALSE)
         DERIV    EQL(1.0/(2.0*SQR (T)))
 TZERO   DERIV    EQL(1000.0)
                  HDR(T,RESULT,SLOPE,DERIV)
                  HDR
                  OUT(T,RESULT,SLOPE,DERIV)
                  FIN(T,0.10)
                  END
1.0         2.0         3.0
0.02        0.02        0.02
0.0
       1.0E0
       1.0E1
       1.0E5
$IBSYS
```

FIGURE 18.1



```
  YDØT
 0.

   T                     RESULT                SLØPE                 DERIV

-0.                   -0.                   0.                    1.00000E 03
 2.00000E-02           1.41421E-01          4.14214E 00           3.53553E 00
 4.00000E-02           2.00000E-01          2.67949E 00           2.50000E 00
 6.00000E-02           2.44949E-01          2.13422E 00           2.04124E 00
 8.00000E-02           2.82843E-01          1.82676E 00           1.76777E 00
 1.00000E-01           3.16228E-01          1.62278E 00           1.58114E 00

  YDØT
 1.00000E 00

   T                     RESULT                SLØPE                 DERIV

-0.                   -0.                   1.00000E 00           1.00000E 03
 2.00000E-02           1.41421E-01          4.14214E 00           3.53553E 00
 4.00000E-02           2.00000E-01          2.67949E 00           2.50000E 00
 6.00000E-02           2.44949E-01          2.13422E 00           2.04124E 00
 8.00000E-02           2.82843E-01          1.82676E 00           1.76777E 00
 1.00000E-01           3.16228E-01          1.62278E 00           1.58114E 00

  YDØT
 1.00000E 01

   T                     RESULT                SLØPE                 DERIV

-0.                   -0.                   1.00000E 01           1.00000E 03
 2.00000E-02           1.41421E-01          4.14214E 00           3.53553E 00
 4.00000E-02           2.00000E-01          2.67949E 00           2.50000E 00
 6.00000E-02           2.44949E-01          2.13422E 00           2.04124E 00
 8.00000E-02           2.82843E-01          1.82676E 00           1.76777E 00
 1.00000E-01           3.16228E-01          1.62278E 00           1.58114E 00

  YDØT
 1.00000E 05

   T                     RESULT                SLØPE                 DERIV

-0.                   -0.                   1.00000E 05           1.00000E 03
 2.00000E-02           1.41421E-01          4.14214E 00           3.53553E 00
 4.00000E-02           2.00000E-01          2.67949E 00           2.50000E 00
 6.00000E-02           2.44949E-01          2.13422E 00           2.04124E 00
 8.00000E-02           2.82843E-01          1.82676E 00           1.76777E 00
 1.00000E-01           3.16228E-01          1.62278E 00           1.58114E 00
```

FIGURE 18.2

A.9.2 Sample Problem 2

Subject : Test of the MIMIC functions FLF, EOR, and LSW

Description : Two logical variables A and B are defined by function switches such that the values of A and B for various values of T are those shown in the following table

T	A	B
≤ 1.0	TRUE	FALSE
1.0 ≤ T ≤ 2.0	FALSE	FALSE
> 2.0	FALSE	TRUE

A third logical variable C was set TRUE.

The three functions FLF, EOR and LSW with logical combinations of A, B, and C were used to define three different logical variables R, RR, and RRR. In turn, these were used to control the printout of an arbitrary numerical value which was defined as characteristic of the value of the logical variable produced by FLF, EOR or LSW. (i.e., R, RR, and RRR respectively).

Program Listing : Figure 19.1

Sample Output : Figure 19.2

Discussion : The functions behaved as expected.

```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
TEST OF THE MIMIC FUNCTIONS FLF,LSW,EOR
         DT        EQL(0.10)
         DTMAX     EQL(0.10)
         DTMIN     EQL(DTMAX)
         C         EQL(TRUE)
         A         FSW((T-1.0),TRUE,TRUE,FALSE)
         B         FSW((T-2.0),FALSE,FALSE,TRUE)
         R         FLF(A,B,C)
         RESULT    EQL(0.0)
 R       RESULT    EQL(10.0)
RR = TRUE FOR A DIFFERENT FROM B.  = FALSE FOR A SAME AS B.
         RR        EOR(A,B)
         ANSWER    EQL(2.0)
 RR      ANSWER    EQL(12.0)
RRR = B FOR A = TRUE.  = C FOR A = FALSE.
         RRR       LSW(A,B,C)
         VALUE     EQL(4.0)
 RRR     VALUE     EQL(14.0)
                   FIN(T,3.0)
                   HDR(T,RESULT,ANSWER,VALUE)
                   HDR
                   OUT(T,RESULT,ANSWER,VALUE)
                   END
$IBSYS
```

FIGURE 19.1

```
   T                        RESULT                   ANSWER                    VALUE

-0.                       1.00000E 01              1.20000E 01              4.00000E 00
 1.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 2.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 3.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 4.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 5.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 6.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 7.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 8.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 9.00000E-01              1.00000E 01              1.20000E 01              4.00000E 00
 1.00000E 00              1.00000E 01              1.20000E 01              4.00000E 00
 1.10000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.20000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.30000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.30000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.40000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.50000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.60000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.70000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.80000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.80000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 1.90000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 2.00000E 00              1.00000E 01              2.00000E 01              1.40000E 00
 2.10000E 00              0.                       1.20000E 01              1.40000E 00
 2.20000E 00              0.                       1.20000E 01              1.40000E 00
 2.30000E 00              0.                       1.20000E 01              1.40000E 00
 2.40000E 00              0.                       1.20000E 01              1.40000E 00
 2.50000E 00              0.                       1.20000E 01              1.40000E 00
 2.60000E 00              0.                       1.20000E 01              1.40000E 00
 2.70000E 00              0.                       1.20000E 01              1.40000E 00
 2.80000E 00              0.                       1.20000E 01              1.40000E 00
 2.90000E 00              0.                       1.20000E 01              1.40000E 00
 3.00000E 00              0.                       1.20000E 01              1.40000E 00
 3.10000E 00              0.                       1.20000E 01              1.40000E 00
```

FIGURE 19.2

A.9.3 Sample Problem 3

Subject : Test of the MIMIC functions DSP and LIM.

Description : The purposes of each of these functions are found in the MIMIC function section of the report.

Program Listing : Figure 20

Sample Output : Figure 20

Discussion : Both functions worked as desired except for the value of R given by DSP at T = 2.0. This value ($-3.72529\ 10^{-9}$) is essentially zero and thus is not grossly in error. It is not understood why this value should appear.

```
$JOB                003105 T NORTHCOTT
$EXECUTE            MIMIC
TEST OF THE MIMIC FUNCTIONS DSP AND LIM
            DTT         EQL(1.0)
            TT          INT(DTT,0.0)
            R           DSP(TT,0.2,0.5)
            RR          LIM(TT,0.2,0.5)
                        FIN(T,1.0)
                        HDR(T,R,RR)
                        HDR
                        OUT(T,R,RR)
                        END
$IBSYS
```

```
    T                            R                             RR

-0.                         -2.00000E-01                  2.00000E-01
 1.00000E-01                -1.00000E-01                  2.00000E-01
 2.00000E-01                -3.72529E-09                  2.00000E-01
 3.00000E-01                 0.                           3.00000E-01
 4.00000E-01                 0.                           4.00000E-01
 5.00000E-01                 0.                           5.00000E-01
 6.00000E-01                 1.00000E-01                  5.00000E-01
 7.00000E-01                 2.00000E-01                  5.00000E-01
 8.00000E-01                 3.00000E-01                  5.00000E-01
 9.00000E-01                 4.00000E-01                  5.00000E-01
 1.00000E 00                 5.00000E-01                  5.00000E-01
```

FIGURE 20

A.9.4 Sample Problem 4

Subject : Test of the MIMIC function RNU

Description : To obtain a list of random numbers having a lower limit of zero, and upper limit of 100., and belonging to a uniform distribution.

Program Listing : Figure 21

Sample Output : Figure 21

Discussion : It is assumed that the step size may be made as small as desired. A new random number appears at each printout. For the 51 numbers shown, the mean was about 51.22.

```
$JOB            003105 T NORTHCOTT
$EXECUTE        MIMIC
TEST OF THE RANDOM NUMBER GENERATOR RNU
                       CON(A,B,C)
           VALUE       RNG(A,B,C)
                       HDR(T,VALUE)
                       HDR
                       OUT(T,VALUE)
                       FIN(T,5.0)
                       END
0.0            100.0          50.0
$IBSYS


    T                               VALUE

 -0.                             2.66235E 01
  1.00000E-01                    7.82349E 01
  2.00000E-01                    5.69458E 01
  3.00000E-01                    3.87817E 01
  4.00000E-01                    7.37427E 01
  5.00000E-01                    1.18286E 01
  6.00000E-01                    3.03955E 00
  7.00000E-01                    9.73755E 01
  8.00000E-01                    4.48364E 01
  9.00000E-01                    9.54224E 01
  1.00000E 00                    9.91333E 01
  1.10000E 00                    5.96924E 00
  1.20000E 00                    6.59302E 01
  1.30000E 00                    2.90161E 01
  1.40000E 00                    4.52271E 01
  1.50000E 00                    6.45630E 01
  1.60000E 00                    3.70239E 01
  1.70000E 00                    1.26099E 01
  1.80000E 00                    4.13208E 01
  1.90000E 00                    7.31567E 01
  2.00000E 00                    5.81177E 01
  2.10000E 00                    4.62036E 01
  2.20000E 00                    8.74146E 01
  2.30000E 00                    3.17505E 01
  2.40000E 00                    2.92114E 01
  2.50000E 00                    2.97974E 01
  2.60000E 00                    8.35083E 01
  2.70000E 00                    4.03442E 01
  2.80000E 00                    5.03052E 01
  2.90000E 00                    6.33911E 01
  3.00000E 00                    2.96021E 01
  3.10000E 00                    9.89380E 01
  3.20000E 00                    2.13989E 01
  3.30000E 00                    4.69849E 01
  3.40000E 00                    2.56958E 01
  3.50000E 00                    7.53174E 00
  3.60000E 00                    4.24927E 01
  3.70000E 00                    8.05786E 01
  3.80000E 00                    7.17896E 01
  3.90000E 00                    6.61255E 01
  4.00000E 00                    1.35864E 01
  4.10000E 00                    6.41724E 01
  4.20000E 00                    6.78833E 01
  4.30000E 00                    7.47192E 01
  4.40000E 00                    3.46802E 01
  4.50000E 00                    9.77661E 01
  4.60000E 00                    1.39771E 01
  4.70000E 00                    3.33130E 01
  4.80000E 00                    5.77393E 00
  4.90000E 00                    8.13599E 01
  5.00000E 00                    1.00708E 01
```

FIGURE 21

A.9.5 Sample Problem 5

Subject : Reactor design

Reference: Chemical Engineering Kinetics, J.M. Smith,
McGraw-Hill, New York, 1956
example 6 - 5, page 162.

Description : The problem which will be solved is to find the length of a tubular reactor of the given diameter such that the conversion of chlorine for the given reactions is 90 percent complete. The temperature profile is also recorded.

Program Listing : Figure 22.1

Sample Output : Figure 22.2, 22.3

Discussion : The assumptions made and the data used are given in the reference. The derivations of the rate and energy equations are also given in the reference. The rate and energy equations are integrated and a check is made to determine when the desired conversion has been obtained. Two pages of output are shown, one near the beginning and one near the end of the run. It may be seen that the required conversion of 90 percent occurs at about 88.7 feet.

```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
REFERENCE   SMITH     CHEMICAL ENGINEERING KINETICS
PRODUCTION OF ALLYL CHLORIDE
                  CON(DT,DTMAX,DTMIN)
                  CON(CPCL,CPP,CPA,CPD,CPH)
                  CON(DELH1, DELH2)
                  CON(AC,AR,F,U,TS)
                  CON(AAA)
         FACT1    EQL((0.8-X1-X2)*(0.2-X1-X2)/((1.-X2)*(1.-X2)))
         R1       EQL(AAA*FACT1*EXP((-13700./TEMP)))
         R2       EQL(46.8*FACT1*EXP((-3460./TEMP)))
         X1       INT((R1*AC/F),0.0)
         X2       INT((R2*AC/F),0.0)
         DELT     EQL(TS-TEMP)
         TEMP     INT(((-R1*DELH1-R2*DELH2)*AC+U*DELT*AR)/FACT2,852.0)
         NCL      EQL(0.85/5.-0.85*X1-0.85*X2)
         NP       EQL(4.*0.85/5.-0.85*X1-0.85*X2)
         NA       EQL(0.85*X1)
         ND       EQL(0.85*X2)
         NH       EQL(0.85*X1)
         FACT2    EQL(NCL*CPCL+NP*CPP+NA*CPA+ND*CPD+NH*CPH)
         XX       EQL((X1+X2)/0.20)
         ABC      FSW((XX-0.90),FALSE,TRUE,TRUE)
                  HDR(T,X1,X2,TEMP)
                  HDR(,XX)
                  HDR
                  OUT(T,X1,X2,TEMP)
                  OUT(,XX)
 ABC              FIN(XX,0.90)
                  FIN(T,200.)
                  END
1.0         0.10        0.10
8.6         25.3        28.0        30.7        7.2
-48000.     -79200.
0.0218      0.524       0.85        5.0         852.0
    8.24E+05
$IBSYS
```

FIGURE 22.1

```
    T                     X1                    X2                    TEMP
                          XX

-0.                     0.                     0.                    8.52000E 02
                        0.
 1.00000E 00            3.91746E-04            3.37889E-03           8.64178E 02
                        1.88532E-02
 2.00000E 00            8.68392E-04            6.88296E-03           8.75360E 02
                        3.87568E-02
 3.00000E 00            1.43455E-03            1.04908E-02           8.85613E 02
                        5.96266E-02
 4.00000E 00            2.09267E-03            1.41810E-02           8.94990E 02
                        8.13684E-02
 5.00000E 00            2.84282E-03            1.79327E-02           9.03536E 02
                        1.03877E-01
 6.00000E 00            3.68263E-03            2.17253E-02           9.11284E 02
                        1.27039E-01
 7.00000E 00            4.60727E-03            2.55390E-02           9.18262E 02
                        1.50731E-01
 8.00000E 00            5.60961E-03            2.93548E-02           9.24491E 02
                        1.74822E-01
 9.00000E 00            6.68042E-03            3.31551E-02           9.29991E 02
                        1.99177E-01
 1.00000E 01            7.80874E-03            3.69230E-02           9.34778E 02
                        2.23659E-01
 1.10000E 01            8.98229E-03            4.06435E-02           9.38868E 02
                        2.48129E-01
 1.20000E 01            1.01879E-02            4.43030E-02           9.42280E 02
                        2.72455E-01
 1.30000E 01            1.14123E-02            4.78894E-02           9.45035E 02
                        2.96508E-01
 1.40000E 01            1.26421E-02            5.13926E-02           9.47157E 02
                        3.20173E-01
 1.50000E 01            1.38648E-02            5.48041E-02           9.48674E 02
                        3.43344E-01
 1.60000E 01            1.50690E-02            5.81172E-02           9.49619E 02
                        3.65931E-01
 1.70000E 01            1.62445E-02            6.13269E-02           9.50031E 02
                        3.87857E-01
 1.80000E 01            1.73831E-02            6.44298E-02           9.49950E 02
                        4.09064E-01
 1.90000E 01            1.84779E-02            6.74238E-02           9.49420E 02
                        4.29508E-01
 2.00000E 01            1.95239E-02            7.03083E-02           9.48488E 02
                        4.49161E-01
 2.10000E 01            2.05176E-02            7.30837E-02           9.47201E 02
                        4.68007E-01
 2.20000E 01            2.14573E-02            7.57514E-02           9.45607E 02
                        4.86043E-01
 2.30000E 01            2.23420E-02            7.83136E-02           9.43752E 02
                        5.03278E-01
 2.40000E 01            2.31723E-02            8.07731E-02           9.41680E 02
                        5.19727E-01
 2.50000E 01            2.39495E-02            8.31332E-02           9.39435E 02
                        5.35413E-01
 2.60000E 01            2.46753E-02            8.53975E-02           9.37055E 02
                        5.50364E-01
 2.70000E 01            2.53522E-02            8.75700E-02           9.34577E 02
```

FIGURE 22.2

```
                        7.97261E-01
5.70000E 01             3.40366E-02          1.26333E-01          8.80232E 02
                        8.01848E-01
5.80000E 01             3.41565E-02          1.27105E-01          8.79364E 02
                        8.06309E-01
5.90000E 01             3.42719E-02          1.27857E-01          8.78533E 02
                        8.10647E-01
6.00000E 01             3.43832E-02          1.28591E-01          8.77739E 02
                        8.14869E-01
6.10000E 01             3.44906E-02          1.29305E-01          8.76979E 02
                        8.18978E-01
6.20000E 01             3.45942E-02          1.30002E-01          8.76251E 02
                        8.22979E-01
6.30000E 01             3.46943E-02          1.30681E-01          8.75553E 02
                        8.26876E-01
6.40000E 01             3.47911E-02          1.31343E-01          8.74884E 02
                        8.30672E-01
6.50000E 01             3.48846E-02          1.31990E-01          8.74241E 02
                        8.34371E-01
6.60000E 01             3.49752E-02          1.32620E-01          8.73625E 02
                        8.37977E-01
6.70000E 01             3.50628E-02          1.33236E-01          8.73032E 02
                        8.41492E-01
6.80000E 01             3.51476E-02          1.33836E-01          8.72462E 02
                        8.44920E-01
6.90000E 01             3.52299E-02          1.34423E-01          8.71914E 02
                        8.48263E-01
7.00000E 01             3.53095E-02          1.34995E-01          8.71386E 02
                        8.51524E-01
7.10000E 01             3.53868E-02          1.35554E-01          8.70877E 02
                        8.54706E-01
7.20000E 01             3.54618E-02          1.36100E-01          8.70386E 02
                        8.57810E-01
7.30000E 01             3.55346E-02          1.36634E-01          8.69913E 02
                        8.60841E-01
7.40000E 01             3.56052E-02          1.37155E-01          8.69456E 02
                        8.63799E-01
7.50000E 01             3.56738E-02          1.37664E-01          8.69015E 02
                        8.66687E-01
7.60000E 01             3.57404E-02          1.38161E-01          8.68589E 02
                        8.69507E-01
7.70000E 01             3.58051E-02          1.38647E-01          8.68177E 02
                        8.72261E-01
7.80000E 01             3.58681E-02          1.39122E-01          8.67778E 02
                        8.74951E-01
7.90000E 01             3.59292E-02          1.39587E-01          8.67392E 02
                        8.77579E-01
8.00000E 01             3.59887E-02          1.40040E-01          8.67018E 02
                        8.80146E-01
8.10000E 01             3.60466E-02          1.40484E-01          8.66656E 02
                        8.82654E-01
8.20000E 01             3.61029E-02          1.40918E-01          8.66305E 02
                        8.85105E-01
8.30000E 01             3.61577E-02          1.41342E-01          8.65964E 02
                        8.87500E-01
8.40000E 01             3.62110E-02          1.41757E-01          8.65634E 02
                        8.89840E-01
8.50000E 01             3.62630E-02          1.42163E-01          8.65314E 02
                        8.92129E-01
8.60000E 01             3.63135E-02          1.42560E-01          8.65003E 02
                        8.94365E-01
8.70000E 01             3.63628E-02          1.42948E-01          8.64701E 02
                        8.96552E-01
8.80000E 01             3.64108E-02          1.43327E-01          8.64407E 02
                        8.98690E-01
8.90000E 01             3.64575E-02          1.43699E-01          8.64122E 02
                        9.00780E-01
```

FIGURE 22.3

A.9.6 Sample Problem 6

Subject : Diffusion into a sphere

Reference: The Mathematics of Diffusion,

J. Crank, Oxford University Press, London 1956,

page 84.

Description : The diffusion equation for a constant diffusion coefficient will be solved for a sphere.

The equation is

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right)$$

Program Listing : Figure 23.1

Sample Output : Figure 23.2, 23.3

Discussion : Finite difference approximations were written for $\frac{\partial^2 C}{\partial r^2}$ and $\frac{\partial C}{\partial r}$ to change the partial differential equation into the following ordinary differential equations

$$\frac{\partial C_n}{dt} = \frac{D}{(\Delta r)^2} \left[(1 + \frac{1}{n}) C_{n+1} - 2 C_n + (1 - \frac{1}{n}) C_{n-1} \right]$$

$$n = 1,2,3$$

The sphere chosen was arbitrarily 1.00 unit in diameter. It was subdivided into 25 radial increments and this differential equation was solved at each increment to yield a concentration profile as a function of time. It was assumed arbitrarily that the surface concentration was 1.0 and the diffusivity was 0.001.

The concentration at the centre point was obtained by the following analysis:

Taylor's series is defined as

$$f(x_o + h) = f(x_o) + h\,f'\,(x_o) + \tfrac{1}{2}\,h^2\,f''\,(x_o) + \;\ldots$$

For this system,

$$C(r_o + \Delta r) = C(r_o) + \Delta r\cdot \left.\frac{\partial C}{\partial r}\right|_{r_o} + \tfrac{1}{2}\cdot(\Delta r)^2 \cdot \left.\frac{\partial^2 C}{\partial r^2}\right|_{r_o} \qquad (1)$$

$$C(r_o + 2\Delta r) = C(r_o) + 2\cdot\Delta r\cdot \left.\frac{\partial C}{\partial r}\right|_{r_o} + 2\cdot(\Delta r)^2\cdot \left.\frac{\partial^2 C}{\partial r^2}\right|_{r_o} \qquad (2)$$

4 x (1)

$$4\cdot C(r_o + \Delta r) = 4\cdot C(r_o) + 4\cdot\Delta r\cdot \left.\frac{\partial C}{\partial r}\right|_{r_o} + 2\cdot(\Delta r)^2\cdot \left.\frac{\partial^2 C}{\partial r^2}\right|_{r_o} \qquad (3)$$

(3) - (2)

$$4\cdot C(r_o + \Delta r) - C(r_o + 2\Delta r) = 3\cdot C(r_o) + 2\cdot\Delta r\cdot \left.\frac{\partial C}{\partial r}\right|_{r_o}$$

But

$$\left.\frac{\partial C}{\partial r}\right|_{r_o} = 0$$

Therefore

$$C(r_o) = [4\cdot C(r_o + \Delta r) - C(r_o + 2\cdot\Delta r)]\,/3.0$$

Two pages of the output are shown, one for the time near zero, and the other at the end of the run.

The negative values for C0 near the beginning of the run are probably caused by the truncation of the Taylor's series expansions for C0. It should be noted that at the end of the run, the interior concentrations are changing relatively rapidly. Steady state would be reached when the concentration throughout the sphere was equal to the surface concentration. It is not known how long the program would have to run to attain this state.

```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
TRIAL SOLUTION OF DIFFUSION IN A SPHERE.
25C IS A SURFACE CONCENTRATION AND IS CONSTANT
D IS THE DIFFUSIVITY OF THE DIFFUSING SUBSTANCE
DELR IS THE INCREMENTAL DISTANCE
                 CON(25C)
                 CON(D,DELR)
         K       EQL(D/(DELR*DELR)
         24C     INT(K*((1.+1./24.)*25C-2.*24C+(1.-1./24.)*23C),0.0)
         23C     INT(K*((1.+1./23.)*24C-2.*23C+(1.-1./23.)*22C),0.0)
         22C     INT(K*((1.+1./22.)*23C-2.*22C+(1.-1./22.)*21C),0.0)
         21C     INT(K*((1.+1./21.)*22C-2.*21C+(1.-1./21.)*20C),0.0)
         20C     INT(K*((1.+1./20.)*21C-2.*20C+(1.-1./20.)*19C),0.0)
         19C     INT(K*((1.+1./19.)*20C-2.*19C+(1.-1./19.)*18C),0.0)
         18C     INT(K*((1.+1./18.)*19C-2.*18C+(1.-1./18.)*17C),0.0)
         17C     INT(K*((1.+1./17.)*18C-2.*17C+(1.-1./17.)*16C),0.0)
         16C     INT(K*((1.+1./16.)*17C-2.*16C+(1.-1./16.)*15C),0.0)
         15C     INT(K*((1.+1./15.)*16C-2.*15C+(1.-1./15.)*14C),0.0)
         14C     INT(K*((1.+1./14.)*15C-2.*14C+(1.-1./14.)*13C),0.0)
         13C     INT(K*((1.+1./13.)*14C-2.*13C+(1.-1./13.)*12C),0.0)
         12C     INT(K*((1.+1./12.)*13C-2.*12C+(1.-1./12.)*11C),0.0)
         11C     INT(K*((1.+1./11.)*12C-2.*11C+(1.-1./11.)*10C),0.0)
         10C     INT(K*((1.+1./10.)*11C-2.*10C+(1.-1./10.)* 9C),0.0)
         9C      INT(K*((1.+1./ 9.)*10C-2.* 9C+(1.-1./ 9.)* 8C),0.0)
         8C      INT(K*((1.+1./ 8.)* 9C-2.* 8C+(1.-1./ 8.)* 7C),0.0)
         7C      INT(K*((1.+1./ 7.)* 8C-2.* 7C+(1.-1./ 7.)* 6C),0.0)
         6C      INT(K*((1.+1./ 6.)* 7C-2.* 6C+(1.-1./ 6.)* 5C),0.0)
         5C      INT(K*((1.+1./ 5.)* 6C-2.* 5C+(1.-1./ 5.)* 4C),0.0)
         4C      INT(K*((1.+1./ 4.)* 5C-2.* 4C+(1.-1./ 4.)* 3C),0.0)
         3C      INT(K*((1.+1./ 3.)* 4C-2.* 3C+(1.-1./ 3.)* 2C),0.0)
         2C      INT(K*((1.+1./ 2.)* 3C-2.* 2C+(1.-1./ 2.)* 1C),0.0)
         1C      INT(K*((1.+1./ 1.)* 2C-2.* 1C+(1.-1./ 1.)* 0C),0.0)
         0C      EQL((4.0*1C-2C)/3.0)
                 FIN(T,20.0)
                 HDR(T,C0,C8,C16,C24)
                 HDR
                 OUT(T,0C,8C,16C,24C)
                 END
1.0
0.001        0.04
$IBSYS
```

FIGURE 23.1

```
      T                    C0                  C8                  C16                 C24

 -0.                    0.                  0.                  0.                  0.
  1.00000E-01           0.                  2.64509E-35         5.60124E-17         6.12381E-02
  2.00000E-01           0.                  3.08378E-30         2.56564E-14         1.15490E-01
  3.00000E-01           0.                  2.70291E-27         8.83056E-13         1.63739E-01
  4.00000E-01          -1.31063E-36         3.20018E-25         1.05375E-11         2.06816E-01
  5.00000E-01          -1.91773E-34         1.26536E-23         7.03981E-11         2.45423E-01
  6.00000E-01          -1.10283E-32         2.50065E-22         3.25951E-10         2.80153E-01
  7.00000E-01          -3.31709E-31         3.06262E-21         1.17209E-09         3.11511E-01
  8.00000E-01          -6.20780E-30         2.64293E-20         3.50349E-09         3.39927E-01
  9.00000E-01          -8.08528E-29         1.74580E-19         9.09517E-09         3.65767E-01
  1.00000E 00          -7.91112E-28         9.34054E-19         2.11295E-08         3.89346E-01
  1.10000E 00          -6.14111E-27         4.21438E-18         4.48751E-08         4.10932E-01
  1.20000E 00          -3.93736E-26         1.65200E-17         8.85128E-08         4.30757E-01
  1.30000E 00          -2.14972E-25         5.75471E-17         1.64092E-07         4.49021E-01
  1.40000E 00          -1.02350E-24         1.81302E-16         2.88595E-07         4.65897E-01
  1.50000E 00          -4.33008E-24         5.23846E-16         4.85079E-07         4.81535E-01
  1.60000E 00          -1.65266E-23         1.40378E-15         7.83864E-07         4.96065E-01
  1.70000E 00          -5.76141E-23         3.52115E-15         1.22372E-06         5.09600E-01
  1.80000E 00          -1.85344E-22         8.33031E-15         1.85305E-06         5.22241E-01
  1.90000E 00          -5.54953E-22         1.87068E-14         2.73099E-06         5.34074E-01
  2.00000E 00          -1.55776E-21         4.00902E-14         3.92840E-06         5.45176E-01
  2.10000E 00          -4.12463E-21         8.23719E-14         5.52884E-06         5.55614E-01
  2.20000E 00          -1.03563E-20         1.62908E-13         7.62925E-06         5.65449E-01
  2.30000E 00          -2.47706E-20         3.11183E-13         1.03406E-05         5.74733E-01
  2.40000E 00          -5.66631E-20         5.75838E-13         1.37885E-05         5.83513E-01
  2.50000E 00          -1.24391E-19         1.03499E-12         1.81130E-05         5.91832E-01
  2.60000E 00          -2.62854E-19         1.81105E-12         2.34694E-05         5.99726E-01
  2.70000E 00          -5.36071E-19         3.09155E-12         3.00277E-05         6.07229E-01
  2.80000E 00          -1.05760E-18         5.15781E-12         3.79723E-05         6.14372E-01
  2.90000E 00          -2.02255E-18         8.42384E-12         4.75020E-05         6.21181E-01
  3.00000E 00          -3.75603E-18         1.34881E-11         5.88294E-05         6.27681E-01
  3.10000E 00          -6.78407E-18         2.12011E-11         7.21799E-05         6.33894E-01
  3.20000E 00          -1.19335E-17         3.27535E-11         8.77914E-05         6.39840E-01
  3.30000E 00          -2.04676E-17         4.97876E-11         1.05913E-04         6.45538E-01
  3.40000E 00          -3.42613E-17         7.45380E-11         1.26804E-04         6.51002E-01
  3.50000E 00          -5.60162E-17         1.10007E-10         1.50735E-04         6.56250E-01
  3.60000E 00          -8.95051E-17         1.60181E-10         1.77981E-04         6.61294E-01
  3.70000E 00          -1.39818E-16         2.30290E-10         2.08828E-04         6.66148E-01
  3.80000E 00          -2.13557E-16         3.27130E-10         2.43567E-04         6.70822E-01
  3.90000E 00          -3.18678E-16         4.59434E-10         2.82492E-04         6.75327E-01
  4.00000E 00          -4.65223E-16         6.38329E-10         3.25904E-04         6.79673E-01
  4.10000E 00          -6.62490E-16         8.77855E-10         3.74103E-04         6.83870E-01
  4.20000E 00          -9.19259E-16         1.19558E-09         4.27394E-04         6.87925E-01
  4.30000E 00          -1.23951E-15         1.61332E-09         4.86079E-04         6.91846E-01
  4.40000E 00          -1.61707E-15         2.15794E-09         5.50462E-04         6.95641E-01
  4.50000E 00          -2.02665E-15         2.86230E-09         6.20843E-04         6.99315E-01
  4.60000E 00          -2.40994E-15         3.76628E-09         6.97520E-04         7.02876E-01
  4.70000E 00          -2.65488E-15         4.91801E-09         7.80789E-04         7.06328E-01
  4.80000E 00          -2.56515E-15         6.37517E-09         8.70938E-04         7.09678E-01
  4.90000E 00          -1.81667E-15         8.20649E-09         9.68253E-04         7.12929E-01
  5.00000E 00           1.03736E-16         1.04934E-08         1.07301E-03         7.16088E-01
  5.10000E 00           3.98295E-15         1.33317E-08         1.18549E-03         7.19157E-01
  5.20000E 00           1.09971E-14         1.68338E-08         1.30594E-03         7.22142E-01
  5.30000E 00           2.28667E-14         2.11307E-08         1.43463E-03         7.25045E-01
  5.40000E 00           4.20633E-14         2.63744E-08         1.57180E-03         7.27872E-01
  5.50000E 00           7.20805E-14         3.27403E-08         1.71770E-03         7.30624E-01
```

FIGURE 23.2

```
1.72000E 01          1.18988E-05          1.04007E-03          8.36253E-02          8.63472E-01
1.73000E 01          1.26994E-05          1.07888E-03          8.46850E-02          8.63981E-01
1.74000E 01          1.35451E-05          1.11872E-03          8.57471E-02          8.64487E-01
1.75000E 01          1.44380E-05          1.15962E-03          8.68113E-02          8.64988E-01
1.76000E 01          1.53803E-05          1.20159E-03          8.78776E-02          8.65484E-01
1.77000E 01          1.63739E-05          1.24465E-03          8.89461E-02          8.65977E-01
1.78000E 01          1.74213E-05          1.28881E-03          9.00165E-02          8.66466E-01
1.79000E 01          1.85246E-05          1.33408E-03          9.10888E-02          8.66950E-01
1.80000E 01          1.96862E-05          1.38048E-03          9.21630E-02          8.67431E-01
1.81000E 01          2.09085E-05          1.42803E-03          9.32390E-02          8.67907E-01
1.82000E 01          2.21941E-05          1.47673E-03          9.43168E-02          8.68380E-01
1.83000E 01          2.35454E-05          1.52661E-03          9.53962E-02          8.68848E-01
1.84000E 01          2.49651E-05          1.57767E-03          9.64772E-02          8.69313E-01
1.85000E 01          2.64559E-05          1.62993E-03          9.75597E-02          8.69775E-01
1.86000E 01          2.80205E-05          1.68342E-03          9.86438E-02          8.70232E-01
1.87000E 01          2.96619E-05          1.73813E-03          9.97293E-02          8.70686E-01
1.88000E 01          3.13829E-05          1.79408E-03          1.00816E-01          8.71137E-01
1.89000E 01          3.31865E-05          1.85129E-03          1.01904E-01          8.71584E-01
1.90000E 01          3.50758E-05          1.90978E-03          1.02994E-01          8.72027E-01
1.91000E 01          3.70538E-05          1.96954E-03          1.04084E-01          8.72467E-01
1.92000E 01          3.91240E-05          2.03061E-03          1.05176E-01          8.72903E-01
1.93000E 01          4.12894E-05          2.09299E-03          1.06269E-01          8.73336E-01
1.94000E 01          4.35535E-05          2.15669E-03          1.07363E-01          8.73766E-01
1.95000E 01          4.59198E-05          2.22173E-03          1.08458E-01          8.74193E-01
1.96000E 01          4.83917E-05          2.28812E-03          1.09554E-01          8.74616E-01
1.97000E 01          5.09728E-05          2.35588E-03          1.10650E-01          8.75036E-01
1.98000E 01          5.36668E-05          2.42501E-03          1.11748E-01          8.75453E-01
1.99000E 01          5.64776E-05          2.49553E-03          1.12846E-01          8.75867E-01
2.00000E 01          5.94088E-05          2.56745E-03          1.13945E-01          8.76278E-01
2.01000E 01          6.24644E-05          2.64078E-03          1.15045E-01          8.76686E-01
```

FIGURE 23.3

A.9.7 Sample Problem 7

Subject : Model of a countercurrent liquid-liquid extraction column.

Reference : Biery, J.C. and D.R. Boylan,
I and E.C. Fund., V.2, No.1, Feb. 1963, pages 44-50.

Description : Biery and Boylan's model 2 is the one being considered. It is a non-equilibrium stage, uniform mixing model. The assumptions made are outlined in the discussion section. The transient response to a step input in feed concentration is considered.

The change in composition of each phase for a given stage may be described by the two following differential equations

$$WR \frac{dx_i}{dt} = FR\ (x_{i-1} - x_i) - K_E a\ V\ (y_i^* - y_i)$$

$$WE \frac{dy_i}{dt} = S\ (y_{i+1} - y_i) + K_E a\ V\ (y_i^* - y_i)$$

where WR is the raffinate phase holdup per stage

WE is the extract phase holdup per stage

FR is the solute free raffinate flow rate

S is the solute free extract flow rate

$K_E a$ is the mass transfer coefficient

V is the stage volume

x is the concentration of the solute in the raffinate phase

y is the concentration of the solute in the extract phase

y^* is the concentration of the solute in the extract phase which would be in equilibrium with the raffinate phase at a given stage.

Program Listing : Figure 24.1, 24.2

Sample Output : Figure 24.3, 24.4

Discussion : A pair of equations of the form outlined was written for each stage and the whole set integrated to give concentration profiles as a function of time.

Another program was used to determine the intial steady state profiles. A step input in feed concentration is imposed on the steady state profiles and the transient profiles are calculated.

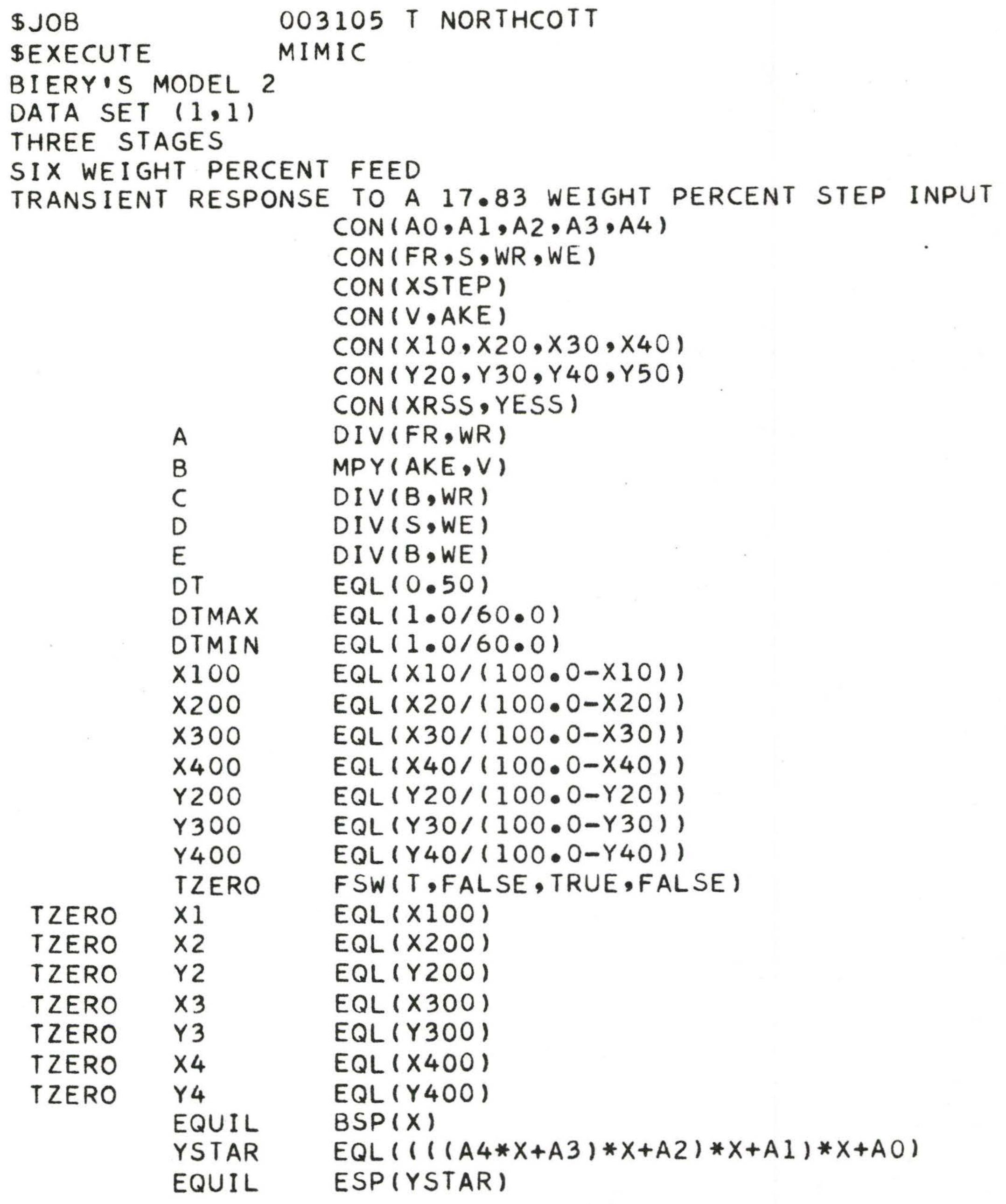
The equilibrium concentration y^* is calculated for each stage by a subprogram EQUIL which uses a regressed equation of the form

$$Y^* = a_o + a_1 x + a_2 x^2 + a_3 x^3$$

Assumptions made for this model include the following:

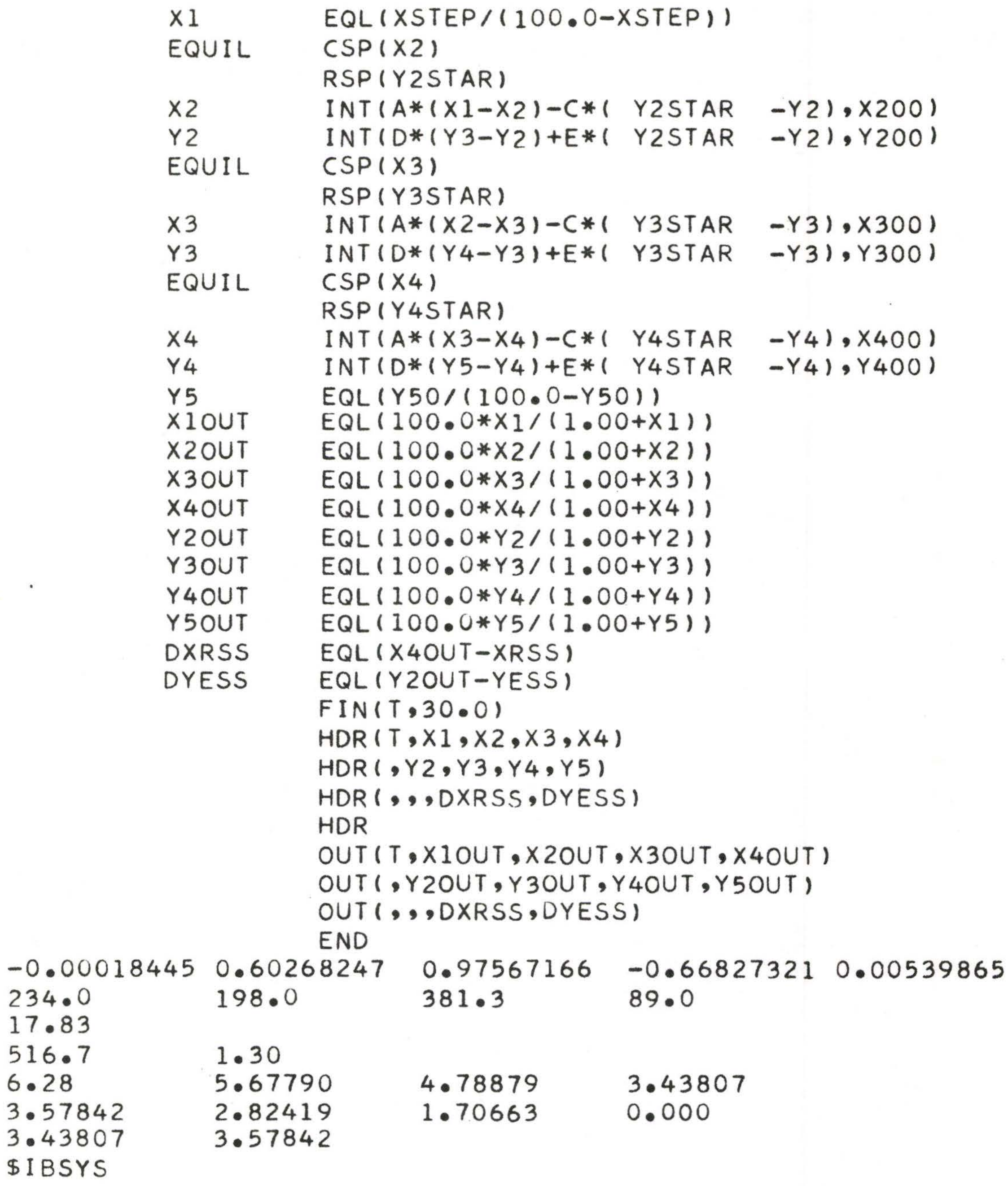
1. The column consists of an arbitrary number of stages.
2. Both streams in each stage are well mixed so that the composition of the outlet stream of each phase from each stage is the same as the composition of that phase in the stage.
3. Solute transfers from the heavy water phase to the lighter organic phase.
4. Each stage is a non-equilibrium stage
5. The flow rate of each phase on a solute-free basis is assumed constant.

6. The holdups of each phase in each stage are assumed constant.
7. The mass transfer coefficient is assumed constant.



```
$JOB         003105 T NORTHCOTT
$EXECUTE     MIMIC
BIERY'S MODEL 2
DATA SET (1,1)
THREE STAGES
SIX WEIGHT PERCENT FEED
TRANSIENT RESPONSE TO A 17.83 WEIGHT PERCENT STEP INPUT
                CON(A0,A1,A2,A3,A4)
                CON(FR,S,WR,WE)
                CON(XSTEP)
                CON(V,AKE)
                CON(X10,X20,X30,X40)
                CON(Y20,Y30,Y40,Y50)
                CON(XRSS,YESS)
        A       DIV(FR,WR)
        B       MPY(AKE,V)
        C       DIV(B,WR)
        D       DIV(S,WE)
        E       DIV(B,WE)
        DT      EQL(0.50)
        DTMAX   EQL(1.0/60.0)
        DTMIN   EQL(1.0/60.0)
        X100    EQL(X10/(100.0-X10))
        X200    EQL(X20/(100.0-X20))
        X300    EQL(X30/(100.0-X30))
        X400    EQL(X40/(100.0-X40))
        Y200    EQL(Y20/(100.0-Y20))
        Y300    EQL(Y30/(100.0-Y30))
        Y400    EQL(Y40/(100.0-Y40))
        TZERO   FSW(T,FALSE,TRUE,FALSE)
 TZERO  X1      EQL(X100)
 TZERO  X2      EQL(X200)
 TZERO  Y2      EQL(Y200)
 TZERO  X3      EQL(X300)
 TZERO  Y3      EQL(Y300)
 TZERO  X4      EQL(X400)
 TZERO  Y4      EQL(Y400)
        EQUIL   BSP(X)
        YSTAR   EQL((((A4*X+A3)*X+A2)*X+A1)*X+A0)
        EQUIL   ESP(YSTAR)
```

FIGURE 24.1



```
          X1        EQL(XSTEP/(100.0-XSTEP))
          EQUIL     CSP(X2)
                    RSP(Y2STAR)
          X2        INT(A*(X1-X2)-C*( Y2STAR  -Y2),X200)
          Y2        INT(D*(Y3-Y2)+E*( Y2STAR  -Y2),Y200)
          EQUIL     CSP(X3)
                    RSP(Y3STAR)
          X3        INT(A*(X2-X3)-C*( Y3STAR  -Y3),X300)
          Y3        INT(D*(Y4-Y3)+E*( Y3STAR  -Y3),Y300)
          EQUIL     CSP(X4)
                    RSP(Y4STAR)
          X4        INT(A*(X3-X4)-C*( Y4STAR  -Y4),X400)
          Y4        INT(D*(Y5-Y4)+E*( Y4STAR  -Y4),Y400)
          Y5        EQL(Y50/(100.0-Y50))
          X1OUT     EQL(100.0*X1/(1.00+X1))
          X2OUT     EQL(100.0*X2/(1.00+X2))
          X3OUT     EQL(100.0*X3/(1.00+X3))
          X4OUT     EQL(100.0*X4/(1.00+X4))
          Y2OUT     EQL(100.0*Y2/(1.00+Y2))
          Y3OUT     EQL(100.0*Y3/(1.00+Y3))
          Y4OUT     EQL(100.0*Y4/(1.00+Y4))
          Y5OUT     EQL(100.0*Y5/(1.00+Y5))
          DXRSS     EQL(X4OUT-XRSS)
          DYESS     EQL(Y2OUT-YESS)
                    FIN(T,30.0)
                    HDR(T,X1,X2,X3,X4)
                    HDR(,Y2,Y3,Y4,Y5)
                    HDR(,,,DXRSS,DYESS)
                    HDR
                    OUT(T,X1OUT,X2OUT,X3OUT,X4OUT)
                    OUT(,Y2OUT,Y3OUT,Y4OUT,Y5OUT)
                    OUT(,,,DXRSS,DYESS)
                    END
-0.00018445 0.60268247  0.97567166  -0.66827321 0.00539865
234.0       198.0       381.3       89.0
17.83
516.7       1.30
6.28        5.67790     4.78879     3.43807
3.57842     2.82419     1.70663     0.000
3.43807     3.57842
$IBSYS
```

FIGURE 24.2

```
  T                     X1              X2              X3              X4
                        Y2              Y3              Y4              Y5
                                                        DXRSS           DYESS
-0.                  1.78300E 01     5.67790E 00     4.78879E 00     3.43807E 00
                     3.57842E 00     2.82419E 00     1.70663E 00     0.
                                                     0.              0.
 5.00000E-01         1.78300E 01     8.66186E 00     5.21099E 00     3.47941E 00
                     5.09351E 00     2.99345E 00     1.72024E 00     0.
                                                     4.13389E-02     1.51509E 00
 1.00000E 00         1.78300E 01     1.05120E 01     6.04970E 00     3.67201E 00
                     6.49415E 00     3.45709E 00     1.80581E 00     0.
                                                     2.33943E-01     2.91573E 00
 1.50000E 00         1.78300E 01     1.17478E 01     6.97903E 00     4.01817E 00
                     7.52754E 00     4.03685E 00     1.97807E 00     0.
                                                     5.80099E-01     3.94912E 00
 2.00000E 00         1.78300E 01     1.26101E 01     7.86122E 00     4.46862E 00
                     8.30523E 00     4.63291E 00     2.21637E 00     0.
                                                     1.03055E 00     4.72681E 00
 2.50000E 00         1.78300E 01     1.32358E 01     8.64660E 00     4.96942E 00
                     8.90440E 00     5.19705E 00     2.49298E 00     0.
                                                     1.53135E 00     5.32598E 00
 3.00000E 00         1.78300E 01     1.37057E 01     9.32532E 00     5.47808E 00
                     9.37635E 00     5.70886E 00     2.78371E 00     0.
                                                     2.04001E 00     5.79793E 00
 3.50000E 00         1.78300E 01     1.40689E 01     9.90385E 00     5.96639E 00
                     9.75526E 00     6.16245E 00     3.07085E 00     0.
                                                     2.52832E 00     6.17684E 00
 4.00000E 00         1.78300E 01     1.43566E 01     1.03941E 01     6.41816E 00
                     1.00643E 01     6.55903E 00     3.34292E 00     0.
                                                     2.98009E 00     6.48587E 00
 4.50000E 00         1.78300E 01     1.45888E 01     1.08089E 01     6.82581E 00
                     1.03195E 01     6.90300E 00     3.59343E 00     0.
                                                     3.38774E 00     6.74108E 00
 5.00000E 00         1.78300E 01     1.47792E 01     1.11600E 01     7.18744E 00
                     1.05323E 01     7.19993E 00     3.81946E 00     0.
                                                     3.74937E 00     6.95390E 00
 5.50000E 00         1.78300E 01     1.49371E 01     1.14574E 01     7.50447E 00
                     1.07111E 01     7.45551E 00     4.02045E 00     0.
                                                     4.06640E 00     7.13269E 00
 6.00000E 00         1.78300E 01     1.50691E 01     1.17098E 01     7.78014E 00
                     1.08621E 01     7.67512E 00     4.19733E 00     0.
                                                     4.34207E 00     7.28372E 00
 6.50000E 00         1.78300E 01     1.51803E 01     1.19243E 01     8.01848E 00
                     1.09902E 01     7.86362E 00     4.35181E 00     0.
                                                     4.58041E 00     7.41183E 00
 7.00000E 00         1.78300E 01     1.52744E 01     1.21069E 01     8.22377E 00
                     1.10992E 01     8.02530E 00     4.48598E 00     0.
                                                     4.78570E 00     7.52082E 00
 7.50000E 00         1.78300E 01     1.53543E 01     1.22624E 01     8.40012E 00
                     1.11922E 01     8.16394E 00     4.60206E 00     0.
                                                     4.96205E 00     7.61377E 00
 8.00000E 00         1.78300E 01     1.54224E 01     1.23951E 01     8.55136E 00
                     1.12716E 01     8.28279E 00     4.70220E 00     0.
                                                     5.11329E 00     7.69315E 00
 8.50000E 00         1.78300E 01     1.54804E 01     1.25084E 01     8.68091E 00
                     1.13395E 01     8.38466E 00     4.78841E 00     0.
                                                     5.24284E 00     7.76103E 00
```

FIGURE 24.3

```
2.10000E 01         1.78300E 01       1.58187E 01       1.31661E 01       9.43479E 00
                    1.17372E 01       8.98271E 00       5.29768E 00       0.
                                                        5.99672E 00       8.15874E 00
2.15000E 01         1.78300E 01       1.58197E 01       1.31681E 01       9.43710E 00
                    1.17384E 01       8.98456E 00       5.29926E 00       0.
                                                        5.99903E 00       8.15997E 00
2.20000E 01         1.78300E 01       1.58206E 01       1.31699E 01       9.43907E 00
                    1.17395E 01       8.98615E 00       5.30061E 00       0.
                                                        6.00100E 00       8.16103E 00
2.25000E 01         1.78300E 01       1.58214E 01       1.31714E 01       9.44077E 00
                    1.17404E 01       8.98751E 00       5.30177E 00       0.
                                                        6.00270E 00       8.16194E 00
2.30000E 01         1.78300E 01       1.58220E 01       1.31726E 01       9.44222E 00
                    1.17411E 01       8.98868E 00       5.30276E 00       0.
                                                        6.00415E 00       8.16272E 00
2.35000E 01         1.78300E 01       1.58226E 01       1.31737E 01       9.44346E 00
                    1.17418E 01       8.98968E 00       5.30361E 00       0.
                                                        6.00539E 00       8.16338E 00
2.40000E 01         1.78300E 01       1.58231E 01       1.31747E 01       9.44453E 00
                    1.17424E 01       8.99054E 00       5.30434E 00       0.
                                                        6.00646E 00       8.16396E 00
2.45000E 01         1.78300E 01       1.58235E 01       1.31755E 01       9.44545E 00
                    1.17429E 01       8.99128E 00       5.30497E 00       0.
                                                        6.00738E 00       8.16445E 00
2.50000E 01         1.78300E 01       1.58239E 01       1.31762E 01       9.44623E 00
                    1.17433E 01       8.99191E 00       5.30550E 00       0.
                                                        6.00816E 00       8.16487E 00
2.55000E 01         1.78300E 01       1.58242E 01       1.31767E 01       9.44690E 00
                    1.17436E 01       8.99245E 00       5.30596E 00       0.
                                                        6.00883E 00       8.16523E 00
2.60000E 01         1.78300E 01       1.58244E 01       1.31772E 01       9.44748E 00
                    1.17440E 01       8.99291E 00       5.30636E 00       0.
                                                        6.00941E 00       8.16554E 00
2.65000E 01         1.78300E 01       1.58247E 01       1.31777E 01       9.44797E 00
                    1.17442E 01       8.99331E 00       5.30670E 00       0.
                                                        6.00990E 00       8.16580E 00
2.70000E 01         1.78300E 01       1.58248E 01       1.31781E 01       9.44840E 00
                    1.17444E 01       8.99365E 00       5.30699E 00       0.
                                                        6.01033E 00       8.16603E 00
2.75000E 01         1.78300E 01       1.58250E 01       1.31784E 01       9.44876E 00
                    1.17446E 01       8.99394E 00       5.30723E 00       0.
                                                        6.01069E 00       8.16622E 00
2.80000E 01         1.78300E 01       1.58252E 01       1.31786E 01       9.44907E 00
                    1.17448E 01       8.99419E 00       5.30745E 00       0.
                                                        6.01100E 00       8.16639E 00
2.85000E 01         1.78300E 01       1.58253E 01       1.31789E 01       9.44934E 00
                    1.17450E 01       8.99440E 00       5.30763E 00       0.
                                                        6.01127E 00       8.16653E 00
2.90000E 01         1.78300E 01       1.58254E 01       1.31791E 01       9.44957E 00
                    1.17451E 01       8.99459E 00       5.30779E 00       0.
                                                        6.01150E 00       8.16665E 00
2.95000E 01         1.78300E 01       1.58255E 01       1.31793E 01       9.44976E 00
                    1.17452E 01       8.99475E 00       5.30792E 00       0.
                                                        6.01169E 00       8.16676E 00
3.00000E 01         1.78300E 01       1.58255E 01       1.31794E 01       9.44993E 00
                    1.17453E 01       8.99488E 00       5.30804E 00       0.
                                                        6.01186E 00       8.16685E 00
```

FIGURE 24.4

A.9.8 Sample Problem 8

Subject : Solution of a set of simulatneous algebraic equations using a Jacobi type calculation.

Reference: Applied Numerical Methods, Prelim. Ed., Carnahan, Luther, Wilkes, Wiley and Sons, New York (1964), page 342.

Description : To solve

$$4 \cdot x_1 + 2 \cdot x_2 + x_3 = 11$$

$$- x_1 + 2x_2 = 3$$

$$2 \cdot x_1 + x_2 + 4 \cdot x_3 = 16$$

Program Listing : Figure 25

Sample Output : Figure 25

Discussion : It should be noted that the matrix of the coefficients of the unknowns has large elements on the diagonal. This condition must hold if the solution is to converge. The set of equations is then rewritten as

$$x_1 = \frac{11}{4} - \tfrac{1}{2} \cdot x_2 - \tfrac{1}{4} \cdot x_3$$

$$x_2 = \frac{3}{2} + \tfrac{1}{2} \cdot x_1$$

$$x_3 = 4 - \tfrac{1}{2} \cdot x_1 - \tfrac{1}{4} \cdot x_2$$

The unknowns on the right hand side of each equation may be thought of as being knowns if values for these quantities are known at any given time. Initiate guesses for x_1, x_2 and x_3 are read in using PAR (x10, x20, x30). The zero-order hold function is used to update the values of x_1, x_2 and x_3 every DTMAX units of time.

```
$JOB               003105 T NORTHCOTT
$EXECUTE           MIMIC
SOLUTION OF SIMULTANEOUS ALGEBRAIC EQUATIONS.
THE LARGE ELEMENTS ARE ON THE DIAGONAL OF THE COEFFICIENT MATRIX.
                          PAR(X10,X20,X30)
            DT            EQL(0.10)
            DTMAX         EQL(DT)
            DTMIN         EQL(DT)
            S             FSW((T-DTMAX),FALSE,TRUE,TRUE)
            X10           ZOH(X1,DTMAX)
            X20           ZOH(X2,DTMAX)
            X30           ZOH(X3,DTMAX)
  S         X1            EQL(2.75-0.50*X20-0.25*X30)
  S         X2            EQL(1.50+0.50*X10)
  S         X3            EQL(4.0-0.50*X10-0.25*X20)
                          HDR(T,X1,X2,X3)
                          OUT(T,X1,X2,X3)
                          HDR
                          FIN(T,1.0)
                          END
0.0             0.0             0.0
10.0            10.0            10.0
$IBSYS
```

```
    X10                         X20                         X30
 0.                          0.                          0.

    T                           X1                          X2                          X3
-0.                          0.                          0.                          0.
 1.00000E-01                 1.00000E 00                 2.87500E 00                 2.25000E 00
 2.00000E-01                 7.50000E-01                 2.00000E 00                 2.78125E 00
 3.00000E-01                 1.05469E 00                 1.87500E 00                 3.12500E 00
 4.00000E-01                 1.03125E 00                 2.02734E 00                 3.00391E 00
 5.00000E-01                 9.85352E-01                 2.01563E 00                 2.97754E 00
 6.00000E-01                 9.97803E-01                 1.99268E 00                 3.00342E 00
 7.00000E-01                 1.00281E 00                 1.99890E 00                 3.00293E 00
 8.00000E-01                 9.99817E-01                 2.00140E 00                 2.99974E 00
 9.00000E-01                 9.99580E-01                 1.99991E 00                 2.99974E 00
 1.00000E 00                 1.00011E 00                 1.99979E 00                 3.00023E 00


    X10                         X20                         X30
 1.00000E 01                 1.00000E 01                 1.00000E 01

    T                           X1                          X2                          X3
-0.                          1.00011E 00                 1.99979E 00                 3.00023E 00
 1.00000E-01                 9.99973E-01                 2.00002E 00                 2.99996E 00
 2.00000E-01                 9.99998E-01                 1.99999E 00                 3.00001E 00
 3.00000E-01                 1.00000E 00                 2.00000E 00                 3.00000E 00
 4.00000E-01                 9.99999E-01                 2.00000E 00                 3.00000E 00
 5.00000E-01                 9.99999E-01                 2.00000E 00                 3.00000E 00
 6.00000E-01                 1.00000E 00                 2.00000E 00                 3.00000E 00
 7.00000E-01                 1.00000E 00                 2.00000E 00                 3.00000E 00
 8.00000E-01                 1.00000E 00                 2.00000E 00                 3.00000E 00
 9.00000E-01                 1.00000E 00                 2.00000E 00                 3.00000E 00
 1.00000E 00                 1.00000E 00                 2.00000E 00                 3.00000E 00
```

FIGURE 25

A.9.9 Sample Problem 9

Subject : Solution of sets of non-linear algebraic equations.

Reference: Applied Numerical Methods, Prelim. Ed.,
Carnahan, Luther, Wilkes, Wiley and Sons, New York (1964),
page 412.

Description : To solve

$$5x_1 = x_2^2 - x_3^2 = 3$$

$$-x_1^2 + 6x_2 - x_3^2 = 4$$

$$-x_1^2 - x_2^2 + 7x_3 = 5$$

Program Listing : Figure 26.1

Sample Output : Figure 26.2

Discussion : The set of equations is written as

$$x_1 = \frac{3}{5} + \frac{1}{5} \cdot x_2^2 + \frac{1}{5} \cdot x_3^2$$

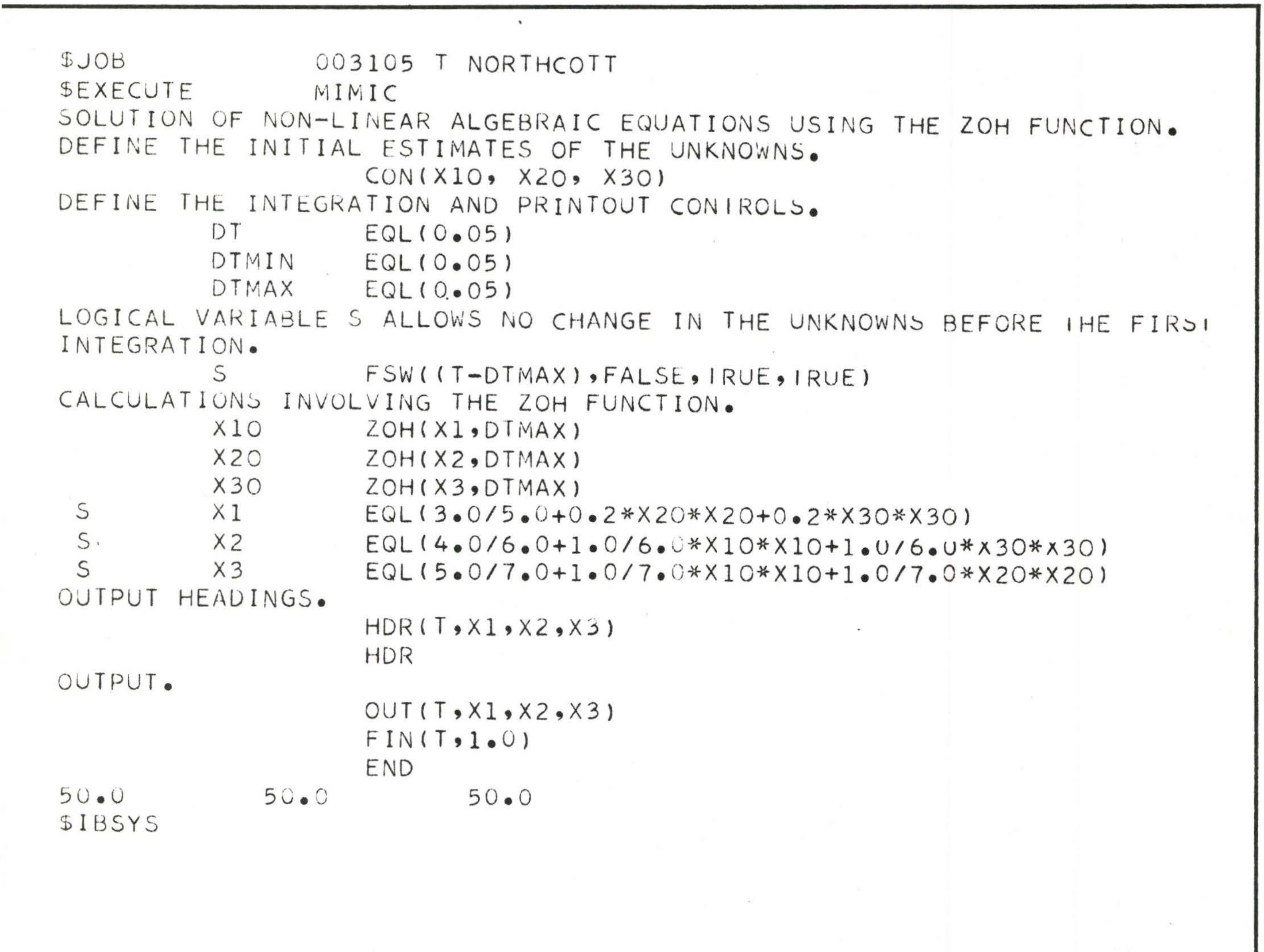
$$x_2 = \frac{4}{6} + \frac{1}{6} \cdot x_1^2 + \frac{1}{6} \cdot x_3^2$$

$$x_3 = \frac{5}{7} + \frac{1}{7} \cdot x_1^2 + \frac{1}{7} \cdot x_2^2$$

The ZOH function was used in the same manner as for sample problem 8.

Further study is needed to establish the criterion for solution of this type of problem.

For the sample output shown, it is noted that the solution has essentially converged to the correct solution (1,1,1).



```
$JOB            003105 T NORTHCOTT
$EXECUTE        MIMIC
SOLUTION OF NON-LINEAR ALGEBRAIC EQUATIONS USING THE ZOH FUNCTION.
DEFINE THE INITIAL ESTIMATES OF THE UNKNOWNS.
                    CON(X10, X20, X30)
DEFINE THE INTEGRATION AND PRINTOUT CONTROLS.
          DT        EQL(0.05)
          DTMIN     EQL(0.05)
          DTMAX     EQL(0.05)
LOGICAL VARIABLE S ALLOWS NO CHANGE IN THE UNKNOWNS BEFORE THE FIRST
INTEGRATION.
          S         FSW((T-DTMAX),FALSE,TRUE,TRUE)
CALCULATIONS INVOLVING THE ZOH FUNCTION.
          X10       ZOH(X1,DTMAX)
          X20       ZOH(X2,DTMAX)
          X30       ZOH(X3,DTMAX)
 S        X1        EQL(3.0/5.0+0.2*X20*X20+0.2*X30*X30)
 S        X2        EQL(4.0/6.0+1.0/6.0*X10*X10+1.0/6.0*X30*X30)
 S        X3        EQL(5.0/7.0+1.0/7.0*X10*X10+1.0/7.0*X20*X20)
OUTPUT HEADINGS.
                    HDR(T,X1,X2,X3)
                    HDR
OUTPUT.
                    OUT(T,X1,X2,X3)
                    FIN(T,1.0)
                    END
50.0         50.0          50.0
$IBSYS
```

FIGURE 26.1

```
     T                       X1                        X2                        X3

 -0.                     0.                        0.                        0.
  5.00000E-02            7.90930E-01               8.11701E-01               8.29206E-01
  1.00000E-01            8.69288E-01               8.85525E-01               8.97775E-01
  1.50000E-01            9.18031E-01               9.26944E-01               9.34260E-01
  2.00000E-01            9.46413E-01               9.52604E-01               9.57429E-01
  2.50000E-01            9.64825E-01               9.68728E-01               9.71879E-01
  3.00000E-01            9.76596E-01               9.79239E-01               9.81332E-01
  3.50000E-01            9.84384E-01               9.86125E-01               9.87521E-01
  4.00000E-01            9.89528E-01               9.90702E-01               9.91636E-01
  4.50000E-01            9.92967E-01               9.93752E-01               9.94379E-01
  5.00000E-01            9.95267E-01               9.95796E-01               9.96218E-01
  5.50000E-01            9.96812E-01               9.97168E-01               9.97452E-01
  6.00000E-01            9.97851E-01               9.98091E-01               9.98282E-01
  6.50000E-01            9.98551E-01               9.98712E-01               9.98842E-01
  7.00000E-01            9.99022E-01               9.99131E-01               9.99218E-01
  7.50000E-01            9.99340E-01               9.99414E-01               9.99473E-01
  8.00000E-01            9.99555E-01               9.99604E-01               9.99644E-01
  8.50000E-01            9.99699E-01               9.99733E-01               9.99760E-01
  9.00000E-01            9.99797E-01               9.99820E-01               9.99838E-01
  9.50000E-01            9.99863E-01               9.99878E-01               9.99891E-01
  1.00000E 00            9.99908E-01               9.99918E-01               9.99926E-01
  1.05000E 00            9.99938E-01               9.99945E-01               9.99950E-01
```

FIGURE 26.2

These updated values in turn become new values of x10, x20 and x30, and ideally the calculated values of x1, x2, and x3 will converge to the correct solution.

The output for two sets of initial conditions is shown. It is seen that both sets have essentially converged after one second of machine time although it is obvious that the second set of initial conditions caused much earlier convergence.

It should be noted that it is not known whether this method will be applicable to other sets of equations. Some study is needed to establish the criterions which govern the solution of similar sets of equations using MIMIC. This example and the next one are included to suggest that MIMIC may have applications in areas other than differential equations.

A.9.10 Sample Problem 10

Subject : Example of integrator mode control.

Description and Discussion : In a major study report (A.11.16) the transient operation of a countercurrent liquid extraction column is considered. The model used to describe the column is basically the same as the one outlined in A.9.7. However, one important difference exists; namely, the mass transfer coefficient is a function of concentration.

In its simplest form, the mass transfer coefficient can be eexpressed as

$$\boxed{K_E a' \;=\; \text{CON1}(f(c))^n}$$

where $K_E a'$ is the overal mass transfer coefficient

CON1 is a "variable constant" which depends upon flowrates and cell parameters

f(c) is some function of concentration

n is some exponent

Now, for a given feed concentration and a given exponent, and with the system at steady state, an iterative operation can be carried out to find a value of CON1 such that the steady state raffinate concentration predicted by the model agrees with the experimental value.

At the end of each iterative run, an error function

$$\boxed{\text{ERROR1} \;=\; \text{XRSS} - \text{X4OUT}}$$

is calculated where

XRSS is the experimental steady state raffinate concentration
X4OUT is the raffinate concentration predicted by the model

The value of CON1 is corrected by

```
CON1 = KK2 - KPRIME * ERROR1
```

where KK2 is the previous value of CON1.
KPRIME is a constant judiciously chosen such that convergence to the correct solution occurs in the minimum number of iterations without the solution oscillating about the correct solution.

In general, the following operations occur during the program. Starting at zero time, the integrators are placed in the OPERATE mode, and they are allowed to integrate up to 20 minutes. Then, the integrators are placed in the HOLD mode, the error function is evaluated and a new value of CON1 is calculated. The integrators are then placed in the RESET mode and the integrators are reset in preparation for another run. The integrators are then placed in the OPERATE mode, and the process repeated until the execution of the FIN statement halts further calculation. It should be noted that both the HOLD mode and the RESET mode are held arbitrarily for one minute each.

In Section A.8.1., it was pointed out that an integration expression takes the form

```
R          INT (A,B,C,D)
```

where A is the expression to be integrated

B is the value of R at zero time

and C and D are logical variables whose values control the mode of the integrator.

It should be noted that C and D are not reserved variables but merely indicate a position in the argument list for INT. Any other logical variables could be used.

In this example program, mode control is achieved by control of the logical variables C and D, which in turn are controlled by other logical variables whose values depend on the values of time, TTIME.

The following table summarizes the logical variables used in the program and their values at various times. TT_{20} represents the end of integration for an iteration

Variable	TT = 0	$0<TT<TT_{20}$	TT_{20}	$TT_{20}+1$	$TT_{20}+2$
B	FALSE	TRUE	FALSE	FALSE	FALSE
B1	TRUE	TRUE	FALSE	FALSE	TRUE
TQ	TRUE	FALSE	FALSE	FALSE	FALSE
NTQ	FALSE	TRUE	TRUE	TRUE	TRUE
S	TRUE	TRUE	FALSE	FALSE	FALSE
H	TRUE	TRUE	TRUE	FALSE	FALSE
O	TRUE	TRUE	TRUE	TRUE	TRUE
C	TRUE	TRUE	FALSE	TRUE	TRUE
CP	FALSE	FALSE	TRUE	FALSE	FALSE
D	TRUE	TRUE	TRUE	FALSE	FALSE

In the next instant after $TT_{20} + 2$, S, H, and O will all become TRUE.

In the program, MIMIC functions such as FSW, COM, IOR, MMV, and AND in combination with logical variables to obtain the desired variable values.

For example, consider the statement

```
NTQ    S    IOR(AND(H, O, B1), AND (B1, COM(O)))
```

From the table given above, it can be seen that this logical combination will produce the correct values for S.

It is interesting to note that if the independent variable is being printed out during an iterative operation, T is not reset to T = 0. for the succeeding iteration, but continues to increase. If values of the independent variable are desired during each iteration, these can be obtained by defining a dummy independent variable such as in the following manner.

```
TTIME          INT (1.0, 0.0, C, D)
```

The dummy independent variable TTIME will reset to the **initial** condition of 0.0 and thus give values equivalent to the independent variable during each iteration. For iterations, the dummy independent variable should also be used in expressions containing the independent variable.

Program Listing : Figures 27.1, 27.2, 27.3

Sample Output : Figures 27.4, 27.5

Comments : Two sections of output are given, one near the beginning out the run (Figure 27.4), and one about the time when one integration is finished and mode changes occur. At T = 20, the integrators transfer to the HOLD mode, and a new value of CON1 (85.8432) appears in the next printout.

Two interesting inaccuracies of the system are noted. **First,** there is a time loss by the dummy independent variable TTIME during the mode change such that at T = 23.0, TTIME = 0.930556, or about 0.07 less than its theoretical value of 1.0. Secondly, the initial conditions are not printed out when the RESET operation occurs i.e., at T = 22.0. This may be explained by the fact that the printout occurs exactly at 22.0 while the RESET operation may occur an instant later. This would also explain the time loss by TTIME.

```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
THREE STAGES
KEA IS BASED ON KARR AND SCHEIBEL'S CORRELATION
ITERATION ON THE CONSTANT TERM FOR A FIXED EXPONENT
                  CON(A0,A1,A2,A3,A4)
                  CON(T0,T1,T2,T3)
                  CON(R0,R1,R2)
                  CON(P0,P1,P2,P3)
                  CON(X10,X20,X30,X40)
                  CON(Y20,Y30,Y40,Y50)
                  CON(XRSS,YESS)
                  CON(FR2,FR3,FR4,S2,S3,S4)
                  CON(WR2,WR3,WR4,WE2,WE3,WE4)
                  CON(V)
                  CON(EPT)
                  CON(KPRIME,CON10)
         DT       EQL(1.0)
         DTMAX    EQL(5.0/60.0)
         DTMIN    EQL(5.0/60.0)
         B1       FSW((TTIME-20.0),TRUE,TRUE,FALSE)
         TQ       FSW(T,FALSE,TRUE,FALSE)
         NTQ      COM(TQ)
 TQ      S        EQL(TRUE)
 NTQ     S        IOR(AND(H,O,B1),AND(B1,COM(O)))
         H        MMV(S,1.0)
         O        MMV(S,2.0)
         C        IOR(AND(S,O,H),AND(COM(S),COM(H)))
         D        AND(H,O)
         CP       COM(C)
         X100     EQL(X10/(100.0-X10))
         X200     EQL(X20/(100.0-X20))
         X300     EQL(X30/(100.0-X30))
         X400     EQL(X40/(100.0-X40))
         Y200     EQL(Y20/(100.0-Y20))
         Y300     EQL(Y30/(100.0-Y30))
         Y400     EQL(Y40/(100.0-Y40))
         TZERO    FSW(TTIME,FALSE,TRUE,FALSE)
 TZERO   X2       EQL(X200)
 TZERO   Y2       EQL(Y200)
 TZERO   X3       EQL(X300)
 TZERO   Y3       EQL(Y300)
 TZERO   X4       EQL(X400)
 TZERO   Y4       EQL(Y400)
         EQUIL    BSP(X)
         YSTAR    EQL((((A4*X+A3)*X+A2)*X+A1)*X+A0)
         EQUIL    ESP(YSTAR)
         KEA      BSP(ARG1,ARG2,FACTOR)
         AKE      EQL(CON1*EXP(EPT,(ARG1/ARG2) *FACTOR))
         KEA      ESP(AKE)
```

FIGURE 27.1

```
         X1          EQL(X100)
         EQUIL       CSP(X2)
                     RSP(Y2STAR)
         DELRO2      EQL(R0+R1*Y2+R2*Y2*Y2)
         SIGMA2      EQL(T0+T1*Y2+T2*Y2*Y2+T3*Y2*Y2*Y2)
         FACT2       EQL(P0+P1*Y2+P2*Y2*Y2+P3*Y2*Y2*Y2)
         CTERM2      EQL(DELRO2/SIGMA2*FACT2)
         KEA         CSP(DELRO2,SIGMA2,FACT2)
                     RSP(AKE2)
         X2          INT(FR2/WR2*(X1-X2)-(AKE2*V/WR2)*(Y2STAR-Y2),X200,C,D)
         Y2          INT(S2/WE2*(Y3-Y2)+(AKE2*V/WE2)*(Y2STAR-Y2),Y200,C,D)
         EQUIL       CSP(X3)
                     RSP(Y3STAR)
         DELRO3      EQL(R0+R1*Y3+R2*Y3*Y3)
         SIGMA3      EQL(T0+T1*Y3+T2*Y3*Y3+T3*Y3*Y3*Y3)
         FACT3       EQL(P0+P1*Y3+P2*Y3*Y3+P3*Y3*Y3*Y3)
         CTERM3      EQL(DELRO3/SIGMA3*FACT3)
         KEA         CSP(DELRO3,SIGMA3,FACT3)
                     RSP(AKE3)
         X3          INT(FR3/WR3*(X2-X3)-(AKE3*V/WR3)*(Y3STAR-Y3),X300,C,D)
         Y3          INT(S3/WE3*(Y4-Y3)+(AKE3*V/WE3)*(Y3STAR-Y3),Y300,C,D)
         EQUIL       CSP(X4)
                     RSP(Y4STAR)
         DELRO4      EQL(R0+R1*Y4+R2*Y4*Y4)
         SIGMA4      EQL(T0+T1*Y4+T2*Y4*Y4+T3*Y4*Y4*Y4)
         FACT4       EQL(P0+P1*Y4+P2*Y4*Y4+P3*Y4*Y4*Y4)
         CTERM4      EQL(DELRO4/SIGMA4*FACT4)
         KEA         CSP(DELRO4,SIGMA4,FACT4)
                     RSP(AKE4)
         X4          INT(FR4/WR4*(X3-X4)-(AKE4*V/WR4)*(Y4STAR-Y4),X400,C,D)
         Y4          INT(S4/WE4*(Y5-Y4)+(AKE4*V/WE4)*(Y4STAR-Y4),Y400,C,D)
         Y5          EQL(Y50/(100.0-Y50))
         X1OUT       EQL(100.0*X1/(1.00+X1))
         X2OUT       EQL(100.0*X2/(1.00+X2))
         X3OUT       EQL(100.0*X3/(1.00+X3))
         X4OUT       EQL(100.0*X4/(1.00+X4))
         Y2OUT       EQL(100.0*Y2/(1.00+Y2))
         Y3OUT       EQL(100.0*Y3/(1.00+Y3))
         Y4OUT       EQL(100.0*Y4/(1.00+Y4))
         Y5OUT       EQL(100.0*Y5/(1.00+Y5))
         ERROR1      EQL(XRSS-X4OUT)
         ERROR2      EQL(YESS-Y2OUT)
         TTIME       INT(1.0,0.0,C,D)
         KK2         TAS(CON1,C,CON10)
CP       CON1        EQL(KK2-COR)
TQ       CON1        EQL(CON10)
         COR         MPY(KPRIME,ERROR1)
                     HDR(T,X1,X2,X3,X4)
                     HDR(TTIME,Y2,Y3,Y4,Y5)
                     HDR(AKE2,AKE3,AKE4,CON)
                     HDR(CTERM2,CTERM3,CTERM4)
                     HDR
```

FIGURE 27.2

```
                  OUT(T,X1OUT,X2OUT,X3OUT,X4OUT)
                  OUT(TTIME,Y2OUT,Y3OUT,Y4OUT,Y5OUT)
                  OUT(AKE2,AKE3,AKE4,CON1)
                  OUT(CTERM2,CTERM3,CTERM4)
                  OUT
                  FIN(T,107.)
                  END
-0.00018445 0.60268247  0.97567166  -0.66827321 0.00539865
10.37768137 -93.5286274 486.3131218 -1040.990753
0.1934      -0.08037897 -0.395827
0.69966979  -5.78837866 48.17870451 -148.2403011
6.12        4.90        4.20        3.55
3.35        1.95        0.90        0.00
3.55        3.35
375.        375.        375.        329.        329.        329.
385.7       385.7       385.7       84.         84.         84.
508.3
1.04778
100.        85.
$IBSYS
```

FIGURE 27.3

```
  EPT
1.04778E 00


  KPRIME                 CØN10
1.00000E 02            8.50000E 01


  T                      X1                     X2                     X3                     X4
  TTIME                  Y2                     Y3                     Y4                     Y5
  AKE2                   AKE3                   AKE4                   CØN
  CTERM2                 CTERM3                 CTERM4

-0.                    6.12000E 00            4.90000E 00            4.20000E 00            3.55000E 00
 0.                    3.35000E 00            1.95000E 00            9.00000E-01            0.
 9.44375E-01           9.17342E-01            9.05663E-01            8.50000E 01
 1.36409E-02           1.32680E-02            1.31067E-02

 1.00000E 00           6.12000E 00            5.28173E 00            4.33181E 00            3.32441E 00
 1.00000E 00           2.95397E 00            2.17295E 00            1.25135E 00            0.
 9.35313E-01           9.20732E-01            9.08813E-01            8.50000E 01
 1.35159E-02           1.33148E-02            1.31502E-02

 2.00000E 00           6.12000E 00            5.38833E 00            4.46963E 00            3.36224E 00
 2.00000E 00           3.03295E 00            2.23713E 00            1.26236E 00            0.
 9.37028E-01           9.21770E-01            9.08924E-01            8.50000E 01
 1.35396E-02           1.33291E-02            1.31517E-02

 3.00000E 00           6.12000E 00            5.43286E 00            4.54866E 00            3.42722E 00
 3.00000E 00           3.07428E 00            2.28395E 00            1.28909E 00            0.
 9.37944E-01           9.22545E-01            9.09195E-01            8.50000E 01
 1.35522E-02           1.33398E-02            1.31555E-02

 4.00000E 00           6.12000E 00            5.45502E 00            4.59318E 00            3.47654E 00
 4.00000E 00           3.09733E 00            2.31322E 00            1.31022E 00            0.
 9.38461E-01           9.23037E-01            9.09413E-01            8.50000E 01
 1.35593E-02           1.33466E-02            1.31585E-02

 5.00000E 00           6.12000E 00            5.46711E 00            4.61857E 00            3.50813E 00
 5.00000E 00           3.11053E 00            2.33069E 00            1.32394E 00            0.
 9.38758E-01           9.23334E-01            9.09556E-01            8.50000E 01
 1.35634E-02           1.33507E-02            1.31605E-02

 6.00000E 00           6.12000E 00            5.47397E 00            4.63321E 00            3.52720E 00
 6.00000E 00           3.11817E 00            2.34096E 00            1.33227E 00            0.
 9.38931E-01           9.23509E-01            9.09644E-01            8.50000E 01
 1.35658E-02           1.33531E-02            1.31617E-02

 7.00000E 00           6.12000E 00            5.47793E 00            4.64169E 00            3.53847E 00
 7.00000E 00           3.12262E 00            2.34696E 00            1.33720E 00            0.
 9.39031E-01           9.23612E-01            9.09696E-01            8.50000E 01
 1.35672E-02           1.33545E-02            1.31624E-02

 8.00000E 00           6.12000E 00            5.48023E 00            4.64663E 00            3.54507E 00
 8.00000E 00           3.12520E 00            2.35046E 00            1.34010E 00            0.
 9.39090E-01           9.23672E-01            9.09726E-01            8.50000E 01
 1.35680E-02           1.33553E-02            1.31628E-02
```

FIGURE 27.4

```
1.60000E 01        6.12000E 00        5.48340E 00        4.65341E 00        3.55418E 00
1.60000E 01        3.12876E 00        2.35528E 00        1.34409E 00        0.
9.39171E-01        9.23755E-01        9.09768E-01        8.50000E 01
1.35691E-02        1.33565E-02        1.31634E-02

1.70000E 01        6.12000E 00        5.48341E 00        4.65345E 00        3.55423E 00
1.70000E 01        3.12878E 00        2.35531E 00        1.34411E 00        0.
9.39171E-01        9.23755E-01        9.09769E-01        8.50000E 01
1.35691E-02        1.33565E-02        1.31634E-02

1.80000E 01        6.12000E 00        5.48342E 00        4.65347E 00        3.55426E 00
1.80000E 01        3.12879E 00        2.35532E 00        1.34413E 00        0.
9.39172E-01        9.23756E-01        9.09769E-01        8.50000E 01
1.35691E-02        1.33565E-02        1.31634E-02

1.90000E 01        6.12000E 00        5.48343E 00        4.65349E 00        3.55428E 00
1.90000E 01        3.12880E 00        2.35533E 00        1.34414E 00        0.
9.39172E-01        9.23756E-01        9.09769E-01        8.50000E 01
1.35692E-02        1.33565E-02        1.31634E-02

2.00000E 01        6.12000E 00        5.48343E 00        4.65349E 00        3.55429E 00
2.00000E 01        3.12880E 00        2.35534E 00        1.34414E 00        0.
9.39172E-01        9.23756E-01        9.09769E-01        8.50000E 01
1.35692E-02        1.33565E-02        1.31634E-02

2.10000E 01        6.12000E 00        5.48335E 00        4.65338E 00        3.55414E 00
2.00417E 01        3.12922E 00        2.35589E 00        1.34487E 00        0.
9.48499E-01        9.32930E-01        9.18802E-01        8.58432E 01
1.35693E-02        1.33566E-02        1.31635E-02

2.20000E 01        6.12000E 00        5.48335E 00        4.65338E 00        3.55414E 00
0.                 3.12922E 00        2.35589E 00        1.34487E 00        0.
9.48499E-01        9.32930E-01        9.18802E-01        8.58432E 01
1.35693E-02        1.33566E-02        1.31635E-02

2.30000E 01        6.12000E 00        5.26917E 00        4.31858E 00        3.32312E 00
9.30556E-01        2.95112E 00        2.17334E 00        1.25664E 00        0.
9.44530E-01        9.29873E-01        9.17883E-01        8.58432E 01
1.35151E-02        1.33149E-02        1.31510E-02

2.40000E 01        6.12000E 00        5.38345E 00        4.46104E 00        3.35401E 00
1.93056E 00        3.03417E 00        2.23808E 00        1.26425E 00        0.
9.46351E-01        9.30931E-01        9.17960E-01        8.58432E 01
1.35400E-02        1.33293E-02        1.31520E-02

2.50000E 01        6.12000E 00        5.43048E 00        4.54317E 00        3.41896E 00
2.93056E 00        3.07724E 00        2.28627E 00        1.29091E 00        0.
9.47316E-01        9.31737E-01        9.18234E-01        8.58432E 01
1.35531E-02        1.33403E-02        1.31558E-02

2.60000E 01        6.12000E 00        5.45368E 00        4.58945E 00        3.46944E 00
3.93056E 00        3.10119E 00        2.31656E 00        1.31258E 00        0.
9.47858E-01        9.32252E-01        9.18460E-01        8.58432E 01
1.35605E-02        1.33474E-02        1.31588E-02
```

FIGURE 27.5

A.10 CONCLUSIONS AND RECOMMENDATIONS

The author feels that MIMIC is an excellent technique for solving many types of problems which engineers often meet, but that MIMIC has certain features which limit its applicability to other problems.

Because MIMIC is able to deal with only one independent variable, many general types of problems such as many fluid mechanics problems cannot be solved using MIMIC. However, partial differential equations with two independent variables can be converted into ordinary differential equations with one independent variable by using finite difference methods.

MIMIC has a restricted value for doing boundary value problems because it is impossible (from the author's limited knowledge) to do a search in a MIMIC program. It has been suggested that the possibility may exist of doing the search in a FORTRAN program and using MIMIC for the rest of the calculation. This process would, in fact, require MIMIC to be called from a FORTRAN program. Discussion with Dr. D.J. Kenworthy of the McMaster Computation Centre has revealed that at the present time this is impossible because of the problems of core capcity and linkage.

A major fault is the impossibility of obtaining an object deck. This means that if a program is rerun, compilation must be redone, and thus computer time is wasted. Compilation time is a large fraction of the total run time of a program, and for many cases, exceeds one-half the total run time. Discussions with Dr. D.J. Kenworthy have occurred, and at the time of writing, he is studying the possibilities of two alternative methods of avoiding the recompilation procedure.

Another drawback is the inadequate diagnostics which result in cases where errors have been made. It is the experience of several people in the department that for large systems and certain types of errors, it is very difficult to determine exactly what the error is and where the error is located.

Some discussion has also been initiated with Dr. Kenworthy on the possibility of obtaining a printout of the actual integration step size being used at any particular time, and also the possibility of getting punched card output.

Unexpected errors may appear. These are the result of the imperfect conversion of MIMIC to the 7040 system. During this study, errors were found in DER and LIN. It was also discovered that a section of core was not being properly erased before a MIMIC run and hence floating point overflows were resulting.

In spite of these shortcomings, MIMIC has several features which make it useful.

MIMIC programs are easy to set up, and the user does not have to be concerned with the order of statements in the program, with the exceptions of control cards, CON, CFN, PAR, PFN, HDR, OUT, END statements, and the order of operations in subroutines. Because of its simplicity, undergraduates can learn and use MIMIC easily, thus ensuring that time allotted for a given problem is spent on the problem itself, and not on the techniques of solution.

MIMIC functions enable many logical and algebraic operations to be carried out with ease, and the ability to add user-written subroutines to a program adds more flexibility. One of the more prominant features is the MIMIC integrator function INT which uses a fourth-order Runge-Kutta variable step size integration technique. This function makes MIMIC ideally suited to solving systems of ordinary differential equations.

In summary, MIMIC is an excellent technique for solving many of the problems faced by chemical engineers, but its shortcomings may limit its application to other types of problems.

A.11 BIBLIOGRAPHY

A.11.1 Franks, R.G.E., and W.E. Schiesser,
"The Evolution of Digital Simulation Programs",
paper presented at the 59th Annual Meeting,
A.I.Ch.E., Detroit, December 4 - 8, 1966.

A.11.2 Linebarger, R.N., and R.D. Brennan,
"A Survey of Digital Simulation : Digital
Analog Simulator Programs",
Simulation 3, No.6, Dec. 1964, pg.22.

All.3 Brennan, R.D., and R.N. Linebarger,
"An Evaluation of Digital Analog Simulators",
paper presented at the Symposium Session
"Hybrid Digital Analog Techniques",
Proceedings I.F.I.P.S. Congress, 1965, vol.27, Part II.

A.11.4 Rideout, V.C.,
"Continuous Systems Simulation, Present Problems
and Future Possibilities",
paper presented at the I.B.M. Symposium on Digital
Simulation of Continuous Systems,
Thomas J. Watson, Research Centre, Yorktown,Heights,
N.Y., June 20 - 22, 1966.

A.11.5 Smith, C.L., Jr.,
"All-Digital Simulation for Process Industries",
I.S.A. Journal, July 1966, page 53.

A.11.6. Harnett, R.T., F.J. Sansom, and L.M. Warshawsky,
MIDAS Programming Guide, Technical Documentary
Report No. SEG-TDR-1, Wright-Patterson Air Force
Base, Ohio, January, 1964.

A.11.7

"MIDAS - An Analog Approach to Digital Computation",
Simulation 3, No.3, September 1964, page 17.

A.11.8 Petersen, H.E., F.J. Sansom, R.T. Harnett, and
L.M. Warshawsky,
"MIDAS - How it Works and How It's Worked",
Proceedings Fall Joint Computer Conference 1964,
October 1964, pages 313-324.

A.11.9 Harley, J.R., and J.J. Skiles,
"DYSAC-4 Digitally Simulated Analog Computer",
Proceedings A.F.I.P.S. Conference, Vol.23, 1963.

A.11.10 Syn, W.M., and R.N. Linebarger,
"DSL/90 - A Digital Simulation Program for Continuous System Modeling",
Proceedings, Spring Joint Computer Conference 1966,
pages 165 - 187.

A.11.11. Syn, W.M., and D.G. Wyman,
"DSL/90, Digital Simulation Language, User's Guide",
I.B.M. Technical Report TR 02.355

A.11.12 Cress, P.
"MIMIC - A Digital Analog Simulator",
A handbook for use at the University of Waterloo,
Waterloo, Ontario, February 1966.

A.11.13 Petersen, H.E., F.J. Sansom, and L.M. Warshawsky,
"MIMIC - A Digital Simulator Program",
SESCA Internal Memo 65-12, Wright Patterson Air Force Base, Ohio, May 1965.

A.11.14 Winegar, G.L.,
"Simulation of the Analog Computer Using the Digital Computer",
M.Sc. thesis, University of Tennessee, June 1967.

A.11.15 Funk, J.E.,
"SLASH ALGOL Simulated Hybrid Computer",
AD 465 935, Frank J. Seiler Research Laboratory,
U.S. Air Force Academy, Colorado.

A.11.16 Northcott, T.H.
"MIMIC - A Study of the Technique and Application to Modeling of an Extraction Column",
M.Eng. Major Study Report, McMaster University, October 1967

A.12 APPENDICES

A.12.1 Diagnostics

The following errors are detected and identified by a diagnostic printout. These will cause deletion of execution.

1. Closed loops
2. No ESP card following a subroutine defined by a BSP card.
3. A CSP card not followed immediately by an RSP card.
4. Use of a function other than the MIMIC functions.

In addition, variable names which have not been assigned a value are identified and given a value of zero. Execution is not deleted.

The usual FORTRAN IV error messages may appear.

Other errors, including the following ones, result in a diagnostic printout.

1. Floating point overflow
2. Interval timer overflow
3. Illegal decimal input character
4. Writing on a restricted section of core

A.12.2 The MIMIC Processor

No extensive discussion will be given on the MIMIC processor, although a short outline will now be presented in order that the reader may have a better understanding of the operations which occur.

The MIMIC processor consists of a number of subroutines written in MAP and FORTRAN. Some of these subroutines themselves contain other subroutines or functions. The basic subroutines will now be discussed.

MIM1 is part of the MIMIC executive program. It controls access to the following locations:

1. Common functions such as SIN, COS, EXP, and SQRT.
2. The MIMIC subroutines MIM2, MIM5, MIM7, MIM8, and MIM9.
3. Functions which deal with floating point traps, exit routines, and with the position in the program.
4. A series of subroutines which are needed repetitively by more than one of the other main routines.

MIM2 (MIMIC) is the compiler. It decomposes the source program into single operation elements in binary coded decimal (BCD) form which are stored in the order in which they are developed. This BCD array is such that the following rules are obeyed.

1. BCD (1,I) = result name
2. BCD (2,I) = function name
3. BCD (3,I) BCD(8,I) = function arguments
4. BCD (9,I) = logical control variable name.

Example* $x = \cos (w * y + z + q) - (\frac{y*z}{w} + T)$

	I=J+1	I=J+2	I=J+3	I=J+4	I-j+5	I=J+6
BCD(1,I)	(001)	(002)	(003)	(004)	(005)	x
BCD(2,I)	MAD	ADD	COS	DIV	MAD	SUB
BCD(3,I)	w	(001)	(002)	z	y	(003)
BCD(4,I)	y	q		w	(004)	(005)
BCD(5,I)	z				T	

---

* This example is taken from Winegar's thesis(14).

MIM2 also sets up vectors recording the names and values of T, DT, N (the number of integrators), DTMAX, DTMIN, integrator result names, TRUE and FALSE.

MIM2 controls access to MIM3, MIM4 and MIM6 and also maintains contact with MIM1 and the IBMAP ASSEMBLY

MIM3 (MIMS0) is the sorting routine. It tests for the following errors:

1. Multiple definitions
2. Missing RSP or ESP
3. Incorrectly entered data
4. Incorrect header, print, and/or plot instructions.
5. Undefined variables
6. Closed loops

MIM3 also sequences the elements of the BCD array into the order needed for execution to the criterion that no operation may contain a variable which has not been previously defined.

MIM4 (MIMIN) is the integration subroutine. It uses a fourth order Runge-Kutta method and contains an internal check to vary the step size between DTMIN and DTMAX such that the maximum step size is used without the integration violating a relative error criterion.

MIM5 (MIMI0) controls the read-in of data and the print-out of data, headings and variables.

MIM6 (MIMAS) assembles the program and converts the program into an executable machine-language subroutine. It links functions in the program to standard functions which are available at other locations in the program.

MIM7 (MIMFN) allows the use of tabulated data for arbitrary functions. It performs a linear interpolation between known data points for functions of one or two variables.

MIM8 (MIMRN) is a random number generating subroutine. It performs either of the two duties defined by MIMIC functions RNG and RNU.

MIM9 (MIMTD) is the routine which generates a time delay.

PART B

APPLICATION OF MIMIC TO THE MODELING OF AN EXTRACTION COLUMN

B.1 INTRODUCTION

B.1.1 General

It is desirable to have a model which will predict steady state and transient responses of a system. Study could then be made of the effect of changes in operating variables on the response of the process. Furthermore, the interaction between the dynamic behaviour of the system with different control modes could be examined without disturbing the actual physical system. Then, when the response characteristics of the system are known, a suitable control mode could be designed.

A major purpose of the present work was to test and extend a model for an existing,mechanically-agitated, countercurrent liquid-liquid extraction column. The resulting model should accurately predict steady-state and transient raffinate and extract concentrations over the whole range of operating conditions for which the column had previously been run. Actual experimental work was done by Pollock(B.6.3), who formed a transient condition by introducing a step change in the feed concentration. The model was to be written in MIMIC - a digital analog simulator language - and an evaluation of the usefulness of MIMIC for this type of simulation was to be made.

All known previous work is based upon the important assumption that both initial and final steady state parameters are known, and, in fact, that the transient between them is known. The mass transfer coefficient, as it is used in previous work, is by definition, a factor which causes the predicted and experimental responses to agree. In reality, what previous models have done is to fit the model to describe a known action. This approach may be valid if the one single transient under study will be the only case to be considered. However, if a number of different transients are to be considered, and if some of these have had no experimental work associated with them, this approach is no longer feasible.

The purpose of a transient model, then, is to predict the response caused by a given step disturbance when the final steady state is not known. The present work is concerned with the construction of a model which will be able to predict the transient responses caused by step changes in the feed concentration, when only the initial steady state flows, holdups, and concentration profiles, and the stage volumes are known. And, unlike previous models, the new model should be able to predict both raffinate and extract responses simultaneously.

In the sections which follow, a brief summary will be made of several important papers of the literature of transient extraction models, a short description of the apparatus on which Pollock obtained data will be given, and the data made available by previous work by Pollock will be outlined.

B.1.2 Literature

B.1.2.1 Work of Biery and Boylan

Biery and Boylan(B.6.1) investigated the theoretical and experimental transient start-up behaviour of a pulsed liquid-liquid extraction column making the following assumptions:

1. The actual pulsing of the column was ignored.
2. Flow rates were on a solute-free basis and were constant.

3. Holdups were constant.
4. The mass transfer coefficient was not a function of concentration or time, but was a function of column height.
5. The equilibrium relationship was nonlinear.

A number of different models were proposed. Seven models were based on an unsteady state material balance over an arbitrary section of column and certain assumptions were made as to the mechanisms of mass transfer and mixing within the section. Two models were based on the fundamental partial differential equations describing the overall transient behaviour. A large number of ordinary differential equations were formed by transforming the height derivative to a divided difference.

It should be noted that, for nonequilibrium stage models, the overall mass transfer coefficient required to make the model reproduce the experimental steady state operation was determined by trial and error. In addition, none of the models contained an axial diffusion term.

Biery concluded from the study that certain of the models were much better than others, the best model being a nonequilibrium stage, nonuniform mixing model in which the driving force at the top of the stage was taken to represent the driving force within the stage.

B.1.2.2 Pollock (M.Eng. thesis)

Pollock(B.6.2) studied the experimental and theoretical operation of a six stage Scheibel type liquid extraction column. Both an equilibrium stage model and a non-equilibrium stage model were used to calculate the steady-state operation, and the non-equilibrium stage model was also used to calculate the transient response to a step change in the feed flow rate. Predicted results were then compared to theoretical results. An overall mass transfer coefficient was calculated using the relation

$$NTU_{OE} = \int_{C_{E2}}^{C_{E1}} \frac{d\,C_E}{C_E^{*} - C_E} + \tfrac{1}{2}\,\ln \frac{1 - C_{E1}}{1 - C_{E2}} + \tfrac{1}{2}\,\ln \frac{C_{E1}\,(r-1)\,+1}{C_{E2}\,(r-1)\,+1} \qquad (1)$$

where

NTU_{OE} is the number of overall transfer units

C_E is the concentration of solute in the solvent phase, weight percent.

r is the ratio of molecular weights of nonsolute to solute.

Then,

$$K_E a = NTU_{OE} \cdot S/V \qquad (2)$$

where

$K_E a$ is the overall mass transfer coefficient

S is the flow rate of the organic phase

V is the volume of a stage

The models were tested in two different ways.

First, the experimentally determined and the calculated mass transfer coefficient variables were substituted into the model and the number of stages required to predict column behaviour accurately was determined.

The second method considered the physical construction of the column. The number of stages in the model was set equal to the number of stages in the column. By using a search technique, a mass transfer coefficient was found which would make the model predict experimental concentrations.

With either method, the outlet concentrations and result curves could be obtained.

Pollock noted that the assumption used to calculate the mass transfer coefficient (i.e. differential length) was not valid for the system. He also noted that experimental holdups and mass transfer coefficient changed between initial and final steady states. Hence, Pollock suggested that a mass transfer coefficient which varied with concentration would provide a better model.

B.1.2.3 Pollock (Ph.D. thesis)

In a very comprehensive study, Pollock$^{(B.6.3)}$ has investigated the theoretical and experimental techniques of single pulse, multiple pulse and step disturbances and has evaluated frequency response methods for dynamic testing. Both the steady state and the transient operation of a countercurrent agitated stage liquid-liquid extraction column were considered, the basic model for the system being the non-equilibrium stage, uniform mixing model.

Pollock included in his report a comprehensive and critical survey of the literature in this area, and also photographs and a description of a very versatile extraction apparatus, designed in a general manner to handle a wide variety of extraction systems.

In this report, Pollock defines and uses different types of mass transfer coefficients discussed in the following paragraphs.

Steady state mass transfer coefficient

This is the coefficient required to cause the predicted steady state outlet concentration to fit the experimental concentration. It is seen that different coefficients are needed for both raffinate and extract streams. In general, for a given flow system, these coefficients decrease as the feed concentration increases. These coefficients were found by using the uniform mixing, nonequilibrium stage model, the experimental steady state parameters, and the Fibonacci search technique.

Transient mass transfer coefficient:

This is the coefficient required to cause the predicted transient response to fit the experimental transient. Again, different coefficients are needed for the raffinate and extract responses. It is noted that these coefficients were calculated in the frequency domain.

From his studies, Pollock concluded that the ideal mixing, non-equilibrium stage model will adequately simulate the response of either the extract or the raffinate separately, but not simultaneously.

Several substudies were completed. The model parameters were evaluated and their sensitivity was tested. And, by assuming a realistic raffinate profile based on internal samples, Pollock was able to determine a strong dependence of the mass transfer coefficient on the assumed concentrations. He suggested that future models should include a concentration-dependent mass transfer coefficient.

B.1.2.4 Karr and Scheibel

Karr and Scheibel(B.6.4) studied extensively the methylisobutyl ketone-acetic acid - water system for a single agitated stage and for countercurrent flow of liquids such that the liquids were contacted only within the stage itself. Activity was used as the driving force for mass transfer. The following two major assumptions were made.

1. The effect of molecular diffusion is small compared to the effect of eddy diffusion.
2. The stage was ideally mixed such that the average concentration of solute in each phase leaving the stage is equal to the average concentration of the solute in that phase within the stage.

These assumptions are valid if the agitation of the stage volume is great enough and if the concentrations are not too high.

Karr and Scheibel derive the relations between the overall mass transfer coefficients based on activity and on concentration arriving at

$$\frac{Ka'}{K_E a'} = \frac{dC_E}{da} \qquad (3)$$

where K is the overall coefficient based on activity as the driving force.

K_E is the overall coefficient based on concentration as the driving force.

C_E is the concentration of the solute in the extract phase

a is the activity of the solute

a' is the surface area per unit volume

Three-and twelve-inch diameter columns with dimensionally similar stages and impellers were used to study the system for a number of different combinations of extractant and direction of transfer.

It was found that the mass transfer coefficients were functions of the following parameters.

1. The coefficients were independent of the continuous phase flow rate.
2. The coefficients were independent of the dispersed phase flow rate or varied linearly with the dispersed phase flow rate, depending on the phase which was dispersed, the extractant phase, and the flow rate. These three factors interact to influence greatly the rate of coalescence and hence the

the interfacial area. For the system Pollock considered (organic phase dispersed, organic phase extractant), Karr and Scheibel found that no coalescence of drops of dispersed phase occurred even at low flow rates, and that the mass transfer coefficient varied linearly with dispersed phase flow rates down to low rates.

3. The coefficients were proportional to the fourth power of the agitator speed when the organic phase was dispersed, and the third power of the agitator speed when the water phase was dispersed.
4. The coefficients varied as the third power of the agitator diameter when the organic phase was dispersed and the 2.7 power of the agitator diameter when the water phase was dispersed.

These observations were based on experiments done with dimensionally similar systems.

For methylisobutyl ketone (MIBK) the extractant, and MIBK also the dispersed phase, Karr and Scheibel found that all the data which was available to them correlated to

$$Ka' = (1.09 \times 10^{-7})(N^{4.0})\ (D^{3.0})\ (S)\ (\frac{\Delta\rho}{\sigma})^{1.5} \qquad (4)$$

where

Ka' is the overall mass transfer coefficient based on activity as the driving force $\frac{(\text{lb. moles})}{(\text{hr.} \times \text{ft.}^3 \times \Delta a}$

N is the agitator RPM

D is the diameter of the agitator (inches)

S is the flow rate of dispersed phase ($\frac{ft.^3}{hr. \times ft.^2}$)

$\Delta\rho$ is the difference in density between the light and heavy phase ($\frac{grams}{ml.}$)

σ is the interfacial tension ($\frac{dynes}{cm.}$)

The term $(\frac{\Delta\rho}{\sigma})^{1.5}$ accounted for the effect of variations in physical properties on the mass transfer coefficient.

Karr and Scheibel presented physical property data for the MIBK - acetic acid - water system, including distribution data and activities at 25°C and densities, viscosities and interfacial tensions of the phases in equilibrium at 25°C.

B.1.3 Experimental Apparatus and Extraction System

Pollock's work was done on a mechanically-agitated, countercurrent liquid-liquid extraction column which he designed and built to meet certain required specifications.

The column, the flow system, and the sampling system were built such that the whole system could be used for a wide variety of extraction studies other than the extraction system studied by Pollock.

The sections which follow are intended to give the reader a general description of the extraction apparatus. Detailed descriptions and photographs may be found in Pollock's thesis.

B.1.3.1 Column Design

The column itself was about 25 inches in height. Constructed of three-inch nominal O.D. pyrex pipe in two - or four-inch sections, the column consisted of three stages plus a cell on either end of the column.

The three stages were formed by four sieve plates spaced at the end of four-inch sections or two two-inch sections. Four-inch sections were used for the first and third stages, while two two-inch sections made up the center stage. The Teflon sieve plates, used in an attempt to eliminate recycle of phases to stages opposite to their main directions of flow, were $1/8$-inch thick and had $5/32$-inch diameter holes on an equilateral pitch such that the free area was twenty percent.

Mixing was provided by three centered impellers, one in each stage. Each impeller consisted for four flat blades with an overall diameter of 1½ inches and a blade width of ¼ inch. These impellers as well as the $5/16$-inch diameter central shaft were of 316 stainless steel.

To prevent vortexing, the end cells were both baffled by four equally spaced baffles each $5/16$-inch wide.

A sparger ring in each end cell near the sieve plate was used to introduce feed (top cell) and solvent (bottom cell) to the column.

About four inches above the raffinate feed sparger in the top cell was the extract removal tube which lead to a drain. In the bottom cell about three inches below the solvent feed sparger was the raffinate outlet tube. This lead to a device which could be adjusted in height to control the upper interface level in the column.

B.1.3.2 Sampling System

Provision was made to remove samples from the coalesced extract phase in the top end cell and from the raffinate phase in the bottom end cell. These samples could be withdrawn through $1/8$-inch Teflon tubes which projected into either coalesced phase to a point near the respective interface. These tubes were connected to a pair of solenoid valves which were in series with an interval timer. Sampling periods could thus be accurately controlled.

Each of the three stages had sample ports containing sampling tubes controlled by solenoid valves. Samples of the concentration profiles along the column could then be obtained. A complete description of this sampling system is found in Pollock's thesis.(B.6.3.)

B.1.3.3 Flow System

All tubing in the system was either stainless steel or Teflon to minimize contamination of solutions.

Feed solution and solvent were stored in large stainless steel tanks, pressurized with nitrogen to provide a driving force for flow. From the tanks, solutions flowed through a constant temperature water bath used to ensure no rotameter variations occurred because of viscosity changes caused by varying liquid temperature. Control valves metered flows to rotameters, from which flows then passed through another water bath.

Two feed streams of different concentrations were connected to a pair of three-way solenoid valves as shown in the following sketch.

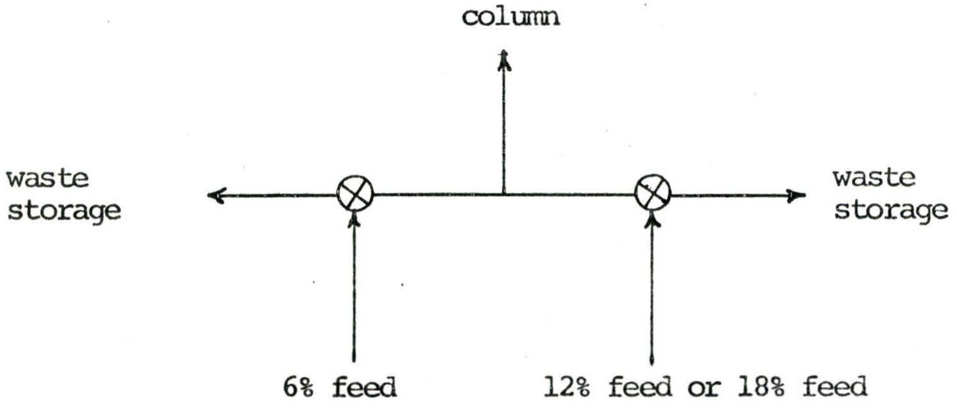


FIGURE 28

The two solenoid valves were controlled by the same switch so that the feed concentration could be changed "instantly" from 6 weight percent feed to 12 or 18 weight percent feed. The distance between the valves and the column was minimized to prevent delays and mixing. Feed solutions flowed to the sparger ring in the end cell at the top of the column, while pure solvent was fed to the sparger ring in the cell at the bottom of the column.

From the column, extract flow went directly to a drain. The raffinate stream went to an overflow device which could be adjusted in height to control the height of the extract interface in the end cell in the top of the column. From this device, the raffinate stream went to a drain.

B.1.3.4 The Extraction System

The extraction system which was used was the methylisobutyl ketone - acetic acid - water system, MIBK being the solvent and acetic acid being the solute. Acetic acid was extracted from the continuous water phase into the dispersed ketone phase.

Four flow systems were studied and these are outlined in Figure 29. For each flow system, step changes in feed concentrations were made from 6 weight percent to either 12 or 18 weight percent solute.

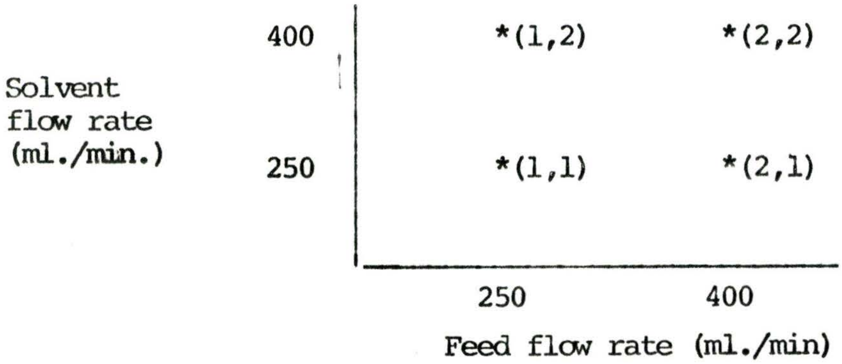


FIGURE 29

Certain characteristics of the system, outlined in a later section, were established for the steady states, and for the transient responses for the step changes in the feed concentration.

B.1.4 Operating Parameters and Data

B.1.4.1 Process Variables

Most of the general process variables have already been defined in Section 2.3.

It should be noted that feed solutions were presaturated with ketone, and solvent was presaturated with water. This was done to ensure that transfer occurred only by diffusion and not by the solution of feed in the solvent.

The system is not highly temperature dependent, but experiments were done with feed and solvent flows at 22 degrees C.

Agitator speed for all runs was 340 RPM.

The primary experimental variables were the feed flow rate, the feed: solvent ratio, and the feed concentration. Only the feed concentration was altered to induce a transient response.

B.1.4.2 Measured Variables

For the experiments performed by Pollock, the measured variables included the following:

1. Feed flow rate
2. Solvent flow rate
3. Feed concentration
4. Raffinate flow rate
5. Extract flow rate
6. Raffinate concentration
7. Extract concentration
8. Concentration profile
9. Agitator RPM

B.1.4.3 Data

For the three steady state concentration levels of each of the four flow systems outlined in Section 2.3.4, the following relevant data were supplied:

1. Feed concentration
2. Steady state raffinate concentration
3. Steady state extract concentration
4. Average solute-free flow rates for both raffinate and extract phases
5. Solute-free raffinate and extract holdups
6. Total volume
7. Weights of phases in the end cells.

Other data which were supplied but not used are the following:

1. The number of theoretical stages
2. The number of transfer units
3. The experimental mass transfer coefficient
4. Dispersed phase volume and total concentration
5. Continuous phase volume and total concentration
6. Settled volumes of extract and raffinate phases

For each of the four flow systems, the experimental transient raffinate and extract concentrations were available for feed concentration steps of both 6 to 12 weight percent and 6 to 18 weight percent.

A steady state modeling program was available which calculated, using a Fibonacci search technique, a mass transfer coefficient to fit the predicted outlet concentrations to those obtained by experiment. Three different coefficients were calculated. One fitted the raffinate concentration, one fitted the extract concentration, and one fitted both concentrations at the same time to give the best possible fit. The program calculated the three coefficients for from one to eight stages.

For each flow system and each step change in feed concentration, transient mass transfer coefficients were available for from one to seven stages. These transient coefficients were obtained by Pollock from frequency domain calculations. Again, three coefficients were available - one to fit the transient raffinate concentration, one to fit the transient extract concentration and one to give the best fit of both these concentrations at the same time.

B.2 MODELING OF A COUNTERCURRENT LIQUID-LIQUID EXTRACTION OPERATION

The purpose of the following section is primarily to review the concepts of the mass transfer coefficient and the overall mass transfer coefficient, and to outline the relationship between the overall coefficient based on concentration and the overall coefficient based on activity. In addition, various liquid-liquid extraction models are outlined and some discussion is given to steady state and transient modeling.

B.2.1 Concept of a Mass Transfer Coefficient

One concept of turbulent flow pictures the existence of eddies - elements of fluid which move about erratically from one place to another in the fluid. Characteristics of the fluid at the point of origin of the eddy are thus transmitted to other areas in the fluid. Hence, in a highly agitated cell, since the fluid motion is turbulent, large numbers of eddies cause the characteristics of the fluid in the cell to become uniform at all positions in the cell. Thus, if the concentration of a dissolved solute is higher at the point of origin of the eddy, a transfer of solute will occur to other parts of the fluid. Eddy diffusivity is a factor which relates the flux of mass by turbulent action and a concentration gradient. Thus,

$$J_A = - \varepsilon \frac{\partial C_A}{\partial Z} \qquad (5)$$

where J_A is the turbulent flux of component A

ε is the eddy diffusivity

and $\frac{\partial C_A}{\partial Z}$ is a concentration gradient of the concentration of component A in the Z direction.

At the same time as eddy diffusion occurs, another diffusion process, molecular diffusion, causes transfer of solute from the "eddy" to the bulk of the fluid. Then, the total flux of component A is the sum of the fluxes caused by each diffusion process.

$$J_{AT} = -(\varepsilon + D_A) \frac{\partial C_A}{\partial Z} \qquad (6)$$

where D_A is the molecular diffusivity of the component A.

Treybal$^{(B.6.5)}$ points out that in the case of fully developed turbulent flow, the eddy diffusivity is many times larger than the molecular diffusivity.

If a dispersed immiscible solvent were to be introduced into a continuous liquid solution in an agitated cell, the droplets of the dispersed phase would be distributed throughout the continuous phase by eddy diffusion. Transfer of solute between phases occurs by molecular diffusion, but the controlling factor is the degree of dispersion of the solvent throughout the continuous phase. This is a function of the turbulence and hence of the eddy diffusion.

In the case of turbulent flow, velocity distributions and the exact nature of eddy diffusion are not known. Mass transfer rates cannot be calculated directly. Thus, in the past, the procedure has been to measure the rates of mass transfer for certain given situations, and to relate these rates to known concentration gradients by means of a factor known as a mass transfer coefficient. Then,

$$N_A = kA\Delta C_A \qquad (7)$$

where N_A is the flux of component A

A is the interfacial area

k is the mass transfer coefficient

ΔC_A is a concentration gradient of component A.

The mass transfer coefficient, k, is a function of the flow characteristics of the fluid and the molecular and eddy diffusivities.

B.2.2 The Overall Mass Transfer Coefficient K_E

In the case of liquid extraction, transfer of mass occurs across the interface between the phases. Consider the raffinate phase (solution) and the extract phase (solvent) to have average concentrations of solute C_R and C_E respectively. The concentrations of the solute at the interface in the raffinate phase and in the extract phase are C_{Ri} and C_{Ei} respectively. These concentrations are not equal, but equilibrium exists at the interface, and hence C_{Ri} is in equilibrium with C_{Ei}. It is seen that a concentration discontinuity exists at the interface. The situation is illustrated in Figure 30.

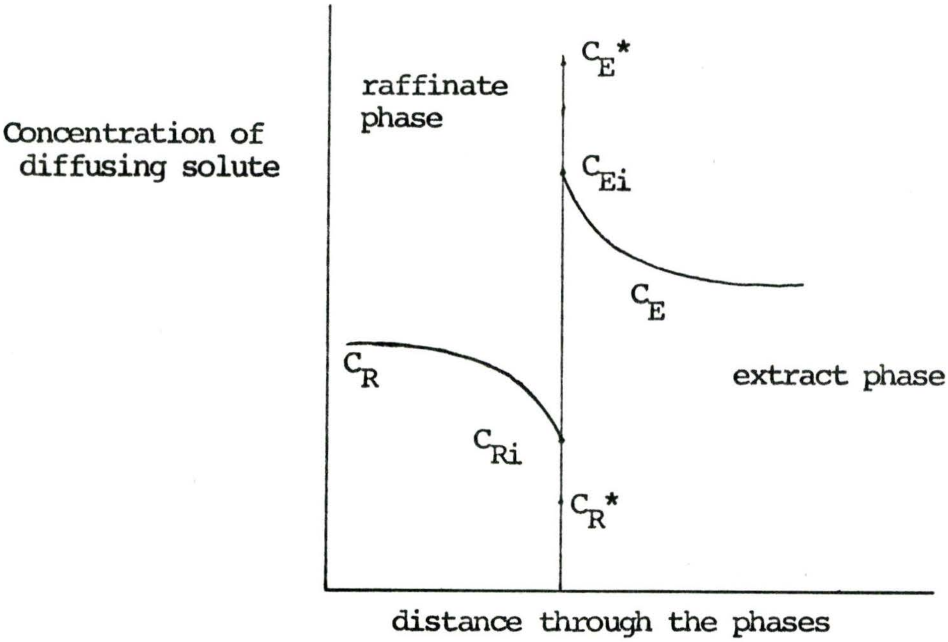


FIGURE 30

An expression for the rate of mass transfer can be written for each phase

$$N_A = k_R A\ (C_R - C_{Ri})$$
$$N_A = k_E A\ (C_{Ei} - C_E) \qquad (8)$$

where k_R and K_E are the mass transfer coefficients for the raffinate phase and the extract phase respectively.

Using the two resistance theory of Whitman the flux can be written in terms of overall mass transfer coefficients where the driving forces have now been altered slightly.

$$N_A = K_E A\ (C_E{}^* - C_E) = K_E A\ (\Delta C_{OE})$$
$$N_A = K_R A\ (C_R - C_R{}^*) = K_R A\ (\Delta C_{OR}) \qquad (9)$$

where K_R and K_E are the overall mass transfer coefficient for the raffinate phase and the extract phase respectively

$C_E{}^*$ is the concentration of solute in the extract phase in equilibrium with the bulk concentration in the raffinate phase C_R.

$C_R{}^*$ is the concentration of solute in the raffinate phase in equilibrium with the bulk concentration in the extract phase C_E.

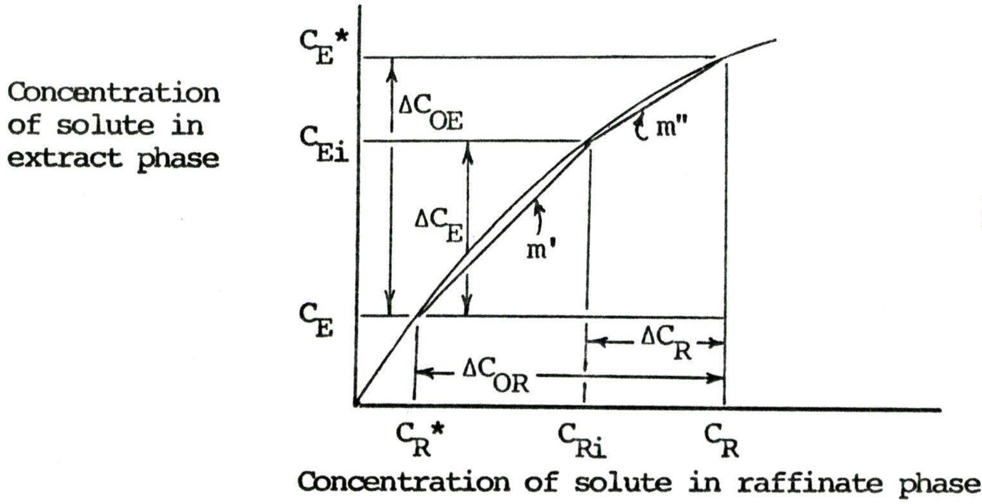


FIGURE 31

From Figure 31, and for the general case of a non-linear equilibrium relationship,

$$\Delta C_{OE} = \Delta C_E + m'' \Delta C_R \tag{10}$$

Therefore,

$$\frac{N_A}{K_E A} = \frac{N_A}{k_E A} + \frac{m'' N_A}{k_R A} \tag{11}$$

and

$$\frac{1}{K_E A} = \frac{1}{k_E A} + \frac{m''}{k_R A} \tag{12}$$

Similarly it can be shown that

$$\frac{1}{K_R A} = \frac{1}{k_R A} + \frac{1}{m' k_E A} \tag{13}$$

B.2.3 The Overall Mass Transfer Coefficient K

Karr and Scheibel point out that Glasstone, Laidler and Eyring have observed that activity is the driving force in diffusion. Then, if the driving force is expressed in terms of activity, for the previous example,

$$N_A = k_{aR} A\ (a_R - a_{Ri}) = k_{aE} A\ (a_{Ei} - a_E) \tag{14}$$

where k_{aR} and k_{aE} are the mass transfer coefficients based on activity for the raffinate phase and the extract phase respectively.

a_R and a_E are the activities of the solute in the bulk raffinate phase and extract phase respectively.

a_{Ri} and a_{Ei} are the activities of the solute at the interface.

Since equilibrium exists at the interface,

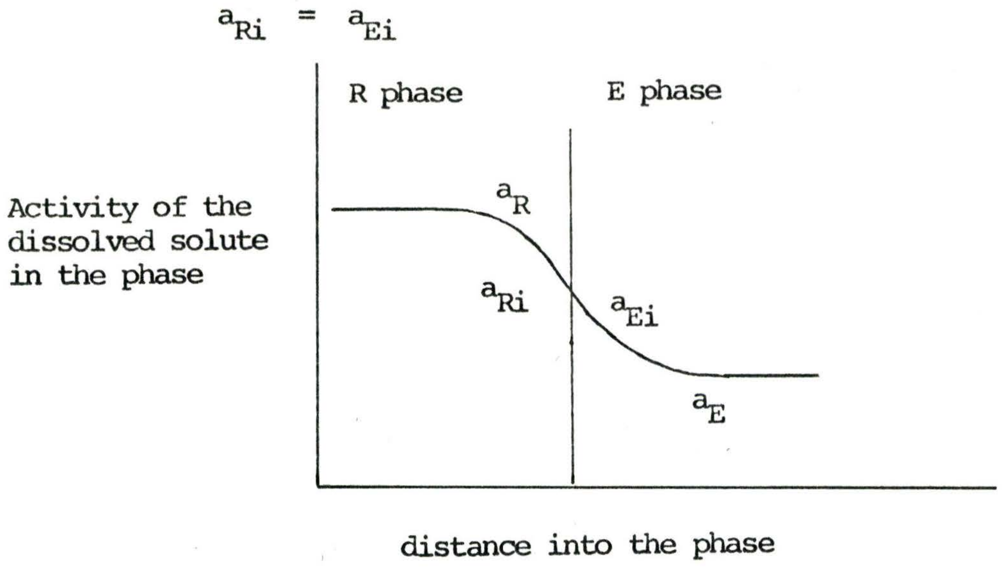


FIGURE 32

Again, the flux can be written in terms of an overall mass transfer coefficient.

$$N_A = K \; A \; (a_R - a_E) \tag{15}$$

where K is the overall mass transfer coefficient based on activity as the driving force.

$$\frac{N_A}{KA} = a_R - a_E = a_R - a_{Ri} + a_{Ei} - a_E = \frac{N_A}{k_{aR}A} + \frac{N_A}{k_{aE}A} \tag{16}$$

Thus

$$\frac{1}{KA} = \frac{1}{k_{aR}A} + \frac{1}{k_{aE}A} \tag{17}$$

It has now been shown that

$$N_A = K_E A \;\; (C_E{}^* - C_E) \tag{9}$$

and

$$N_A = KA\ (a_R - a_E) \tag{15}$$

These can be written

$$N_A = K_E a'V\ (C_E{}^* - C_E) \tag{9'}$$

and

$$N_A = K\,a'V\ (a_R - a_E) \tag{15'}$$

where a' is the interfacial area per unit volume

V is the total volume

Then,

$$K_E a'\ V\ (C_E{}^* - C_E) = Ka'\ V(a_R - a_E) \tag{16}$$

and

$$\frac{Ka'}{K_E a'} = \frac{C_E{}^* - C_E}{a_R - a_E} \tag{16'}$$

Now since a is usually small for practical purposes$^{(B.6.4)}$, then

$$\frac{Ka'}{K_E a'} = \frac{\Delta C_E}{\Delta a} = \frac{dC_E}{da} \tag{17}$$

and

$$K_E a' = Ka'\ \left(\frac{da}{dC_E}\right) \tag{17'}$$

It should be noted that for highly turbulent systems, the interfacial area per unit volume (a') is usually kept grouped with the mass transfer coefficient and the group ($K_E a'$) or (Ka') is used in correlations.

In some of the literature, the group ($K_E a'$) or (Ka') is defined as the overall mass transfer coefficient. In the discussions which follow, this definition will be used.

The overall mass transfer coefficient, then, is a function of the interfacial area. This in turn is a function of the holdup and the diameter of the droplets of dispersed phase. Karr and Scheibel point out that Hayworth and Treybal found that interfacial tension and density difference between phases to have the greatest effect on the diameter of drops issuing from nozzles. These two properties are functions of concentration, and therefore, the overall mass transfer coefficient should be a function of concentration.

Karr and Scheibel have shown that for a given degree of agitation, and for agitated cells of certain dimensions,

$$Ka' = (\text{constant}) \left(\frac{\Delta\rho}{\sigma}\right)^{1.5} \tag{4'}$$

where $\Delta\rho$ is the density difference between phases

σ is the surface tension at the interface. Thus, using equation 4' and equation 17'

$$K_E a' = (\text{constant}) \left(\frac{da}{dC_E}\right) \left(\frac{\Delta\rho}{\sigma}\right)^{1.5} \tag{18}$$

and then $K_E a$ is a complex function of concentration. A relation of this general form will be used to calculate the overall mass transfer coefficient in the present work.

B.2.4 Countercurrent Liquid Extraction Models

Two fundamental types of countercurrent mass transfer operation may be considered.- continuous or stagewise. Although equations describing continuous operation can be written, since much of the experimental work done thus far has been with staged or plate columns, stagewise models are much more common. The two fundamental stagewise models are the equilibrium stage model, and the non-equilibrium stage model.

B.2.4.1 The Equilibrium Stage Model

This model has the following assumptions as its basis:

1. The phases in each stage are ideally mixed.
2. The phases in each stage are in equilibrium.
3. The holdups and flow rates of each phase are constant.
4. Backmixing of either phase between stages is not allowed.

The differential equations which describe the mass balance about a given stage, i, can be written in the form

$$\begin{aligned} WR \frac{dx_i}{dt} &= FR\ x_{i-1} - FR\ x_i \\ WE \frac{dy_i}{dt} &= S\ y_{i+1} - S\ y_i \end{aligned} \qquad (19)$$

where WR and WE are the holdups per stage of raffinate phase and extract phase respectively (weight of solute-free phase).

x_i and y_i are the raffinate composition and the extract composition respectively of stage i (weight of solute)/(weight of solute-free phase)

FR and S are raffinate flow rate and extract flow rate respectively $\left(\frac{\text{weight of solute free phase}}{\text{time}}\right)$

The assumption of ideal mixing means that the concentration of the solute in the phases leaving a stage is the same as the concentration of the solute in the phases in the stage.

The assumption of equilibrium between phases means that the contact time is sufficiently long for this condition to be approached.

Constant phase holdups and flow rates defines the phases to be completely immiscible.

The equilibrium stage model is useful in certain specific areas only, since it assumes a stage efficiency of 100 per cent.

B.2.4.2 The Non-Equilibrium Stage Model Ideal Mixing (B.6.1)

The non-equilibrium stage model has been the basis of many of the available models for countercurrent liquid extraction. Several different non-equilibrium stage models can be formulated, depending upon the assumptions which are made about the degree of mixing, and hence the driving force term.

The ideal mixing, non-equilibrium model incorporates the following assumptions:

1. The phases in each stage are ideally mixed but are not in equilibrium.
2. Holdups and flows of each phase are constant.
3. No backmixing of either phase to the stage from which it occurs is allowed.

Then, for stage i, the differential equations describing the mass balance about the stage can be written

$$\begin{aligned} WR \frac{dx_i}{dt} &= FR \quad (x_{i-1} - x_i) - K_E a'V(y_i{}^* - y_i) \\ WE \frac{dy_i}{dt} &= S \quad (y_{i+1} - y_i) + K_E a'V(y_i{}^* - y_i) \end{aligned} \qquad (20)$$

B.2.4.3 Non-Equilibrium Stage Model, Non-ideal Mixing (B.6.1)

Biery presented two models which considered non-uniform mixing. In one of these models, the driving force for mass transfer is taken to be across the top of the stage. Thus

$$WR \frac{dx_i}{dt} = FR \quad (x_{i-1} - x_i) - K_E a'V \; (y_{i-1}{}^* - y_i)$$

$$WE \frac{dy_i}{dt} = S \quad (y_{i+1} - y_i) + K_E a'V \; (y_{i-1}{}^* - y_i) \qquad (21)$$

The other model considered the driving force for mass transfer to be taken across the bottom of the stage. Thus,

$$WR \frac{dx_i}{dt} = FR \quad (x_{i-1} - x_i) - K_E a'V \; (y_i{}^* - y_{i+1})$$

$$WE \frac{dy_i}{dt} = S \quad (y_{i+1} - y_i) + K_E a'V \; (y_i{}^* - y_{i+1}) \qquad (22)$$

B.2.4.4 Other Models

Biery(B.6.1) has presented other models in which he has used averaging methods for the derivative term or central difference methods for the driving force term.(B.6.6)

Foster presented a model which was basically the uniform mixing, non-equilibrium stage model, but a term was added to represent backmixing between stages. End cells were also added to each end of the column to represent areas in the actual column where phases separated but no mass transfer occurred.

Pollock's(B.6.3) model was basically the uniform-mixing, non-equilibrium stage model, with separation cells on either end of the column.

B.2.5 Steady State and Transient Modeling

B.2.5.1 Steady State

In order to properly define parameters and conditions for the transient model, the steady state concentration profile must be known. At least two methods to solve for this profile are available, and both assume that steady state holdups and flows and the mass transfer coefficient are known.

B.2.5.1.1 Matrix Solution

The derivatives of the differential equations are set to zero and a set of simultaneous algebraic equations results. Pollock(B.6.3) describes a method for reducing these equations to matrix form and obtaining the solution by an iterative process. In the present study, initial trials to solve a series of simultaneous non-linear equations were made using MIMIC and the method was abandoned in favour of the integration solution.

B.2.5.1.2 Integration Solution

Initial estimates of the steady state concentration profiles were used as the initial conditions to the sets of differential equations. The differential equations were then integrated until no further changes in the dependent variables resulted, thus producing the steady state profiles. These were then used as the initial profiles for the transient responses.

B.2.5.2 Transient

The transient condition was brought about by introducing a step change in the feed concentration. Several techniques are available to obtain the transient response. Pollock(B.6.3.) used two methods, the Runge-Kutta-Gill method and an iterative matrix method. He compared the solution times needed for each method. For up to 4 stages, solution times are similar. For more than 4 stages, the solution time required for the iterative matrix increased exponentially with the number of stages while the solution time required for the Runge-Kutta-Gill method increased linearly with time.

In the present model, as in Pollock's proposed model, the following features are allowed:

1. Holdups do not have to be equal in all stages.
2. Stage volumes may vary.
3. The equilibrium relationship may be nonlinear
4. A single phase cell is added at each end of the column. Mixing of different concentrations of a phase occurs in these cells.

In addition, the present model allows the overall mass transfer coefficient to vary along the column as a function of concentration.

B.3 COMPUTATION AND RESULTS

The section which follows deals with the analytical and computer techniques used in this study, and with the results of the work completed.

B.3.1 MIMIC

MIMIC, one of several digital analog simulator programs which have appeared during the past several years, has several features which should be useful for modeling. By using MIMIC functions, which are black-box units, a wide variety of algebraic and logical operations can be carried out with ease. Special operations not handled by MIMIC functions can be carried out by user-written subroutines. And, except for a few special cases, the order in which statements are placed in the program is not important because an internal sorting routine in MIMIC arranges the program into an order of calculation. In addition, MIMIC is easy to learn, and MIMIC programming is fast and efficient.

In order to evaluate MIMIC as a tool for modeling and to gain experience in the application of MIMIC, this technique was used to solve the equations describing the transient operation of the liquid extraction column.

A complete description of MIMIC, the MIMIC functions, and instructions for writing MIMIC programs are found in Part A of this report.

B.3.2 Description of the Model

The model used in this study was essentially the same as the one used by Pollock; namely, the non-equilibrium stage model with uniform mixing of each phase in each stage, and with phase separation cells at either end of the column. To correspond with the actual laboratory column, the model has three stages each of the same constant volume In addition, the model used allows the mass transfer coefficient to vary as a function of concentration. The equations presented represent the model as it has been described.

$$
\begin{aligned}
HE \quad \frac{dy_1}{dt} &= S \quad (y_2 - y_1) \\
WR \quad \frac{dx_2}{dt} &= FR \quad (x_1 - x_2) - K_E a_2' \quad V \quad (y_2^* - y_2) \\
WE \quad \frac{dy_2}{dt} &= S \; ((y_3 - y_2) + K_E a_2' \quad V \quad (y_2^* - y_2) \\
WR \quad \frac{dx_3}{dt} &= FR \quad (x_2 - x_3) - K_E a_3' \quad V \quad (y_3^* - y_3) \\
WE \quad \frac{dy_3}{dt} &= S \quad (y_4 - y_3) + K_E a_3' \quad V \quad (y_3^* - y_3) \qquad (23) \\
WR \quad \frac{dx_4}{dt} &= FR \quad (x_3 - x_4) - K_E a_4' \quad V \quad (y_4^* - y_4) \\
WE \quad \frac{dy_4}{dt} &= S \quad (y_5 - y_4) + K_E a_4' \quad V \quad (y_4^* - y_4) \\
HR \quad \frac{dx_5}{dt} &= FR \quad (x_4 - x_5)
\end{aligned}
$$

where HE is the weight of solute-free phase in the organic phase separation cell at the top of the column.

HR is the weight of solute-free phase in the raffinate phase separation cell at the bottom of the column.

To provide equations of a form which could be solved by MIMIC, these equations were rearranged slightly so that each equation had only the derivative term on the left hand side of the equation.

Figure 33 presents a diagram of the theoretical column.

B.3.3 The Equilibrium Relationship

It is noted that in the equations describing the model, the concentration of solute in the solvent phase which would be in equilibrium with the concentration of solute in the raffinate stream from a stage is required for each stage.

In all programs used in this study, the equilibrium concentrations are calculated by a subroutine in the program which is essentially a fourth-order polynomial equation respresentation of the equilibrium relationships. The coefficients for this polynomial were found by regressing the same data used by Pollock to a polynomial of given order by using the FORTRAN library program DLESQ which provides a least-squares fit. Several different orders of polynomial were fitted and the order which gave the best recalculation of the data points was chosen.

B.3.4 The Mass Transfer Coefficient

Equation (18) in Section B.2.3 showed that the overall mass transfer coefficient expressed in terms of a concentration driving force can be written as

$$K_E a' = (\text{constant}) \left(\frac{da}{dc_E}\right) \left(\frac{\Delta\rho}{\sigma}\right)^{1.5} \qquad (18)$$

where $\frac{da}{dc_E}$, $\Delta\rho$ and σ are all functions of the concentration of solute in the extract phase.

In the present work all three functions are repsented by polynomials. Using the data of Karr and Scheibel and the FORTRAN library routine DLESQ, the coefficients of the polynomials were found. Each data set was fitted

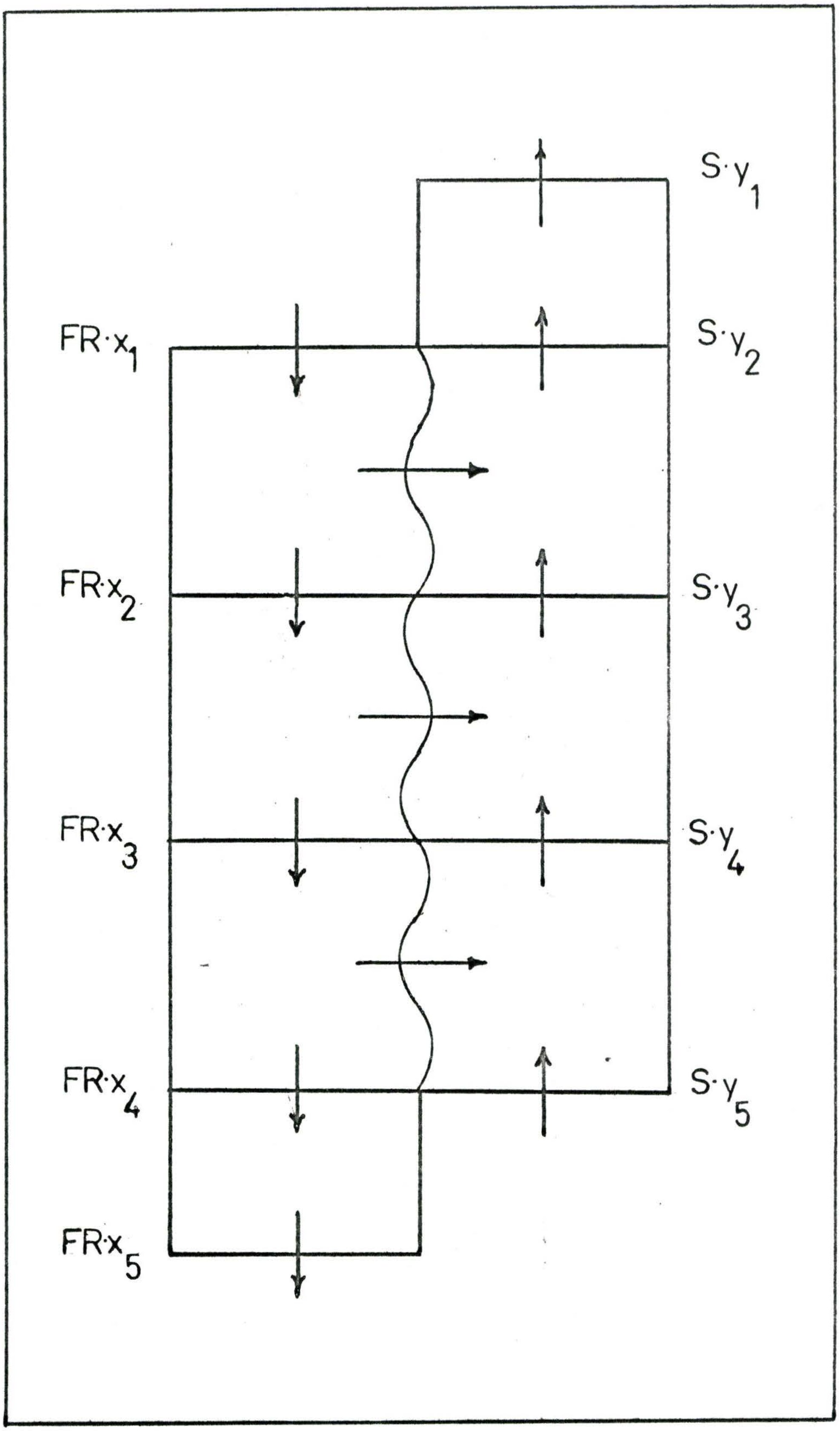


FIGURE 33

by polynomials of several different orders, and the order which gave the best recalculation of the data points was chosen.

In all programs used in this work, the mass transfer coefficient for each stage is calculated by means of a subprogram.

B.3.4.1 Initial Computation of K_Ea'

Some initial trials were completed using the mass transfer coefficient as defined by equation (18). It was found that the value of the constant term (see equation (4)) could not be used.

By using an iterative technique (see A.9 .10), values of the constant term (CON1) required to cause the steady state raffinate concentration predicted by the model to match the actual experimental steady state raffinate concentration were found for all three concentration levels of each of the flow systems.

B.3.4.2 Results, Initial Computation of K_Ea'

The results of the calculations outlined in B.3.4.1 are shown in Table 1.

It can be seen that the value of the constant term and therefore the value of the mass transfer coefficient depends not only upon the dispersed phase flow rate and the concentration but also on the continuous phase flow rate. This fact is contrary to the observations of Karr and Scheibel. In addition, it is noted that the predicted and the experimental extract concentrations do not agree when the predicted and experimental raffinate concentrations match. However, calculations show that the mass balance is obeyed by the model, and therefore that the model is algebraically sound.

TABLE 1 : VALUES OF THE CONSTANT TERM AT STEADY STATES

FLOW SYSTEM	FEED CONCENTRATION Wt. percent	CON1	EXPERIMENTAL RAFFINATE CONC. Wt. Percent	PREDICTED RAFFINATE CONC. Wt. Percent	EXPERIMENTAL EXTRACT CONC. Wt. Percent	PREDICTED EXTRACT CONC. Wt. Percent
(1,1)	6	270.6	3.72	3.71895	3.33	3.2454
	12	236.632	6.81	6.80997	6.93	6.76440
	18	160.156	9.68	9.67983	10.57	9.76389
(2,1)	6	321.148	4.40	4.40026	3.72	3.53558
	12	238.161	8.42	8.42000	7.94	7.43406
	18	195.957	11.74	11.7403	12.37	11.4224
(1,2)	6	376.262	2.76	2.76032	2.76	2.65190
	12	309.133	5.15	5.15005	5.68	5.37323
	18	272.263	7.03	7.02999	8.58	8.15094
(2,2)	6	464.835	3.55	3.54969	3.35	3.13411
	12	406.643	6.66	6.65962	7.18	6.70846
	18	393.858	9.07	9.06992	10.68	10.6256

B.3.4.3 Final Form of the Mass Transfer Coefficient

Because the initial form of the mass transfer coefficient used in B.3.4.1 showed behaviour contrary to that observed by Karr and Scheibel, the relationship for the overall mass transfer coefficient was modified. To have as simple a form as possible, the modified relationship was written as

$$K_E a' = \text{(constant)} \left(\frac{da}{dc_E} \times \frac{\Delta\rho}{\sigma}\right)^n \qquad (24)$$

where n is some exponent.

For each of the three concentration levels of system (1,1) and for fixed values of the constant term over a wide range (5.0 to 850.0), the corresponding values of the exponent were obtained such that the steady states predicted and experimental raffinate concentrations matched.

The purpose of these calculations was to find a value of the constant term such that the value of the exponent would be the same at each of the three concentration levels. This would mean that the value of that particular constant and the corresponding exponent value could be used to predict the mass transfer coefficients across the range of concentrations dealt with in the system (1,1). Then, a similar operation could be carried out to determine constants and exponents for the other flow systems.

Similar calculations were carried out for the 6 percent feed level only of flow systems (2,1), (1,2), and (2,2).

B.3.4.4 Results, Final Form of $K_E a'$

The results of the calculations described in B.3.4.3 are given in Table 2, Table 3 and Figure 34.

TABLE 2 : VALUES OF EXPONENTS FOR FIXED CONSTANT TERMS, SYSTEM (1,1)

CON1	FEED 6%		FEED 12%		FEED 18%	
5	0.513870	3.72027	0.515124	6.81094	0.585436	9.67799
10	0.674470	3.72012	0.67818	6.81000	0.751659	9.67903
50	1.04778	3.71993	1.05739	6.81061	1.13708	9.67916
100	1.20818	3.71999	1.22068	6.81093	1.30308	9.68002
150	1.30217	3.71993	1.31575	6.80925	1.40006	9.68000
270.6	1.43795	3.71005	1.45479	6.80978	1.54119	9.67994
400	1.52956	3.71973	1.54688	6.81013	1.63466	9.67974
550	1.60298	3.71931	1.62157	6.80887	1.71028	9.67582
700	1.66038	3.72221	1.67649	6.80092	1.76784	9.67511
850	1.70379	3.71909	1.72426	6.80980	1.81482	9.67969

NOTE : The second column under each feed concentration in the steady state raffinate concentration predicted by the accompanying exponent value and the corresponding value of CON1.

TABLE 3 : CALCULATED CON1 FOR SIX PERCENT FEED CONCENTRATION

FLOW SYSTEM	EXPONENT VALUES							
	0.513870	0.67447	1.04778	1.30213	1.52939	1.60298	1.66038	1.70379
1,2		13.5239	68.2710	204.706	545.833	751.721		1158.76
2,1	6.07293		60.2018	178.723	479.077	658.721	845.656	985.935
2,2			85.8185		685.626	942.301		

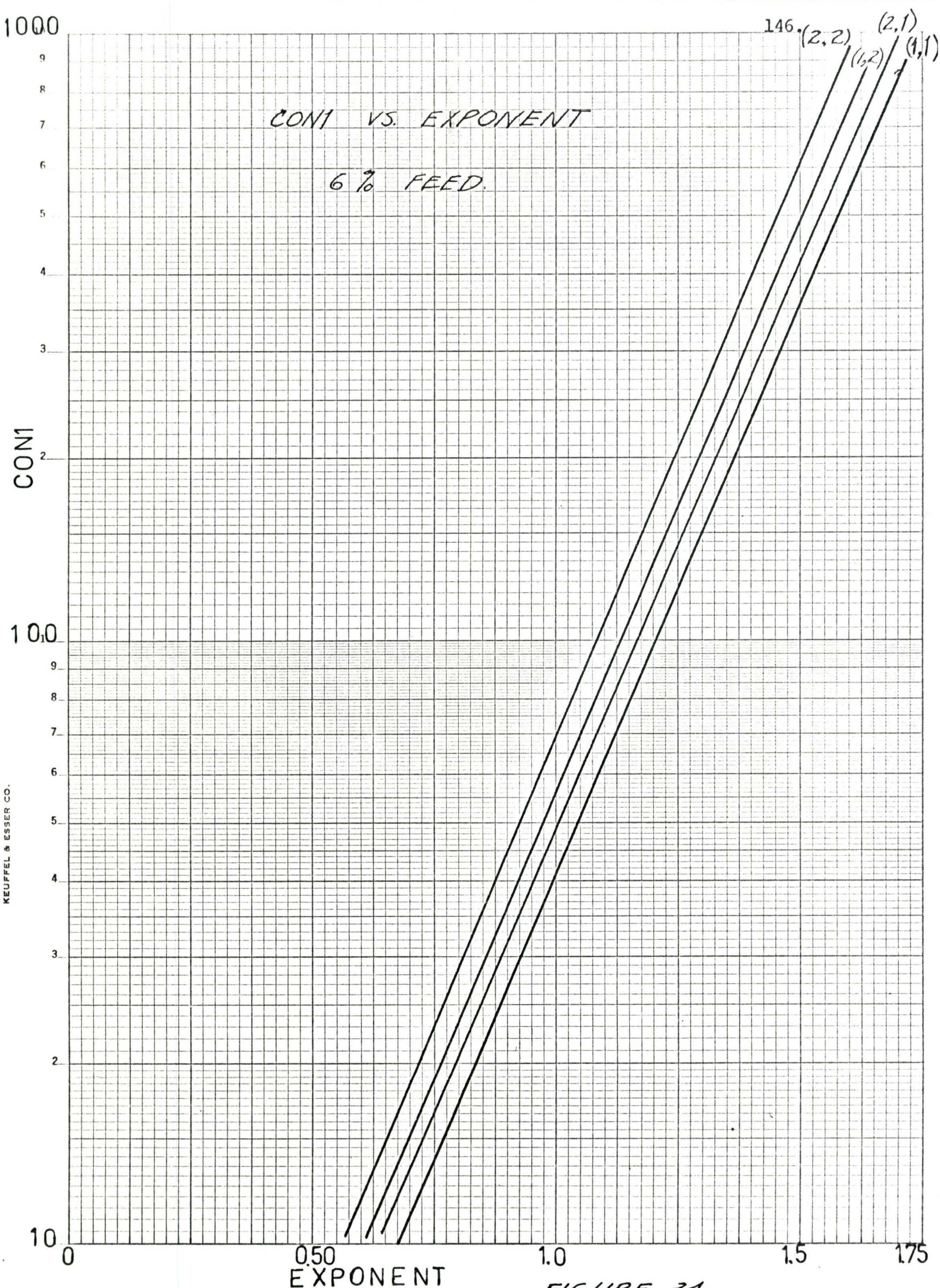

CON1 VS. EXPONENT
6 % FEED
(2,2)
(1,2)
(2,1)
(1,1)
CON1
1000
100
10
9
8
7
6
5
4
3
2
EXPONENT
0
0.50
1.0
1.5
1.75

FIGURE 34

It is evident that no value of the constant term CON1 in the range 5.0 to 50.0 will provide a non-varying exponent over the three levels of concentration.

Again, it is obvious that the dispersed (organic) phase flow rate, the concentration and the continuous phase flow rates all affect the value of the exponent and therefore the value of the mass transfer coefficient.

B.3.5 Transient Studies

Step changes of feed concentration from six weight percent to twelve or eighteen weight percent produced transient responses.

Using the six percent feed steady state values of the flows, concentration profiles and holdups, at least two runs were completed for each transient with large and small values of the constant term and the corresponding exponent found at the six percent feed concentration level.

It should be noted that this technique uses parameters which can be found at the original steady state level only, and does not assume any knowledge of the transient or of the final steady state conditions. On the other hand, Pollock's transient model uses a mass transfer coefficient which is obtained by fitting the model response to the experimental response in the frequency domain, and hence assumes knowledge of the transient.

In this study, integration of the differential equations is carried out for twenty experimental minutes using a step size of 1.0 second, and the departures of the raffinate and extract concentrations from the six percent steady state values were recorded as a function of time. Printouts of thirty second intervals gave the concentration profiles, the deviations of raffinate and extract phase concentrations from steady state and the mass transfer coefficients for each stage.

B.3.6 Results, Transient Studies

Experimental and theoretical transient responses for all four flow systems are shown in Figures 35 to 50. For comparison, plots of the transients calculated using Pollock's transient mass transfer coefficients and the six percent steady state coefficients are also shown. Information found in these figures leads to several conclusions about the transient response study undertaken. In almost every system, the following information may be noted:

1. The raffinate concentration curve is fitted best using the transient raffinate mass transfer coefficient calculated by Pollock.
2. The extract concentration curve is fitted best by the six percent steady state raffinate mass transfer coefficient.
3. The raffinate curve is fitted better using a high value of CON1 and the corresponding exponent. On the other hand, the extract concentration curve is fitted better using a low value of CON1 and the corresponding exponent.
4. The worst fit of the extract concentration curve occurs when the transient raffinate mass transfer coefficient is used.
5. In addition, the present model with the concentration-dependent mass transfer coefficient is still predicting too much mass transfer.

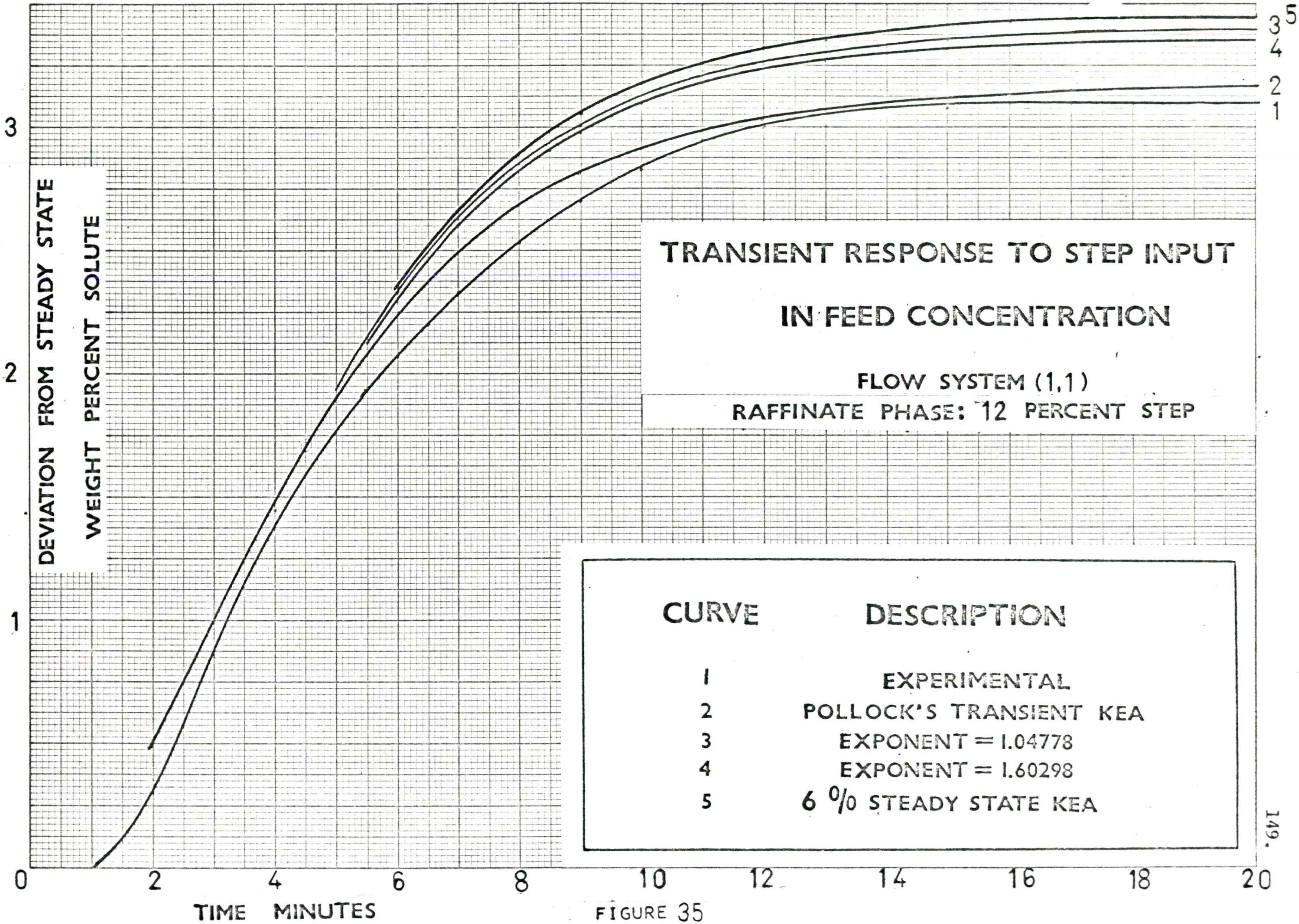
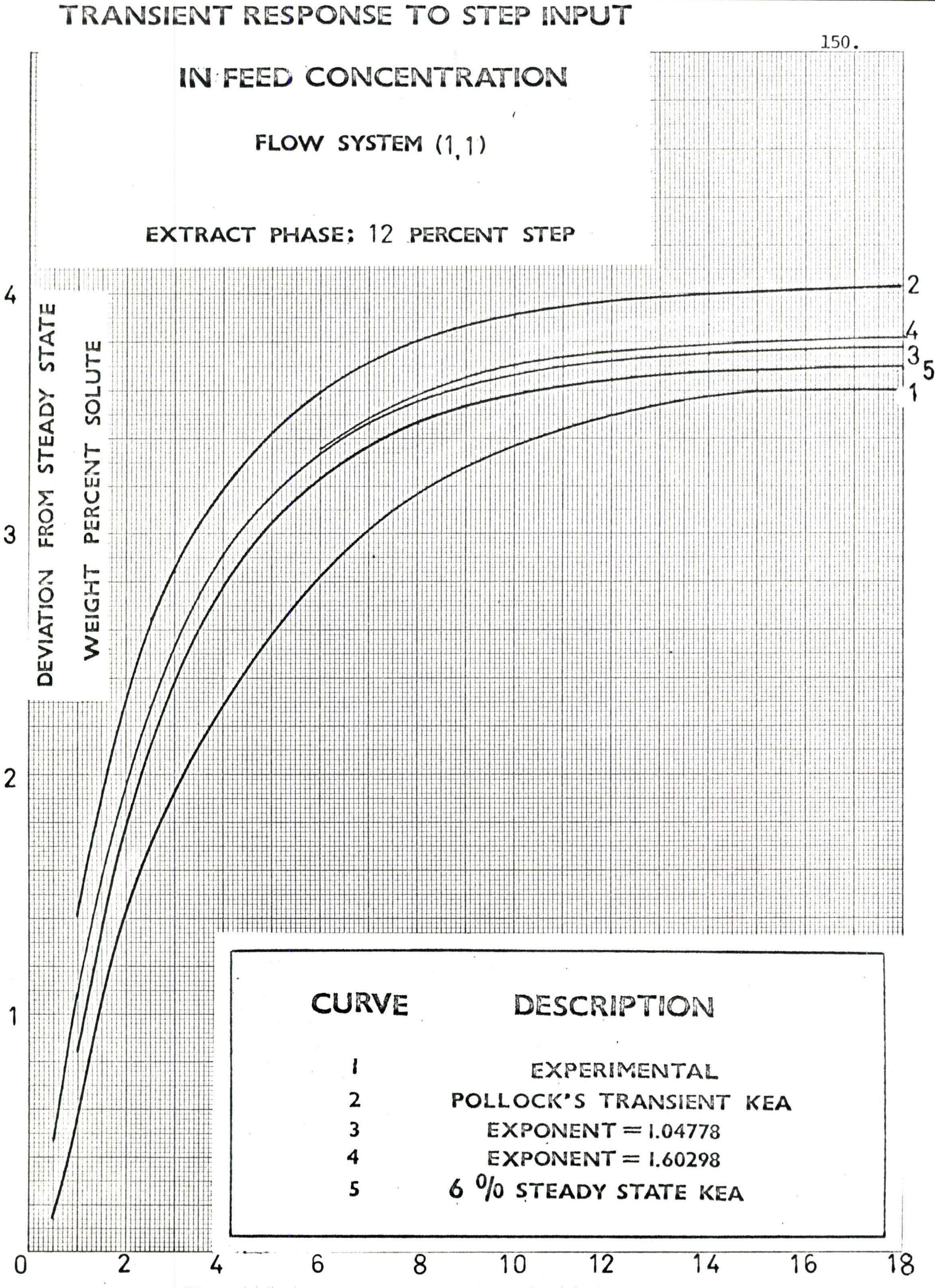

TRANSIENT RESPONSE TO STEP INPUT
IN FEED CONCENTRATION
FLOW SYSTEM (1,1)
RAFFINATE PHASE: 12 PERCENT STEP
DEVIATION FROM STEADY STATE
WEIGHT PERCENT SOLUTE
TIME MINUTES
0
1
2
3
0
2
4
6
8
10
12
14
16
18
20
5
3
4
2
1
CURVE
DESCRIPTION
1
EXPERIMENTAL
2
POLLOCK'S TRANSIENT KEA
3
EXPONENT = 1.04778
4
EXPONENT = 1.60298
5
6 % STEADY STATE KEA

FIGURE 35



TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION

FLOW SYSTEM (1,1)

EXTRACT PHASE: 12 PERCENT STEP

FIGURE 36

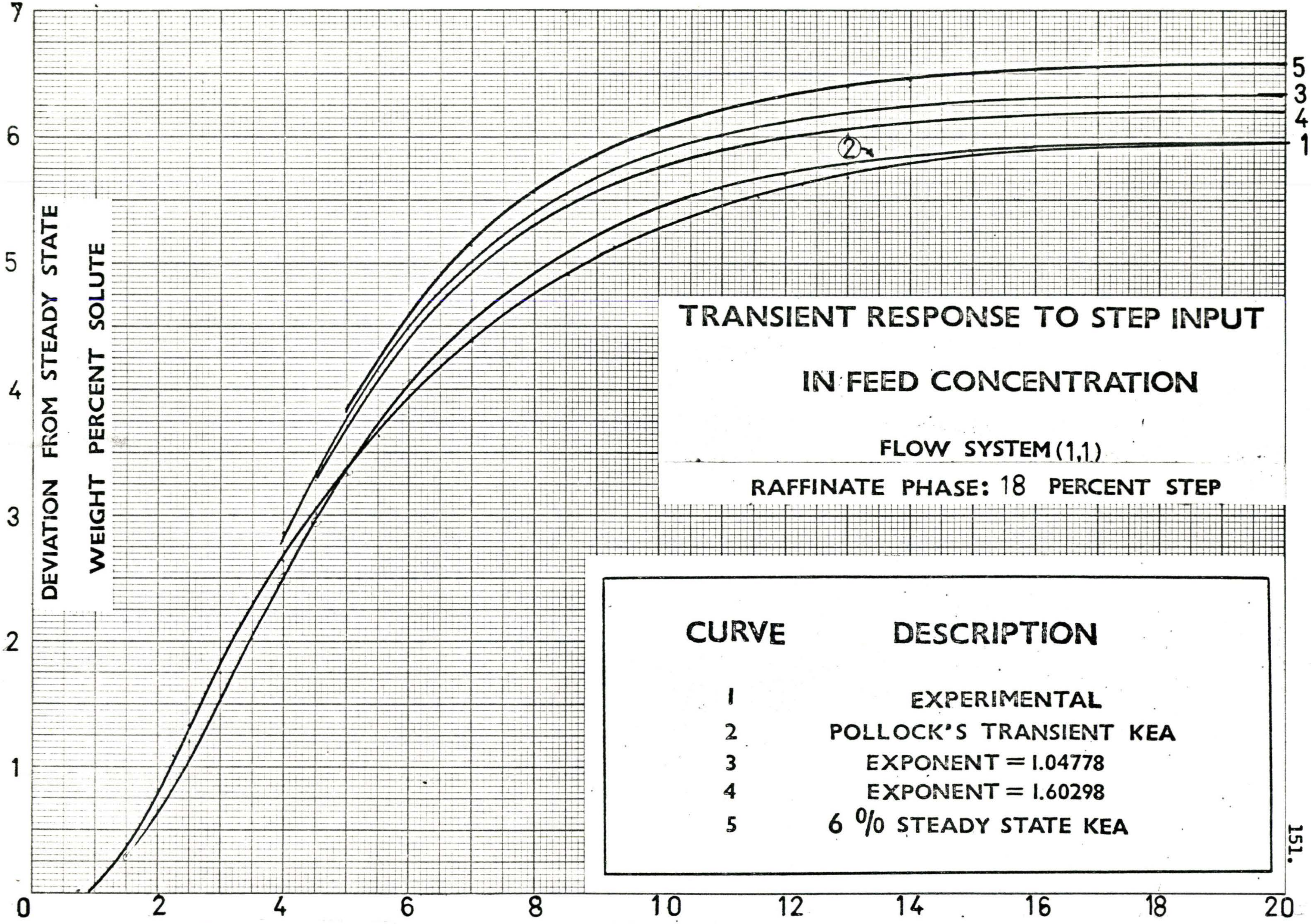

TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION
FLOW SYSTEM (1,1)
RAFFINATE PHASE: 18 PERCENT STEP
CURVE
DESCRIPTION
1 EXPERIMENTAL
2 POLLOCK'S TRANSIENT KEA
3 EXPONENT = 1.04778
4 EXPONENT = 1.60298
5 6 % STEADY STATE KEA
DEVIATION FROM STEADY STATE
WEIGHT PERCENT SOLUTE
TIME MINUTES
0
1
2
3
4
5
6
7
0
2
4
6
8
10
12
14
16
18
20
5
3
4
1
2

FIGURE 37

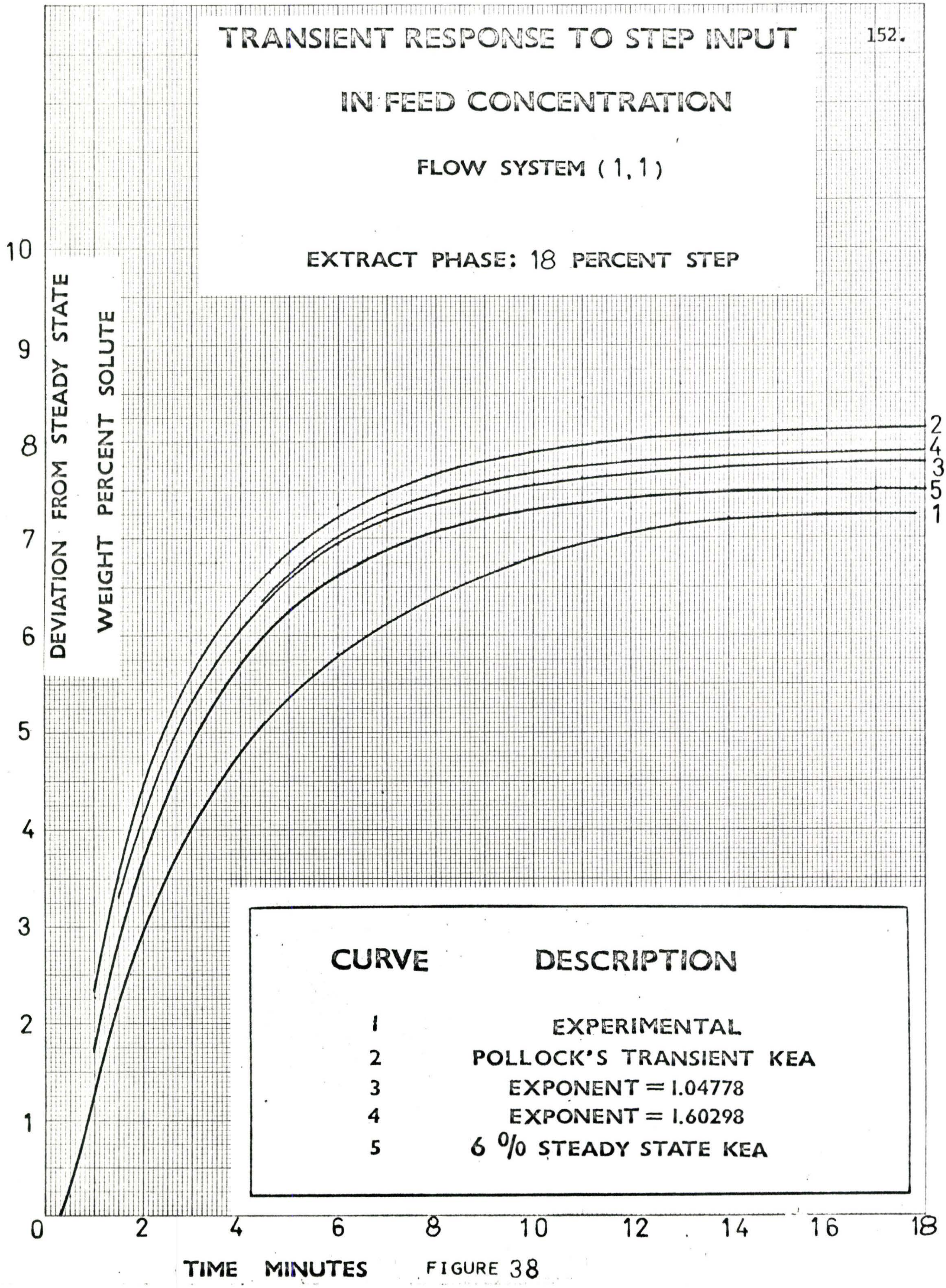
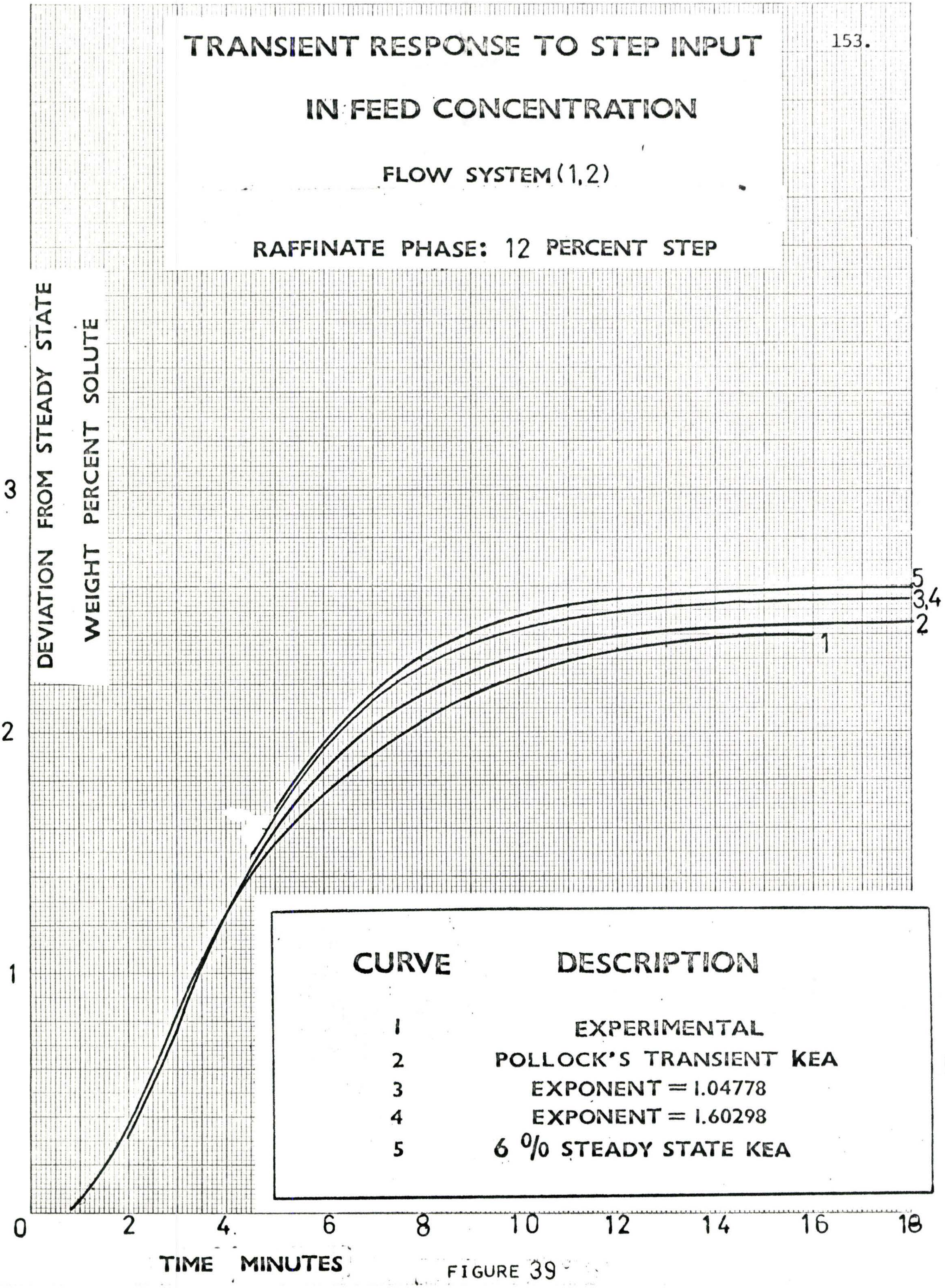

TRANSIENT RESPONSE TO STEP INPUT
IN FEED CONCENTRATION
FLOW SYSTEM (1,1)
EXTRACT PHASE: 18 PERCENT STEP
DEVIATION FROM STEADY STATE
WEIGHT PERCENT SOLUTE
10
9
8
7
6
5
4
3
2
1
0
2
4
6
8
10
12
14
16
18
TIME MINUTES
2
4
3
5
1
CURVE
DESCRIPTION
1 EXPERIMENTAL
2 POLLOCK'S TRANSIENT KEA
3 EXPONENT = 1.04778
4 EXPONENT = 1.60298
5 6 % STEADY STATE KEA

FIGURE 38


TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION

FLOW SYSTEM (1,2)

RAFFINATE PHASE: 12 PERCENT STEP

FIGURE 39

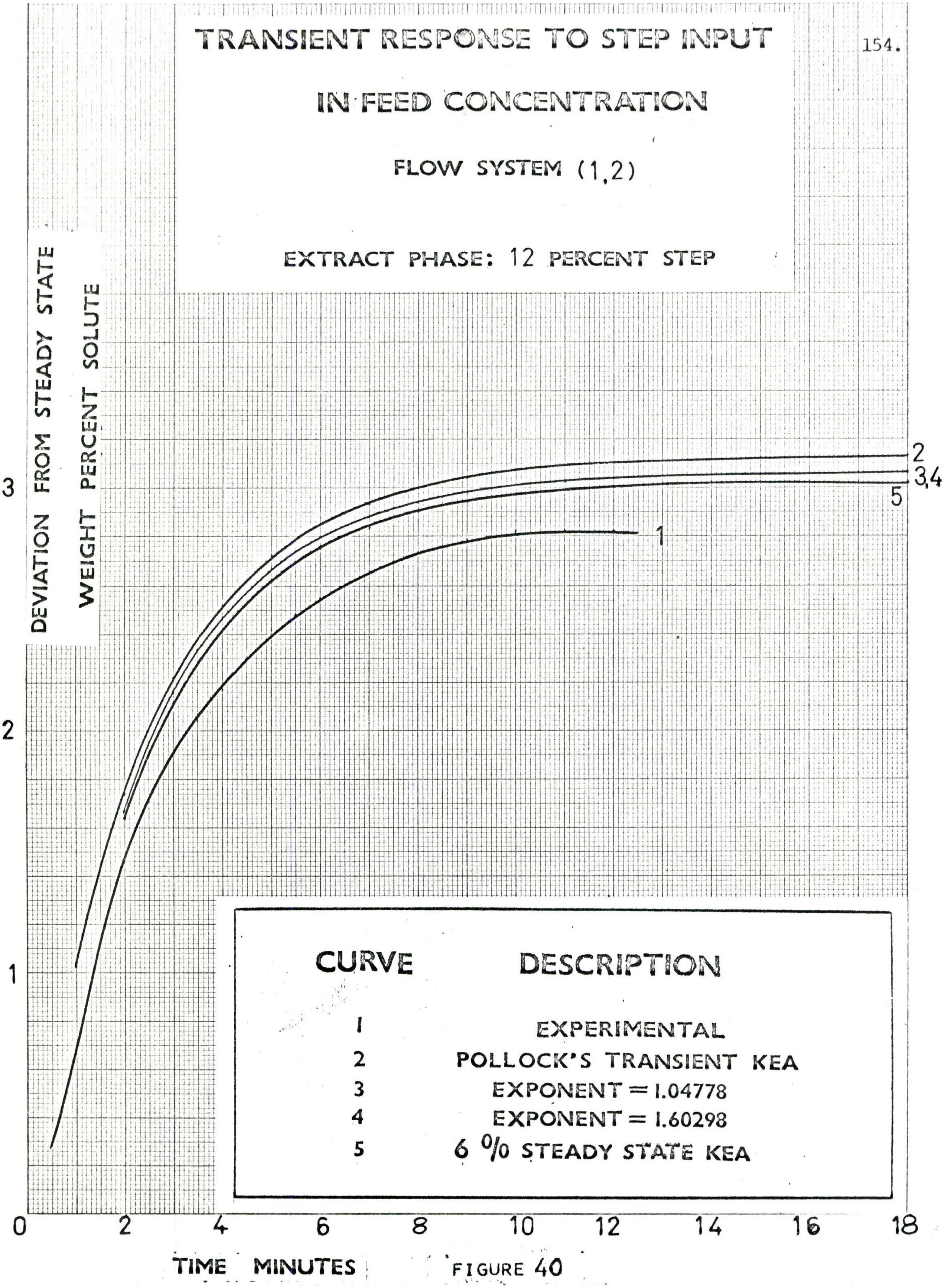

TRANSIENT RESPONSE TO STEP INPUT
IN FEED CONCENTRATION
FLOW SYSTEM (1,2)
EXTRACT PHASE: 12 PERCENT STEP
DEVIATION FROM STEADY STATE
WEIGHT PERCENT SOLUTE
1
2
3
0
2
4
6
8
10
12
14
16
18
TIME MINUTES
1
2
3,4
5
CURVE
DESCRIPTION
1 EXPERIMENTAL
2 POLLOCK'S TRANSIENT KEA
3 EXPONENT = 1.04778
4 EXPONENT = 1.60298
5 6 % STEADY STATE KEA

FIGURE 40

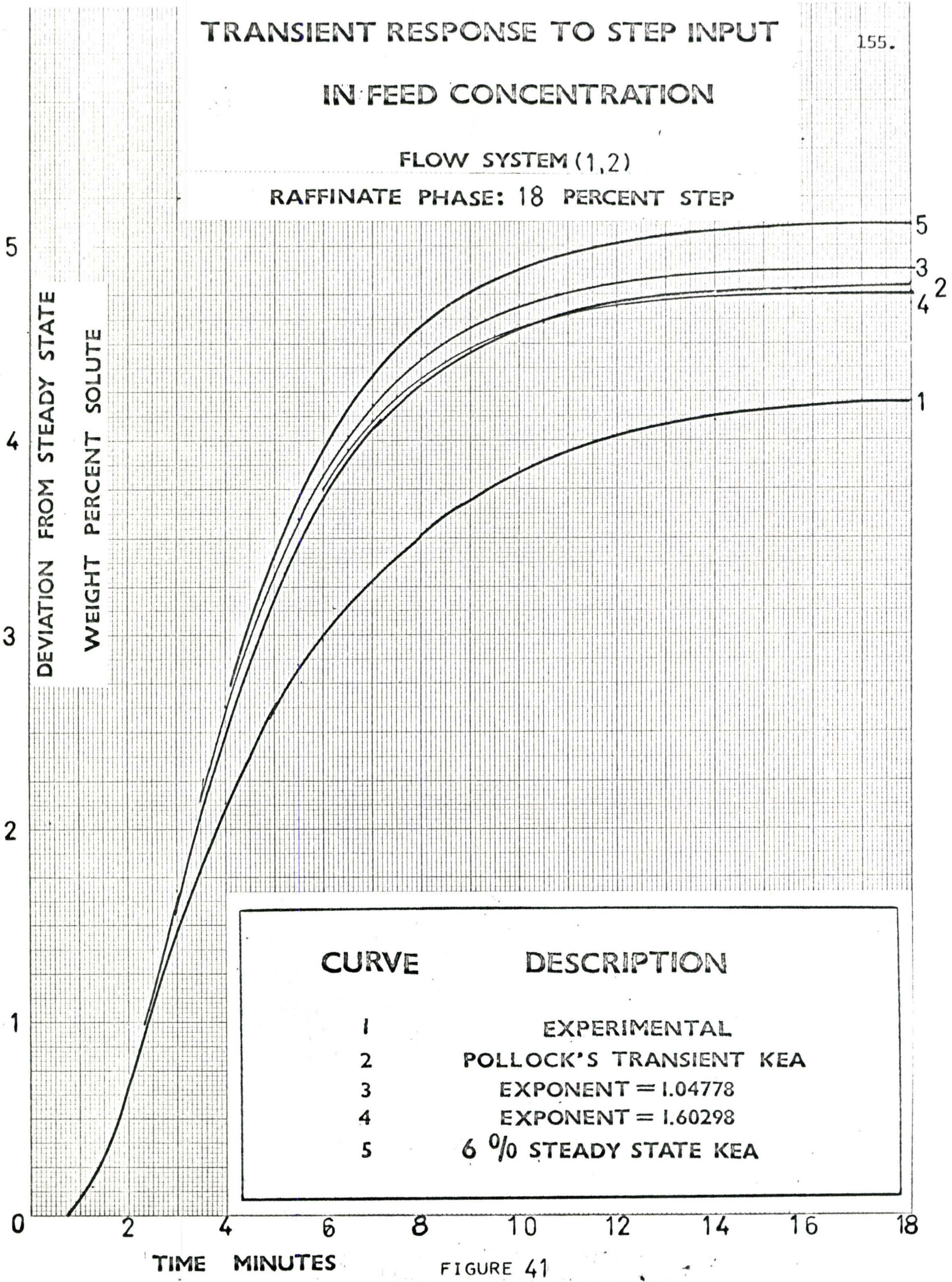
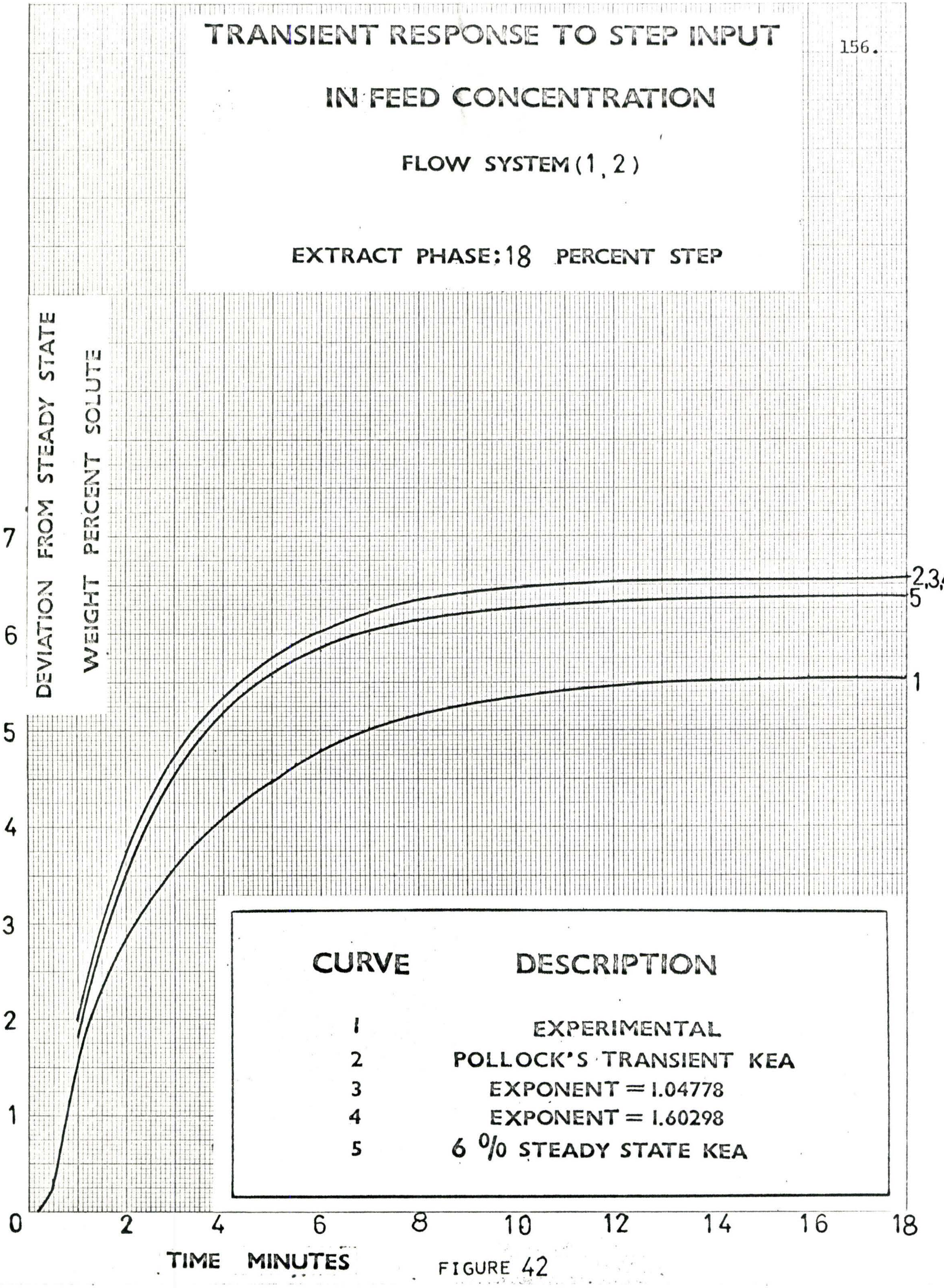

TRANSIENT RESPONSE TO STEP INPUT
IN FEED CONCENTRATION
FLOW SYSTEM (1,2)
RAFFINATE PHASE: 18 PERCENT STEP
DEVIATION FROM STEADY STATE
WEIGHT PERCENT SOLUTE
0
1
2
3
4
5
0
2
4
6
8
10
12
14
16
18
TIME MINUTES
5
3
2
4
1
CURVE
DESCRIPTION
1 EXPERIMENTAL
2 POLLOCK'S TRANSIENT KEA
3 EXPONENT = 1.04778
4 EXPONENT = 1.60298
5 6 % STEADY STATE KEA

FIGURE 41



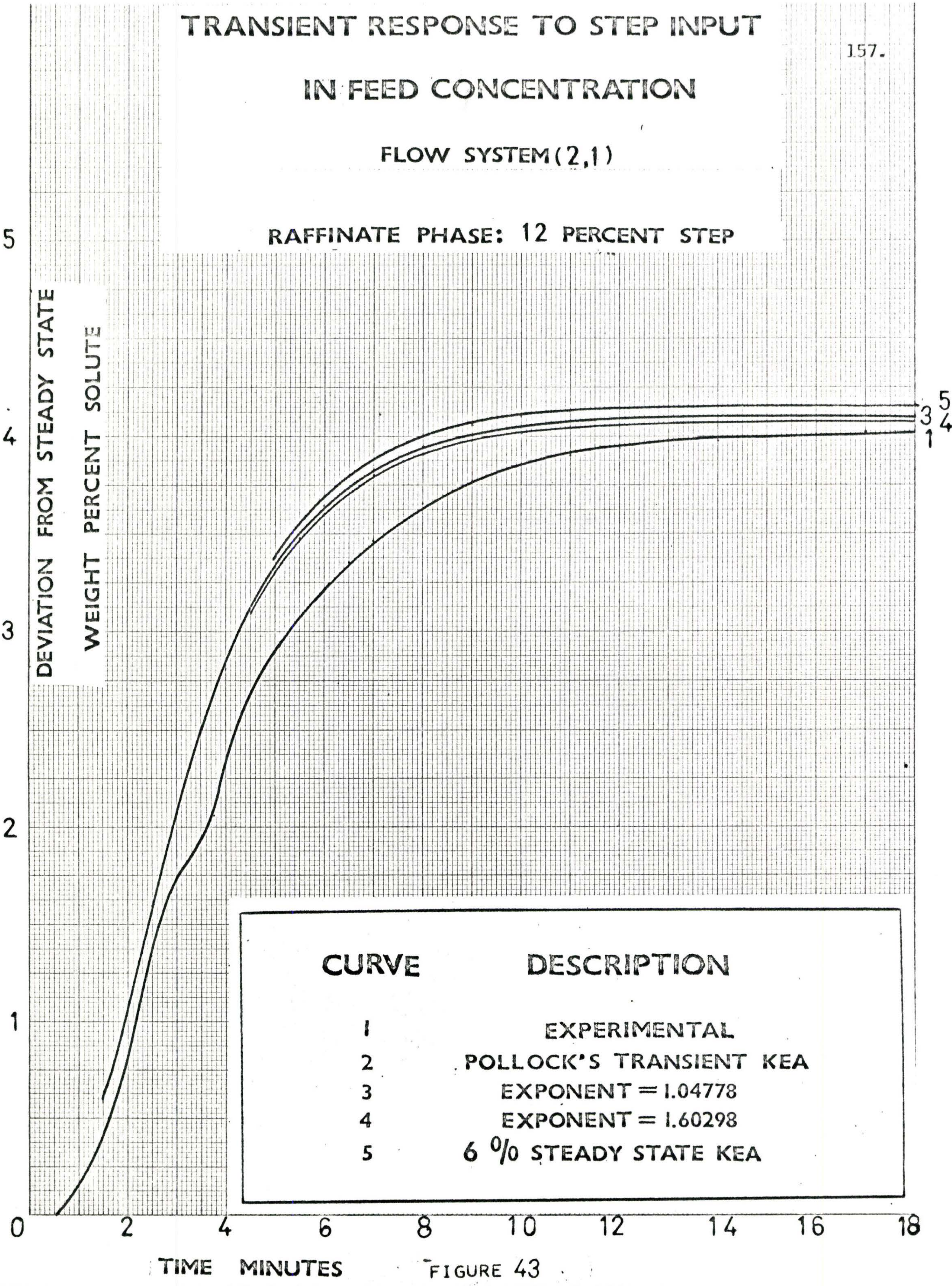
TRANSIENT RESPONSE TO STEP INPUT

IN FEED CONCENTRATION

FLOW SYSTEM (1, 2)

EXTRACT PHASE: 18 PERCENT STEP

FIGURE 42



TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION

FLOW SYSTEM (2,1)

RAFFINATE PHASE: 12 PERCENT STEP

FIGURE 43

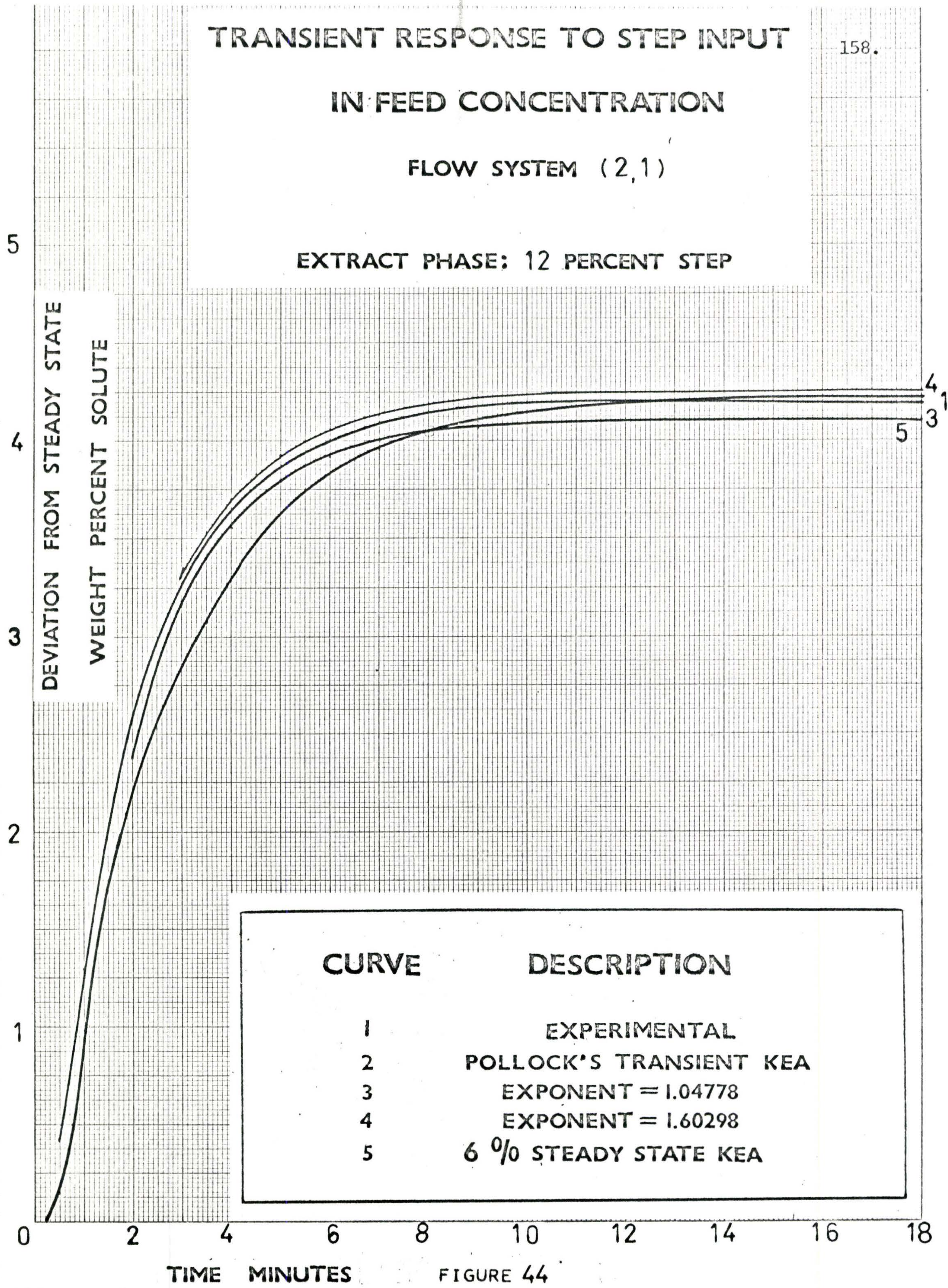
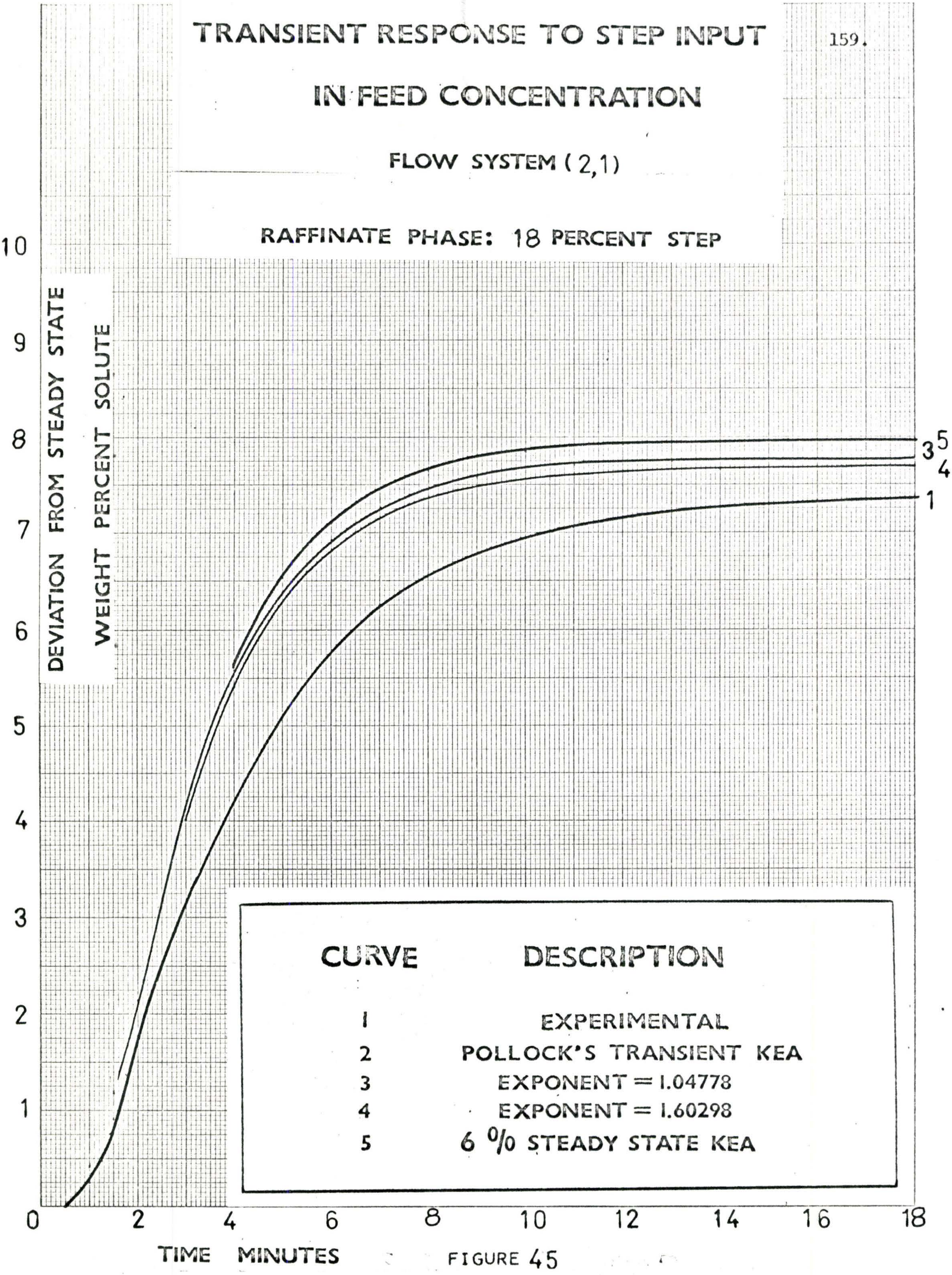

TRANSIENT RESPONSE TO STEP INPUT
IN FEED CONCENTRATION
FLOW SYSTEM (2,1)
EXTRACT PHASE: 12 PERCENT STEP
DEVIATION FROM STEADY STATE
WEIGHT PERCENT SOLUTE
0
1
2
3
4
5
2
4
6
8
10
12
14
16
18
TIME MINUTES
4
1
3
5
CURVE
DESCRIPTION
1 EXPERIMENTAL
2 POLLOCK'S TRANSIENT KEA
3 EXPONENT = 1.04778
4 EXPONENT = 1.60298
5 6 % STEADY STATE KEA

FIGURE 44

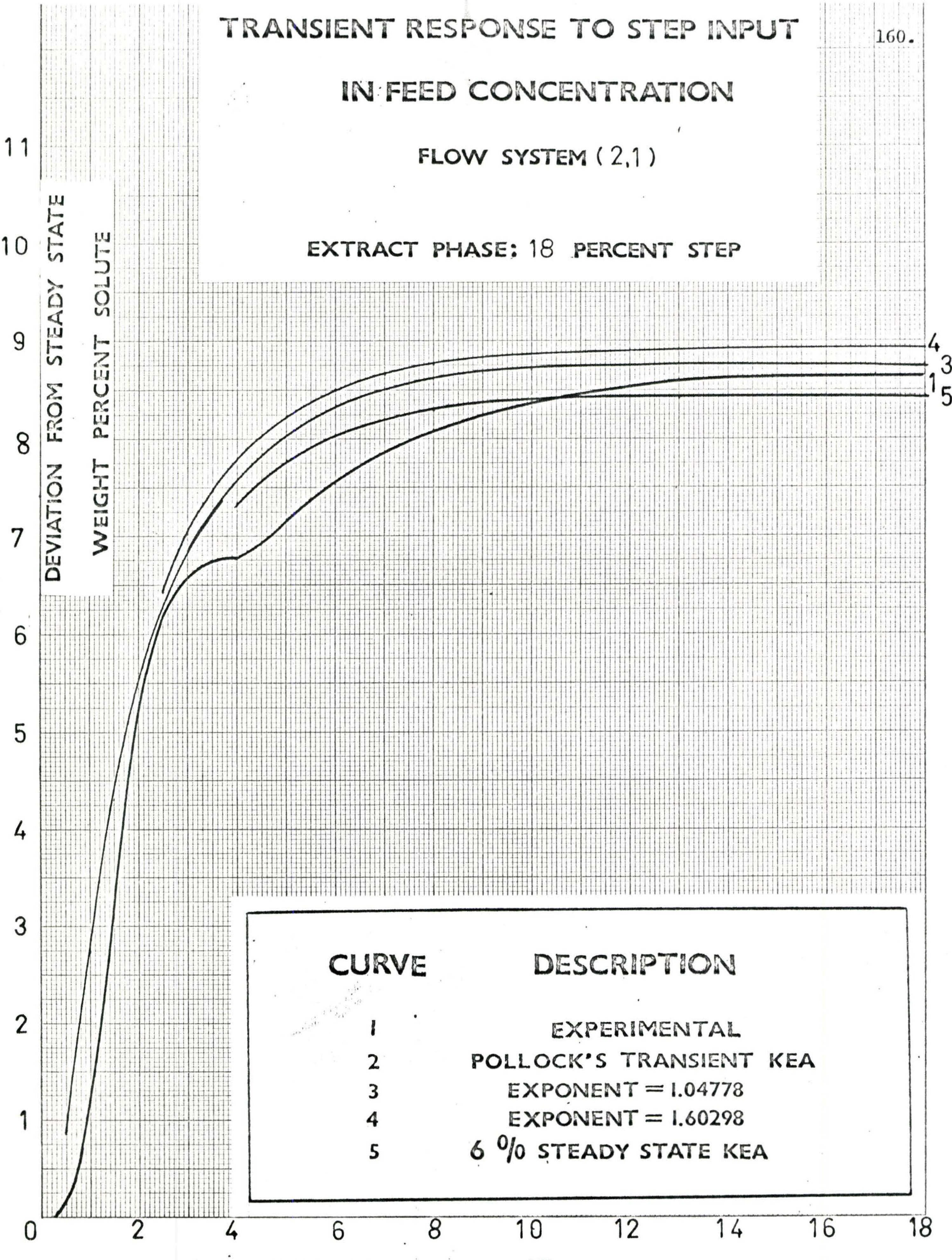


TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION

FLOW SYSTEM (2,1)

RAFFINATE PHASE: 18 PERCENT STEP

FIGURE 45



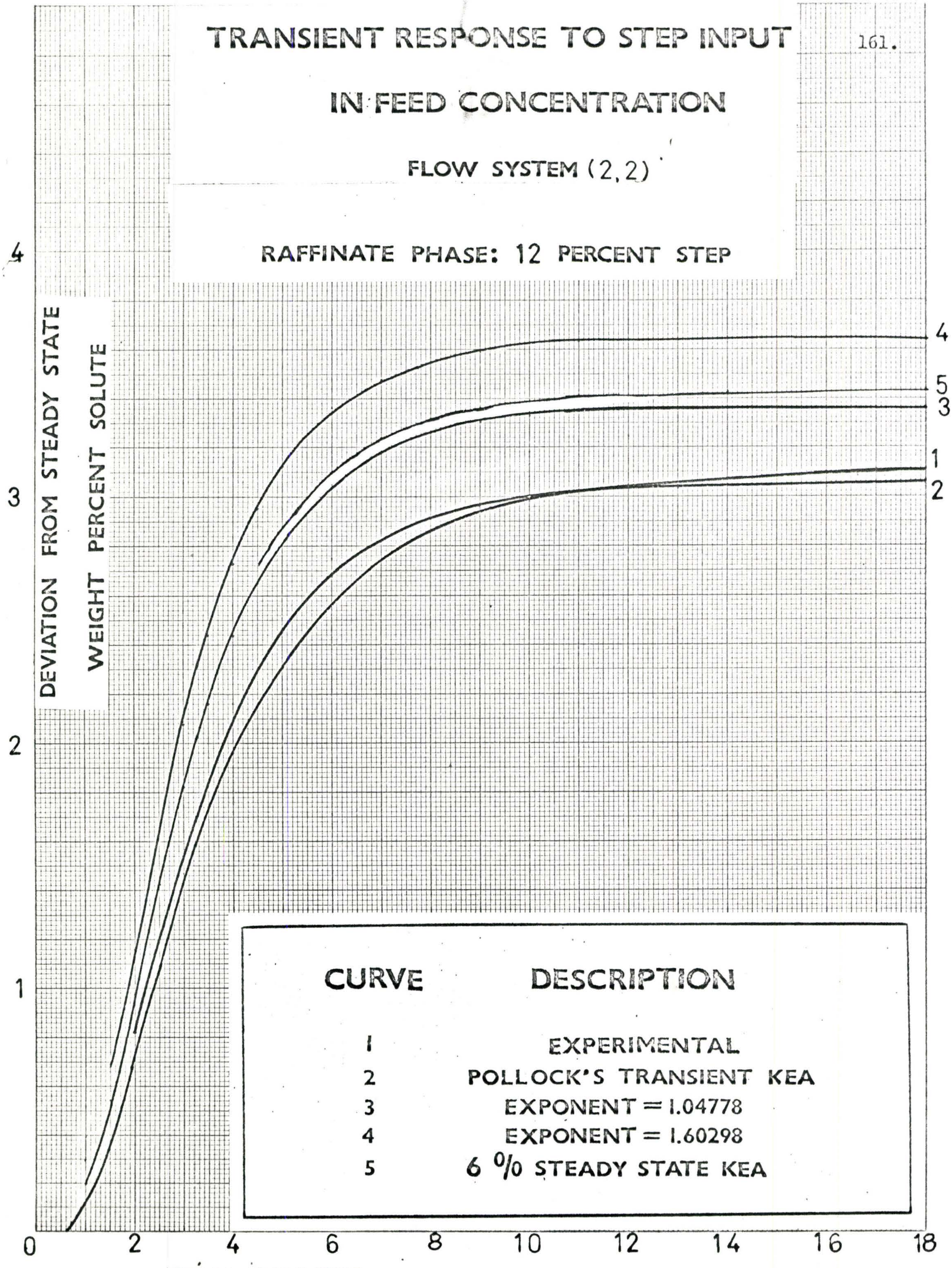
TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION

FLOW SYSTEM (2,1)

EXTRACT PHASE: 18 PERCENT STEP

CURVE	DESCRIPTION
1	EXPERIMENTAL
2	POLLOCK'S TRANSIENT KEA
3	EXPONENT = 1.04778
4	EXPONENT = 1.60298
5	6 % STEADY STATE KEA

FIGURE 46



TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION

FLOW SYSTEM (2,2)

RAFFINATE PHASE: 12 PERCENT STEP

FIGURE 47

TRANSIENT RESPONSE TO STEP INPUT

IN FEED CONCENTRATION

FLOW SYSTEM (2,2)

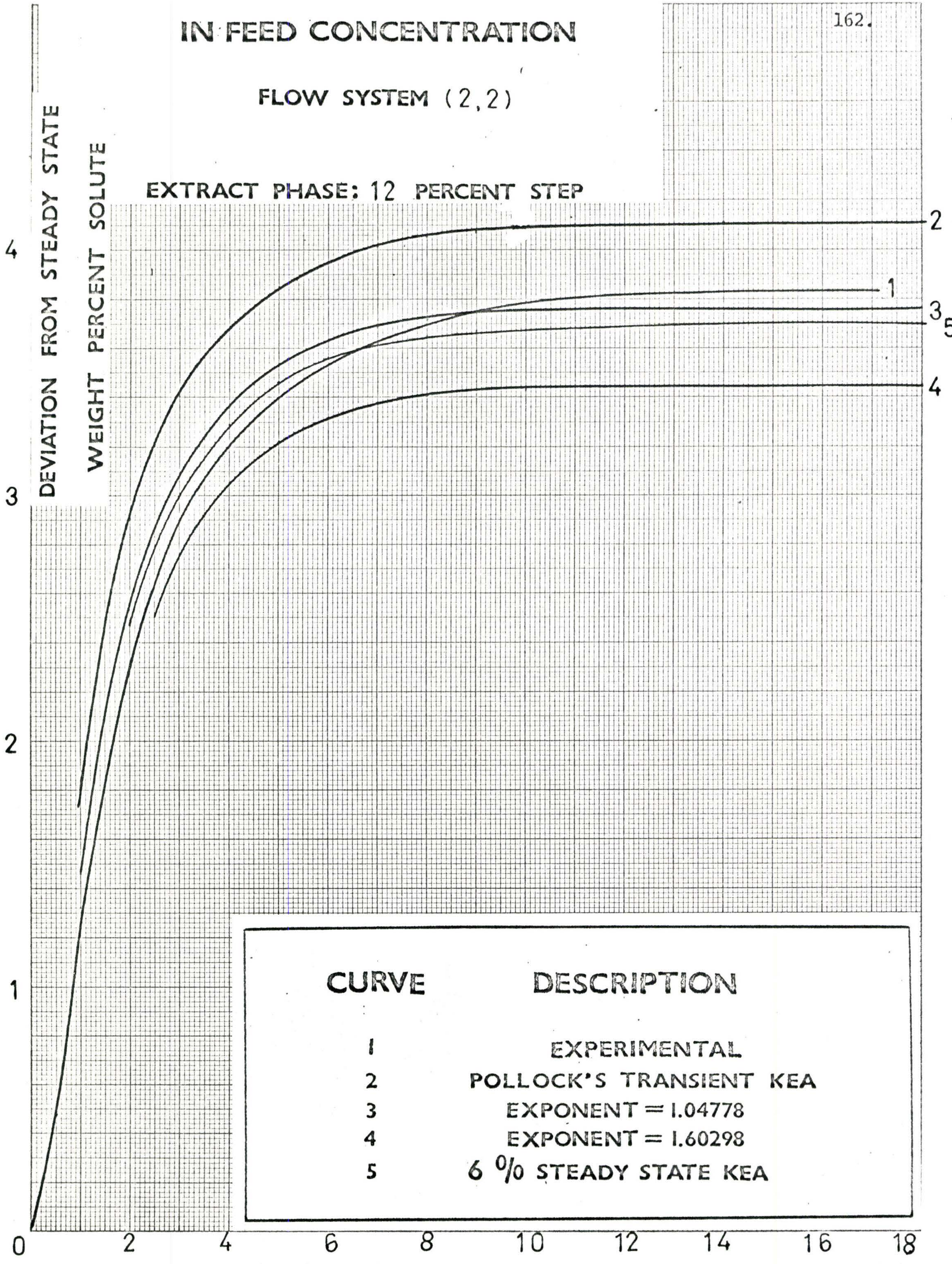


FIGURE 48

TRANSIENT RESPONSE TO STEP INPUT IN FEED CONCENTRATION

FLOW SYSTEM (2,2)

RAFFINATE PHASE: 18 PERCENT STEP

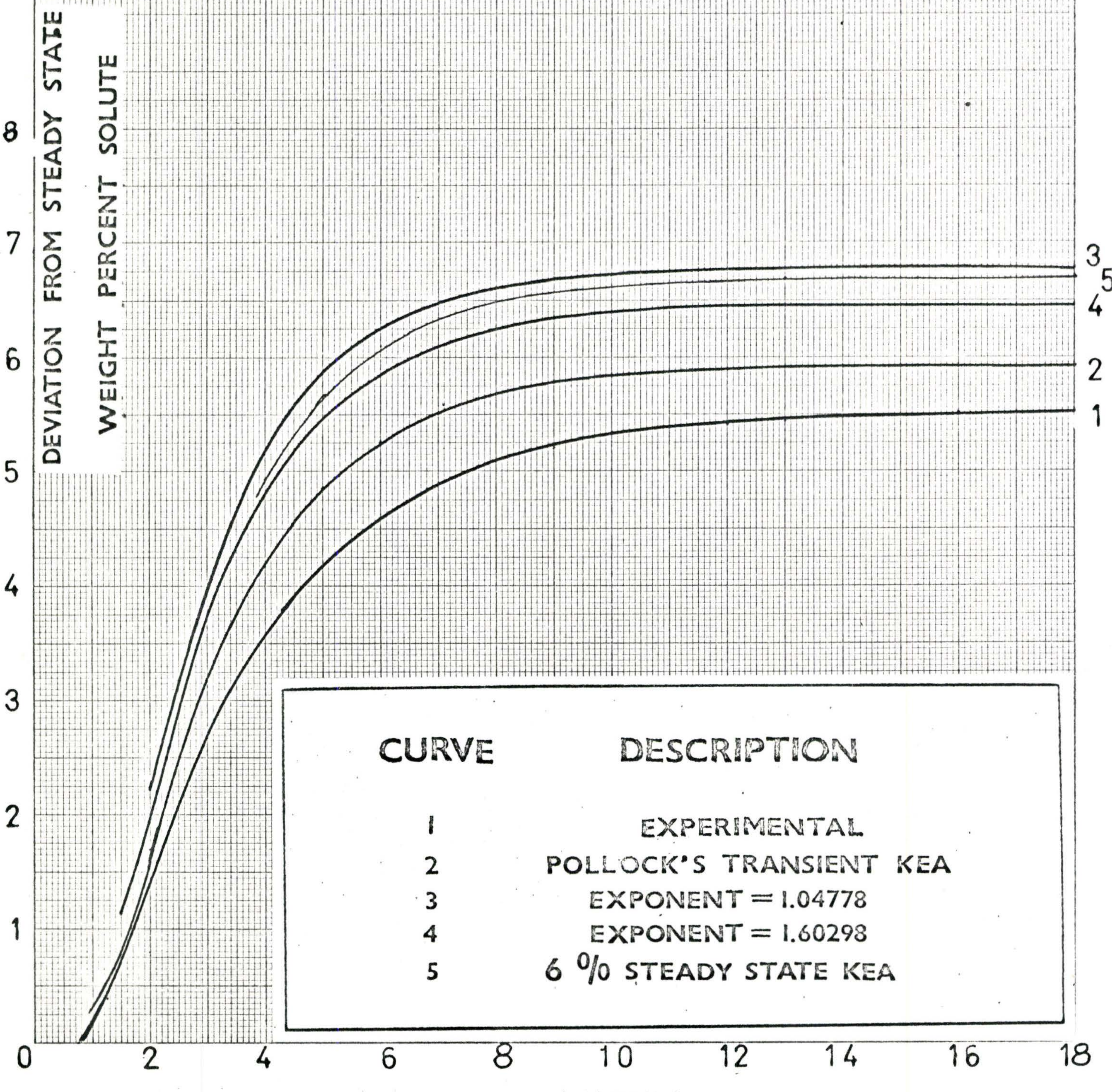


FIGURE 49

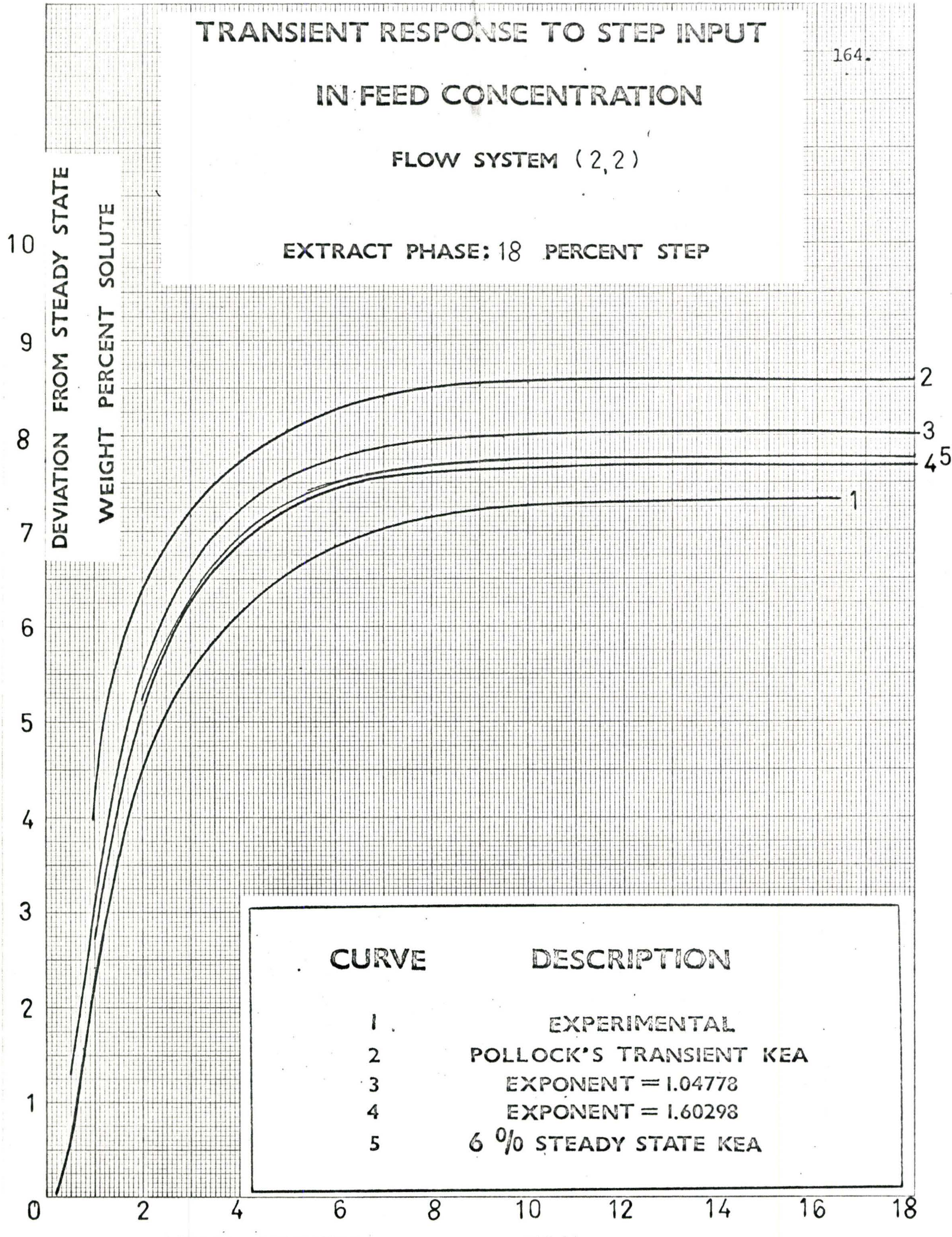

TRANSIENT RESPONSE TO STEP INPUT
IN FEED CONCENTRATION
FLOW SYSTEM (2,2)
EXTRACT PHASE: 18 PERCENT STEP
DEVIATION FROM STEADY STATE
WEIGHT PERCENT SOLUTE
0
1
2
3
4
5
6
7
8
9
10
2
4
6
8
10
12
14
16
18
TIME MINUTES
2
3
4
5
1
CURVE
DESCRIPTION
1 . EXPERIMENTAL
2 POLLOCK'S TRANSIENT KEA
3 EXPONENT = 1.04778
4 EXPONENT = 1.60298
5 6 % STEADY STATE KEA

FIGURE 50

B.4 RECOMMENDATIONS AND CONCLUSIONS

From results obtained in the study, the conclusions were made that the Karr-Scheibel relationship is not valid for this system and that the modified relationship is also not valid.

There are several factors which help to explain why this may be so. Karr and Scheibel's stage is not dimensionally similar to the stages used by Pollock, and stage shape would have a large effect on the mixing patterns in the stage. In addition, Karr and Scheibel's stage was specially constructed so that the heavy phase entering a mixing section does not countercurrently contact the light phase leaving the section, and the heavy phase leaving a mixing section does not contact the light phase entering the section. Thus, the operation of the two columns is under somewhat different sets of conditions. It may be postulated too that, although precautions were taken by both Karr and Scheibel and Pollock to avoid contamination of their feed streams, some surfactant may be present in either of the experiments in sufficient quantity to markedly influence experimental results.

Nevertheless, Karr and Scheibel's relationship did provide a starting point for varying the mass transfer coefficient as a function of concentration, and it is thought that a more successful model could be found if more work were given in an extension of this study. In particular, if future work is undertaken on this project, the following areas of study are suggested:

1. The mass transfer coefficient should be expressed in the form

$$K_E a' = (\text{constant})\ \Delta\rho^{n1}\ \sigma^{n2}\ \mu_o^{n3}\ \rho_o^{n4}$$

where n1, n2, n3 and n4 are exponents. The interfacial tension term is the major parameter influencing the drop size and its effect will be much greater than the effect of the density difference.

For example, from 0 - 19.3 weight percent solute in the aqueous phase, the density difference changes by about 15 percent. However, from 0. - 18.4 weight percent solute in the aqueous phase, the interfacial tension changes about 58 percent. In addition, it is thought that the effect that the density and viscosity of the continuous phase would have on the mixing within the cell should be taken into account. Other parameters which would influence the mixing within a stage are the measurements of the cell, the agitator measurements and speed, and the stream flow rates. However, these parameters have been collected into the constant term for this analysis.

If an equation of this form is used for the mass transfer coefficient, some type of search routine in FORTRAN will have to be used to calculate the variables (constant), n1, n2, n3, and n4 for a given steady state condition. Calculation of these variables using MIMIC would be extremely difficult, if not impossible.

2. Study should be given to methods which would provide accurate sampling of the concentration profiles along the column. Knowledge of these profiles at the steady states would be useful in evaluating a proposed model, because the profiles predicted by the model and the actual experimental profiles at the steady states should agree.

   At the present time, only the predicted outlet concentrations can be compared to the experimental outlet concentrations, and nothing is known about the comparison of the predicted and experimental profiles. Any realistic model should be able to predict the steady state profiles as well as the outlet concentrations.

3. From mass relationships, it is possible to calculate the final solute-free raffinate flow resulting from a step change in feed concentration. Then, it may be possible to determine a scheme to vary the raffinate flow from the initial flow to the final flow as a function of concentration. Or, it may be desirable to immediately define the raffinate flow as the final steady state flow all through the column. Changes of raffinate flow may be as large as 14.5 percent, and the ability to account for a changing raffinate flow would make the model more physically realistic.

   However, it is thought that changes in extract flow and phase holdups could not be predicted. Experimentally, extract flow changes are small, about 3.5 percent at the most, and holdup changes appear to be random.

4. In the present program, data obtained under equilibrium conditions are used in the relations for $\Delta\rho$, σ and $\frac{da}{dc_E}$. However, the two phases in each cell are probably not at equilibrium. Karr and Scheibel noted that most of their data indicated a 65 percent or higher approach to equilibrium and they used the average of the interfacial tensions based on the concentrations in the two phases. The present programs use a relationship based only on the concentration in the extract phase. Then, to obtain values for the surface tension which may be more realistic, another relationship based on the concentration in the aqueous phase is required. This can be obtained from the data of Karr and Scheibel. Then, the average of the surface tension found by each relationship could be found.

In conclusion, it may be said that a model has been tested in which the mass transfer coefficient varies as a function of concentration. However, it is thought that the correlation presented for the mass transfer coefficient is not suitable, and a new form of the mass transfer coefficient is presented for consideration in future work.

B.5 NOMENCLATURE

A	the total interfacial area
a	activity
a'	the interfacial area per unit volume
C	concentration of solute in a phase
CON1	a "variable constant" formed by combining the effects of impeller speed, impeller size, and the extract flow rate in equation (4).
D	diameter of the impeller
$\mathcal{D}$	diffusion coefficient.
FR	the flow rate of the raffinate phase, weight of solute-free phase per unit time.
HE	the weight of the solute-free phase in the extract separation cell at the top of the column.
HR	the weight of the solute-free phase in the raffinate separation cell at the bottom of the column.
J	the turbulent flux of a component due to the presence of eddies
K	the overall mass transfer coefficient based on activities.
K_E	the overall mass transfer coefficient based on the concentration of solute in the extract phase.
k	a single phase mass transfer coefficient
N	the impeller speed; the flux of a component referred to a stationary point.
NTU	the number of transfer units
r	the ratio of molecular weights of nonsolute to solute
S	the extract phase flow rate, weight of solute-free phase per unit time.

V	the volume of a stage.
WR	the weight of solute-free raffinate holdup per stage
WE	the weight of solute-free extract holdup per stage
x	the concentration of solute in the raffinate phase, weight of solute per unit weight of solute-free phase.
XRSS	the 6 percent feed steady state outlet raffinate concentration, weight percent solute.
y	the concentration of solute in the extract phase, weight of solute per unit weight of solute-free phase.
YESS	the 6 percent steady state outlet extract concentration, weight percent solute.

GREEK LETTERS

ε	the eddy diffusivity
$\Delta\rho$	the density difference between raffinate and extract phases
σ	the surface tension between phases

SUBSCRIPTS

A	of component A
aR	based on activity difference in the raffinate phase.
aE	based on activity difference in the extract phase
E	in the extract phase
i	at the interface
O	overall
R	in the raffinate phase
T	Total.

B.6 BIBLIOGRAPHY

B.6.1 Biery, J.C., and D.R. Boylan,
"Dynamic Simulation of a Liquid-Liquid Extraction Column",
I. and E.C. Fundamentals, 2, No.1, page 44, February 1963.

B.6.2 Pollock, G.G.,
"Simulation of a Mixer-Settler Liquid Extraction Column",
M.Eng. Thesis, McMaster University, January 1964.

B.6.3 Pollock, G.G.,
"Simulation and Dynamic Response of a Liquid-Liquid Extraction Process",
Ph.D. Thesis, McMaster University, October 1967.

B.6.4 Karr, A.E., and E.G. Scheibel,
"Mass Transfer Between Immiscible Liquids in Continuous Flow in an Agitated Chamger",
C.E.P. Symposium Series, 10, 73 (1964).

B.6.5 Treybal, R.E.,
Liquid Extraction,
McGraw-Hill, 1963, page 169

B.6.6 Foster, H.R. Jr., and A.L. Babb, private communication.

B.7 APPENDICES

B.7.1 Computation Time

Since at the present time no "object deck" is available in MIMIC, and therefore recompilation of a program must be made if the program is rerun, computation time for the programs used in this work tends to be high.

Dr. D.J. Kenworthy of the McMaster Computation Centre is investigating the possibilities of a method involving dumping core onto tape at the point where compilation has been completed but immediately before data are read into the computer. At this point, the "circuit diagram" has been completed. The output onto tape would make this "diagram" available for reruns of the same program. However, as yet, no real work has been done to modify the system to carry out this operation.

Table 4, which was obtained by analyzing the run times of a number of cases shows estimates of compilation times and actual integration times for the programs used in this study.

Certain conclusions can be made about the relative times taken by given operations. For instance, the compilation time required for program 1, i.e. the program with the iterative loop, is much longer than for the other programs. This is because the "circuit diagram" for the program is more complicated; since at the end of each iteration, integration modes change, an error function has to be calculated, and the value of a parameter (either the exponent or CON1) has to be adjusted.

PROGRAM	SEARCH FOR CON1 OR EXPONENT. EXAMPLE IN A.10.10	$K_E a'$ IN SUBROUTINE	$K_E a'$ IS FIXED
PRINTOUT INTERVAL (MINUTES)	1.0	0.5	0.5
INTEGRATION STEP SIZE (SECONDS)	5.0	1.0	1.0
COMPILATION TIME (ESTIMATE) (SECONDS)	190 ± 20	110 ± 10	94 ± 5
	CALCULATION TIME (SECONDS/MINUTE OF INTEGRATION TIME)		
INTEGRATION INTERVAL (MINUTES)			
20. MIN		9.25 ± 0.50	3.47 ± 0.25
86. MIN	1.66 ± 0.23		
107 MIN	1.81 ± 0.19		
108 MIN	1.72 ± 0.18		
216 MIN	1.62 ± 0.08		

TABLE 4

B.7.2 Program Listings

This section contains listings and brief discussions on two of the three main types of programs used in this study. The third program, which contains an iteration for calculation of CON1 or the exponent, is given as a sample problem in Section A.9.10, and a full discussion of the program is provided.

The two programs given here are the transient programs. The first program, listed in Figures 51, 52, and 53, gives the transient response when the mass transfer coefficient is in the final form (Section B.3.4.3). Some further description should be given about certain statements in the program.

The first four statements beginning with CON cause coefficients for equations representing equilibrium concentrations, surface tensions, density differences and activity derivatives as a function of solute concentration in the extract phase to be defined.

Concentrations are read in in terms of weight percent solute. Then, they are converted to units of weight of solute per unit weight of solute-free phase and used in these units until printout, when they are again converted to units of weight percent solute.

A subroutine EQUIL calculates equilibrium concentrations.

Another subroutine KEA calculates an overall mass transfer coefficient as a function of concentration.

The calculation in the listed program is for the 12 and 18 percent steps for flow system (1,1).

The value of the exponent EPT was found by using a program similar to A. 9.10 for a fixed value of CON1 = 550. The steady state profiles obtained in this same program when the exponent has been calculated correctly are used as the initial profiles in this run.

The program listed in Figures 54 and 55 is similar to the first, except that the mass transfer coefficient used in Pollock's transient raffinate coefficient which is constant for a given flow system. The program is ready to calculate the response of twelve and eighteen percent steps in feed concentration for flow systems (1,2) and (2,2).

```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
MODIFIED POLLOCK'S MODEL
KEA IS A FUNCTION OF CONCENTRATION
THREE STAGES
SIX WEIGHT PERCENT FEED
FLOW SYSTEM (1,1)
TRANSIENT RESPONSES FOR 12 AND 18 PERCENT STEPS
                  CON(A0,A1,A2,A3,A4)
                  CON(T0,T1,T2,T3)
                  CON(R0,R1,R2)
                  CON(P0,P1,P2,P3)
                  CON(FR2,FR3,FR4,S2,S3,S4)
                  CON(WR2,WR3,WR4,WE2,WE3,WE4)
                  CON(V)
                  CON(HR,HE)
                  PAR(X10,X20,X30,X40,X50)
                  PAR(Y10,Y20,Y30,Y40,Y50)
                  PAR(XRSS,YESS)
                  PAR(EPT)
                  PAR(CON1)
                  PAR(XSTEP)
         DT       EQL(0.5)
         DTMAX    EQL(1.0/60.0)
         DTMIN    EQL(1.0/60.0)
         C        EQL(TRUE)
         D        EQL(TRUE)
         X100     EQL(X10/(100.0-X10))
         X200     EQL(X20/(100.0-X20))
         X300     EQL(X30/(100.0-X30))
         X400     EQL(X40/(100.0-X40))
         X500     EQL(X50/(100.0-X50))
         Y100     EQL(Y10/(100.0-Y10))
         Y200     EQL(Y20/(100.0-Y20))
         Y300     EQL(Y30/(100.0-Y30))
         Y400     EQL(Y40/(100.0-Y40))
         TZERO    FSW(T,FALSE,TRUE,FALSE)
 TZERO   Y1       EQL(Y100)
 TZERO   X1       EQL(X100)
 TZERO   X2       EQL(X200)
 TZERO   Y2       EQL(Y200)
 TZERO   X3       EQL(X300)
 TZERO   Y3       EQL(Y300)
 TZERO   X4       EQL(X400)
 TZERO   Y4       EQL(Y400)
 TZERO   X5       EQL(X500)
```

FIGURE 51

```
EQUIL     BSP(X)
YSTAR     EQL((((A4*X+A3)*X+A2)*X+A1)*X+A0)
EQUIL     ESP(YSTAR)
KEA       BSP(ARG1,ARG2,FACTOR)
AKE       EQL(CON1*EXP(EPT,(ARG1/ARG2) *FACTOR))
KEA       ESP(AKE)
X1        EQL(XSTEP/(100.0-XSTEP))
Y1        INT((S2/HE)*(Y2-Y1),Y100,C,D)
EQUIL     CSP(X2)
          RSP(Y2STAR)
DELRO2    EQL(R0+R1*Y2+R2*Y2*Y2)
SIGMA2    EQL(T0+T1*Y2+T2*Y2*Y2+T3*Y2*Y2*Y2)
FACT2     EQL(P0+P1*Y2+P2*Y2*Y2+P3*Y2*Y2*Y2)
KEA       CSP(DELRO2,SIGMA2,FACT2)
          RSP(AKE2)
X2        INT(FR2/WR2*(X1-X2)-(AKE2*V/WR2)*(Y2STAR-Y2),X200,C,D)
Y2        INT(S2/WE2*(Y3-Y2)+(AKE2*V/WE2)*(Y2STAR-Y2),Y200,C,D)
EQUIL     CSP(X3)
          RSP(Y3STAR)
DELRO3    EQL(R0+R1*Y3+R2*Y3*Y3)
SIGMA3    EQL(T0+T1*Y3+T2*Y3*Y3+T3*Y3*Y3*Y3)
FACT3     EQL(P0+P1*Y3+P2*Y3*Y3+P3*Y3*Y3*Y3)
KEA       CSP(DELRO3,SIGMA3,FACT3)
          RSP(AKE3)
X3        INT(FR3/WR3*(X2-X3)-(AKE3*V/WR3)*(Y3STAR-Y3),X300,C,D)
Y3        INT(S3/WE3*(Y4-Y3)+(AKE3*V/WE3)*(Y3STAR-Y3),Y300,C,D)
EQUIL     CSP(X4)
          RSP(Y4STAR)
DELRO4    EQL(R0+R1*Y4+R2*Y4*Y4)
SIGMA4    EQL(T0+T1*Y4+T2*Y4*Y4+T3*Y4*Y4*Y4)
FACT4     EQL(P0+P1*Y4+P2*Y4*Y4+P3*Y4*Y4*Y4)
KEA       CSP(DELRO4,SIGMA4,FACT4)
          RSP(AKE4)
X4        INT(FR4/WR4*(X3-X4)-(AKE4*V/WR4)*(Y4STAR-Y4),X400,C,D)
Y4        INT(S4/WE4*(Y5-Y4)+(AKE4*V/WE4)*(Y4STAR-Y4),Y400,C,D)
X5        INT((FR4/HR)*(X4-X5),X500,C,D)
Y5        EQL(Y50/(100.0-Y50))
X1OUT     EQL(100.0*X1/(1.00+X1))
X2OUT     EQL(100.0*X2/(1.00+X2))
X3OUT     EQL(100.0*X3/(1.00+X3))
X4OUT     EQL(100.0*X4/(1.00+X4))
X5OUT     EQL(100.0*X5/(1.00+X5))
Y1OUT     EQL(100.0*Y1/(1.00+Y1))
Y2OUT     EQL(100.0*Y2/(1.00+Y2))
Y3OUT     EQL(100.0*Y3/(1.00+Y3))
Y4OUT     EQL(100.0*Y4/(1.00+Y4))
Y5OUT     EQL(100.0*Y5/(1.00+Y5))
DXRSS     EQL(X5OUT-XRSS)
DYESS     EQL(Y1OUT-YESS)
```

FIGURE 52

```
               HDR(T,X1,X2,X3,X4,X5)
               HDR(,Y1,Y2,Y3,Y4,Y5)
               HDR(AKE2,AKE3,AKE4,DXRSS,DYESS)
               HDR
               OUT(T,X1OUT,X2OUT,X3OUT,X4OUT,X5OUT)
               OUT(,Y1OUT,Y2OUT,Y3OUT,Y4OUT,Y5OUT)
               OUT(AKE2,AKE3,AKE4,DXRSS,DYESS)
               OUT
               FIN(T,20.)
               END
-0.00018445 0.60268247  0.97567166  -0.66827321 0.00539865
10.37768137 -93.5286274 486.3131218 -1040.990753
0.1934      -0.08037897 -0.395827
0.69966979  -5.78837866 48.17870451 -148.2403011
234.        234.        234.        198.        198.        198.
381.3       381.3       381.3       89.         89.         89.
516.7
123.        43.5
6.28        5.65183     4.82454     3.71931     3.71931
3.24506     3.24506     2.45263     1.40542     0.0
3.71931     3.24506
1.60298
550.
12.33
6.28        5.65183     4.82454     3.71931     3.71931
3.24506     3.24506     2.45263     1.40542     0.0
3.71931     3.24506
1.60298
550.
17.83
$IBSYS
```

FIGURE 53

```
$JOB           003105 T NORTHCOTT
$EXECUTE       MIMIC
MODIFIED POLLOCK'S MODEL
THREE STAGES
TRANSIENT RESPONSES USING THE TRANSIENT KEA'S
DATA SETS (1,2), AND (2,2)
                  CON(A0,A1,A2,A3,A4)
                  PAR(FR,S,WR,WE)
                  PAR(V,AKE)
                  PAR(HR,HE)
                  PAR(X10,X20,X30,X40,X50)
                  PAR(Y10,Y20,Y30,Y40,Y50)
                  PAR(XRSS,YESS)
                  PAR(XSTEP)
         A        DIV(FR,WR)
         B        MPY(AKE,V)
         C        DIV(B,WR)
         D        DIV(S,WE)
         E        DIV(B,WE)
         DT       EQL(1.0)
         DTMAX    EQL(1.0/60.0)
         DTMIN    EQL(1.0/60.0)
         X100     EQL(X10/(100.0-X10))
         X200     EQL(X20/(100.0-X20))
         X300     EQL(X30/(100.0-X30))
         X400     EQL(X40/(100.0-X40))
         X500     EQL(X50/(100.0-X50))
         Y100     EQL(Y10/(100.0-Y10))
         Y200     EQL(Y20/(100.0-Y20))
         Y300     EQL(Y30/(100.0-Y30))
         Y400     EQL(Y40/(100.0-Y40))
         TZERO    FSW(T,FALSE,TRUE,FALSE)
 TZERO   X1       EQL(X100)
 TZERO   Y1       EQL(Y100)
 TZERO   X2       EQL(X200)
 TZERO   Y2       EQL(Y200)
 TZERO   X3       EQL(X300)
 TZERO   Y3       EQL(Y300)
 TZERO   X4       EQL(X400)
 TZERO   Y4       EQL(Y400)
 TZERO   X5       EQL(X500)
         EQUIL    BSP(X)
         YSTAR    EQL((((A4*X+A3)*X+A2)*X+A1)*X+A0)
         EQUIL    ESP(YSTAR)
         X1       EQL(XSTEP/(100.0-XSTEP))
         Y1       INT(S/HE*(Y2-Y1),Y100)
         EQUIL    CSP(X2)
                  RSP(Y2STAR)
         X2       INT(A*(X1-X2)-C*( Y2STAR  -Y2),X200)
         Y2       INT(D*(Y3-Y2)+E*( Y2STAR  -Y2),Y200)
         EQUIL    CSP(X3)
                  RSP(Y3STAR)
         X3       INT(A*(X2-X3)-C*( Y3STAR  -Y3),X300)
         Y3       INT(D*(Y4-Y3)+E*( Y3STAR  -Y3),Y300)
         EQUIL    CSP(X4)
                  RSP(Y4STAR)
         X4       INT(A*(X3-X4)-C*( Y4STAR  -Y4),X400)
         Y4       INT(D*(Y5-Y4)+E*( Y4STAR  -Y4),Y400)
         X5       INT(FR/HR*(X4-X5),X500)
```

FIGURE 54

```
          Y5        EQL(Y50/(100.0-Y50))
          X1OUT     EQL(100.0*X1/(1.00+X1))
          X2OUT     EQL(100.0*X2/(1.00+X2))
          X3OUT     EQL(100.0*X3/(1.00+X3))
          X4OUT     EQL(100.0*X4/(1.00+X4))
          X5OUT     EQL(100.0*X5/(1.00+X5))
          Y1OUT     EQL(100.0*Y1/(1.00+Y1))
          Y2OUT     EQL(100.0*Y2/(1.00+Y2))
          Y3OUT     EQL(100.0*Y3/(1.00+Y3))
          Y4OUT     EQL(100.0*Y4/(1.00+Y4))
          Y5OUT     EQL(100.0*Y5/(1.00+Y5))
          DXRSS     EQL(X5OUT-XRSS)
          DYESS     EQL(Y1OUT-YESS)
                    FIN(T,20.)
                    HDR(T,X1,X2,X3,X4,X5)
                    HDR(,Y1,Y2,Y3,Y4,Y5)
                    HDR(,,,DXRSS,DYESS)
                    HDR
                    OUT(T,X1OUT,X2OUT,X3OUT,X4OUT,X5OUT)
                    OUT(,Y1OUT,Y2OUT,Y3OUT,Y4OUT,Y5OUT)
                    OUT(,,,DXRSS,DYESS)
                    END
-0.00018445 0.60268247  0.97567166  -0.66827321 0.00539865
234.        321.        369.7       93.7
500.        0.959
124.        63.
6.17        5.056       3.87659     2.60041     2.60042
2.76851     2.76851     1.89900     0.983902    0.0
2.60042     2.76851
12.22
234.        321.        369.7       93.7
500.        0.959
124.        63.
6.17        5.056       3.87659     2.60041     2.60042
2.76851     2.76851     1.89900     0.983902    0.0
2.60042     2.76851
18.14
375.        329.        385.7       84.
508.3       3.25
123.        53.
6.12        5.51313     4.60486     3.20061     3.20061
3.53235     3.53235     2.80116     1.70380     0.00
3.20061     3.53235
12.23
375.        329.        385.7       84.
508.3       3.25
123.        53.
6.12        5.51313     4.60486     3.20061     3.20061
3.53235     3.53235     2.80116     1.70380     0.00
3.20061     3.53235
18.14
$IBSYS
```

FIGURE 55

C. CONCLUSIONS

An extensive study has been made of MIMIC, and a model has been written in MIMIC to simulate the transient response of a liquid-liquid extraction column to step inputs in feed concentration.

During this work several shortcomings have been noted.

1. Some of the MIMIC functions (e.g. DER, FUN) are limited.
2. Problems may arise with systems with over 20-25 integrators.
3. Diagnostics may be inadequate or nonexistent.
4. Application of MIMIC to boundary value problems is limited.
5. Recompilation of a program must occur if the program is rerun.
6. Errors still exist in the system from the imperfect translation from the 7090/94 system to the 7040/44 system.

At the same time, many advantageous features of MIMIC were noted.

1. Complicated systems of differential equations can be easily solved without becoming mired in numerical or programming techniques.
2. MIMIC is easy to learn and retain.
3. Programming is fast and efficient.

Formats are simple, and MIMIC functions allow many logical and algebraic operations to be carried out with ease.

In the opinion of the author, these advantages outweighed the disadvantages and therefore he recommends MIMIC as a technique to be considered for solving many of the types of problems faced by chemical engineers.

D. ACKNOWLEDGEMENTS

I wish to thank a number of people for their assistance during this work, in particular the following:

My research supervisor, Dr. A.I. Johnson, for his constructive advice and his constant encouragement;

Gary G. Pollock, whose data I used and who spent hours discussing the problem with me;

Dr. C.M. Crowe, for several interesting discussions about MIMIC;

Dr. D.J. Kenworthy of the McMaster Computation Centre, who provided valuable assistance in correcting errors found in the McMaster version of MIMIC, and in explaining some of the internal workings of MIMIC;

Mrs. Sally Gravestock, for her skilful typewriting.

In addition, I wish to acknowledge the original Wright-Patterson MIMIC manual(A.11.13) and a handbook by P. Cress of the University of Waterloo as the bases of Part A of the report.

Finally, I thank McMaster University for financial support during the study.