REFERENCES

1. A. Benallou, D.E. Seborg and D.A. Mellichamp, Dynamic Compartmental Models for Separation Processes, AIChE Journal Vol. 32, No.7, July 1986.
2. Bequette B. W. and T. F. Edgar, Noninteracting control system design methods in distillation, Computers chem. Engng 13, pp. 641-650, 1989.
3. Cho, Y. S., and B. Joseph, The development of Simple Dynamic Models for Separation Processes, Paper 2d, 73rd Ann. AIChE Meet., Chicago, 1980.
4. Crockett, W. E., Approximate Distillation Dynamics from Steady State Data, Proc. JACC, Vol. 1, pp. 223, 1978.
5. David M. Himmelblau, Basic Principles and Calculations in Chemical Engineering, Prentice-Hall International Editions, Fifth edition, 1989.
6. Eckert, E., and V. Hlavacek, Calculation of Multicomponent Distillation of Nonideal Mixtures by a Shortcut Method, Chem. Eng. Sci., Vol. 33, pp. 77, 1978.
7. Edmister, W. G., Absorption and Stripping-Factor Functions for Distillation Calculation by Manual- and Digital-Computer Methods, AIChE J., Vol. 3, pp. 165, 1957.
8. Ernest J. Henley and J. D. Seader, Equlibrium-Stage Separation Operations in Chemical Engineering, John Wiley & Sons Inc., New York, 1981.
9. Espana, M., and I. D. Landau, Reduced-Order Bilinear Models for Distillation Columns, Automatica, Vol. 14, pp. 345, 1978.
10. Fleischer, M. T., and D. M. Prett., Simplified Techniques for Simulating Complex Columns, Chem. Eng. Prog., Vol. 77., pp. 72, 1981.

11. Hendrick C. Van Ness and Michael M. Abbott, Classical Thermodynamics of Nonelectrolyte Solutions With Applications to Phase Equlibria, McGraw-Hill Book Company, New York, 1982.

12. Holland C. D., Multicomponent Distillations, Prentice-Hall Inc., Englewood Cliffs, N.J. 1963.

13. Kuznik, J., and R. Kzyzanowski, Calculated Designations of the Dynamic Properties of Simplified Models of Distillation Columns, Int. Chem. Eng., Vol. 15, pp. 553, 1975.

14. _____, Numerical Determination of the Dynamic Properties of a Distillation Column and a Measurement Verification Test of the Column Model, Int. Chem. Eng., Vol. 17, pp. 360, 1977.

15. L. John Ribar, Fortran Programming for Windows, McGraw-Hill Book Company, New York, 1993.

16. Marshall, W. R., and R. L. Pigford, The application of Differential Equations to Chemical Engineering Problems, Univ. Delaware Press, Newark, DE, 1947.

17. Marshall, S. A., An Approximate Methode for Reducing the Order of a Linear System, Control, Vol. 10, pp. 642, 1966.

18. Moczek, J. S., R. E. Otto, and T. J. Williams, Approximation Models for the Dynamic Response of Large Distillation Columns, CEP Symp. Ser., Vol. 61, pp. 136, 1965.

19. Osborne, W. G., Jr., et al., A Simplified Model for transient Behavior of Distillation Columns, AIChE-ICE Symp. Ser., Vol. 1, pp. 84, 1965.

20. Robert H. Perry and Don Green, Perry's Chemical Engineering Handbook, 6th edition, McGraw-Hill International Editions, 1984.

21. Robert E. Treybal, Mass-Transfer Operations, McGraw-Hill Book Company, New York, 1981.

22. Robert H. Hammond, Introduction to Fortran 77 and the Personal Computer, McGraw-Hill Book Company, Computer Science Series 1987.

23. R.R. Horton, B.W. Bequette and T.F. Edgar, Improvements in Dynamics Compartmental Modeling for Distillation, Computer Chemical Engineering, Vol. 15, No. 3, pp. 197-201, 1991.

24. Stewart, W. E., K. L. Levien, and M. Morari, A New Model Reduction Technique for Staged Separation Operations, paper 55c, 74th. Ann. AIChE Meet., New Orleans, 1981.

25. Wahl, E. F., and P. Harriott, Understanding and Prediction of the dynamic Behavior of Distillation Columns, IEC Proc. Des. Dev., Vol. 9, pp 396, 1970.

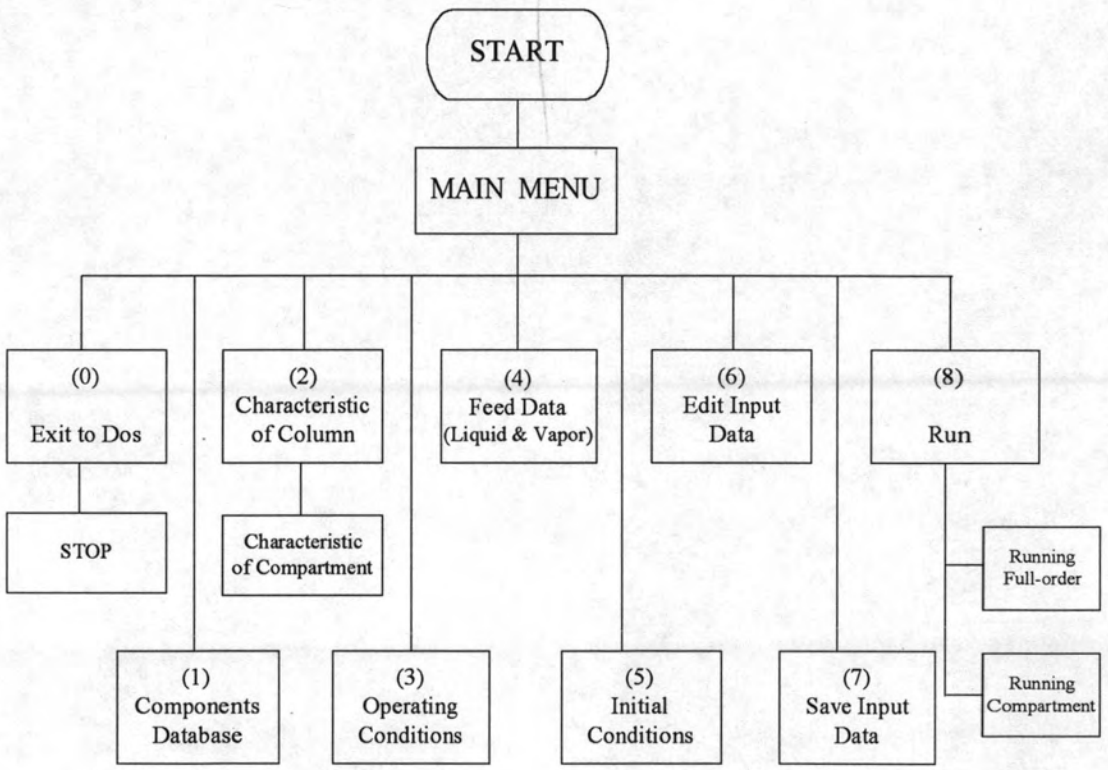
26. W. Jeferey Cook, John Klatt and Coleman B. Brosilow, Simulation of Large Scale Dynamic System-II. A Modular Simulator for the Dynamics of Distillation Systems, Computer Chemical Engineering Vol. 11, No. 3, pp. 255-264, 1987.

27. W. L. Luyben, Practical Distillation Control, Van Nostrand Reinhold, New York, 1992.

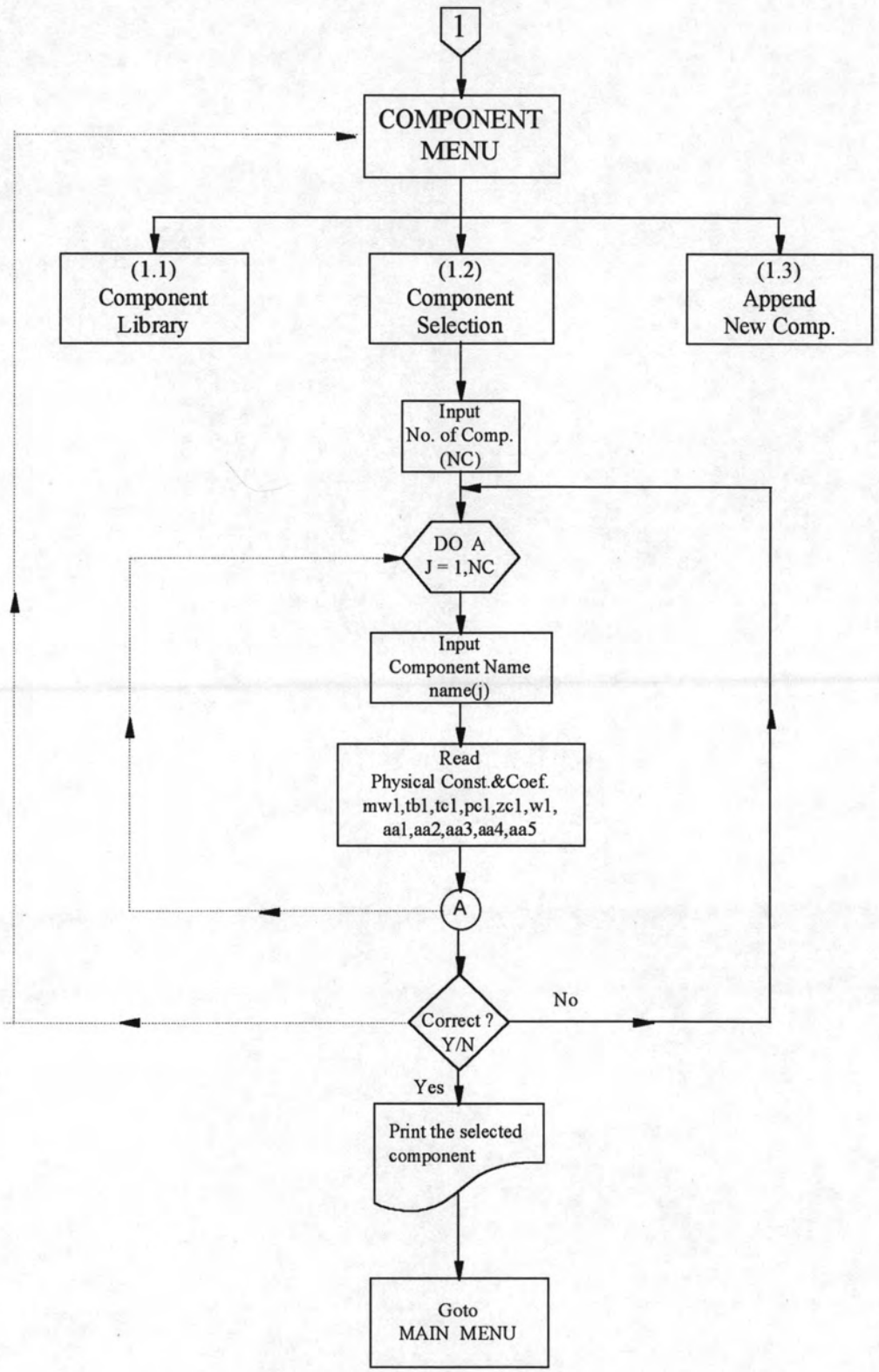
28. W. L. Luyben, Process Modeling Simulation and Control for Chemical Engineers, McGraw-Hill International Editions, 1974

Appendix A

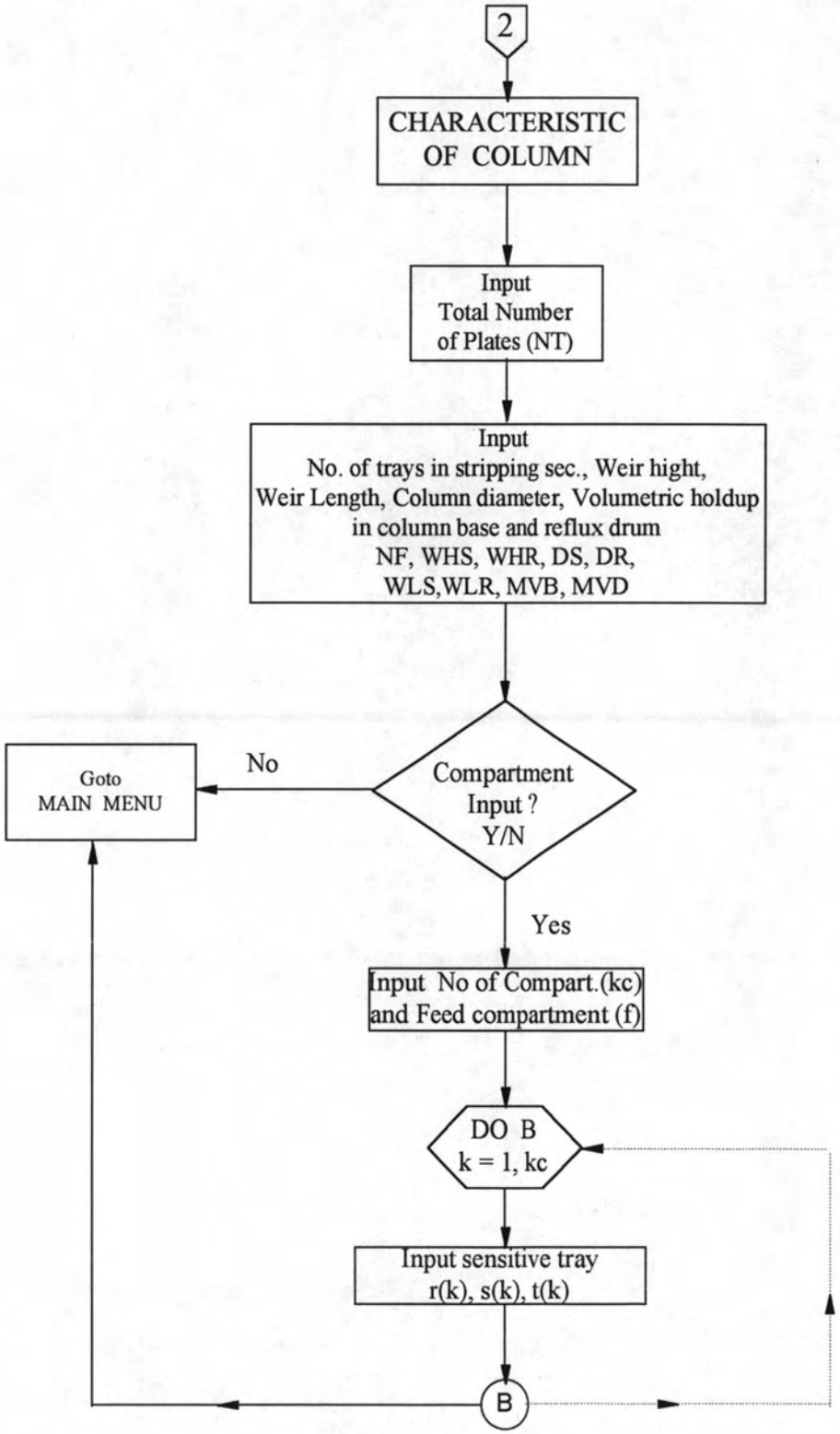
Computer Program Flow Chart



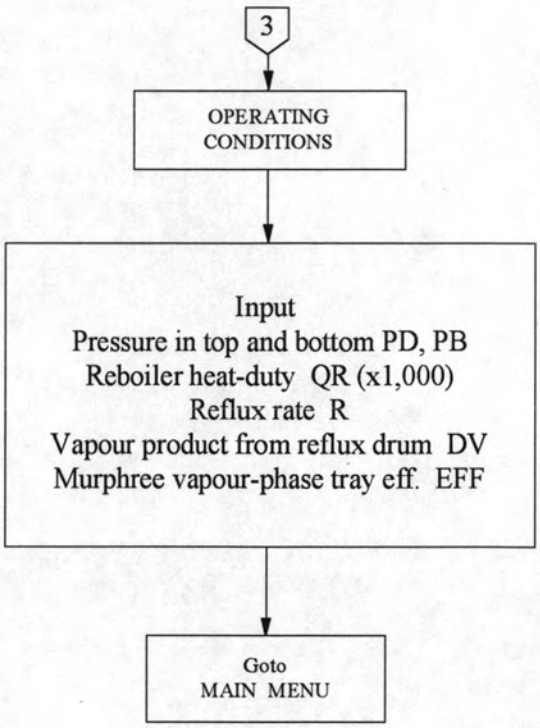
A) Program Structure



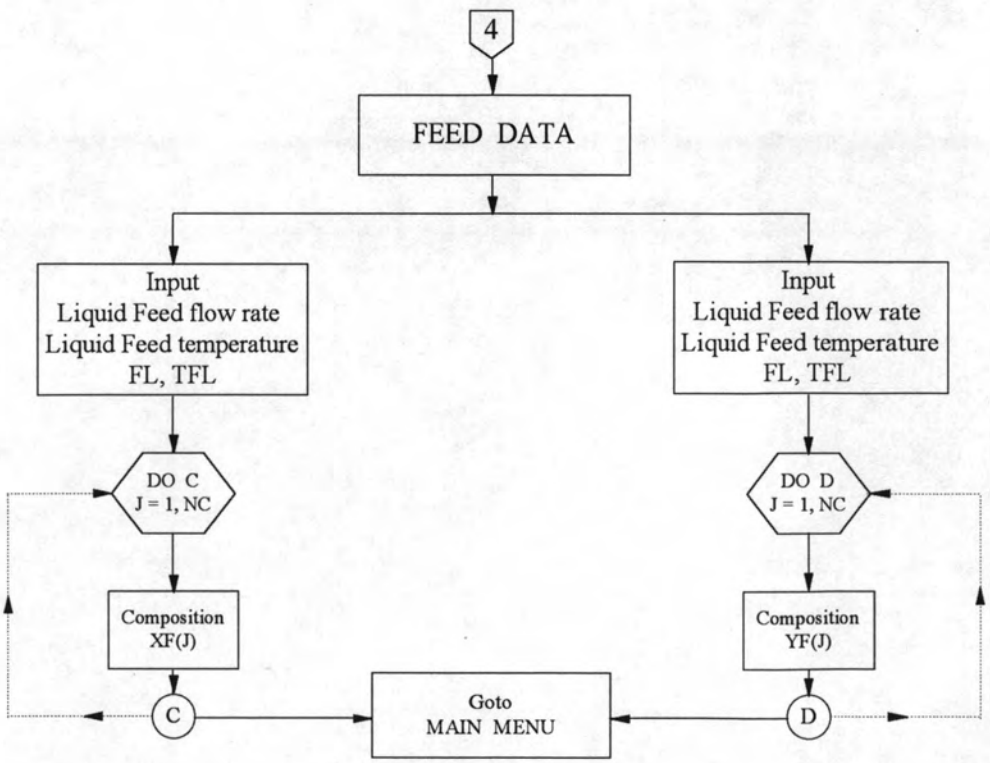
1) Component Database



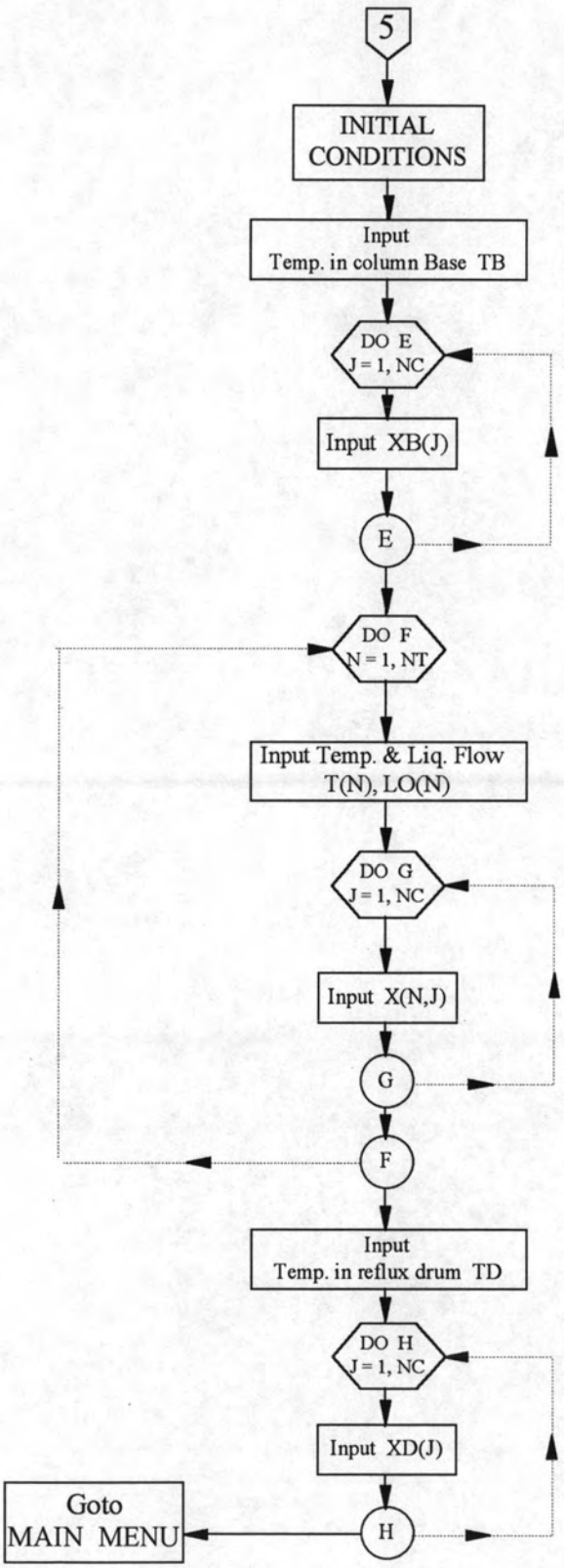
2) Characteristic of Column



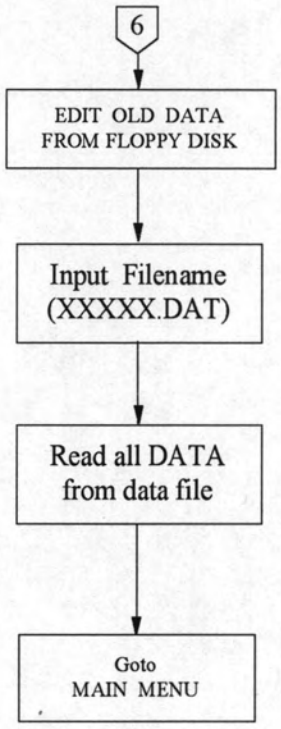
3) Operating Conditions



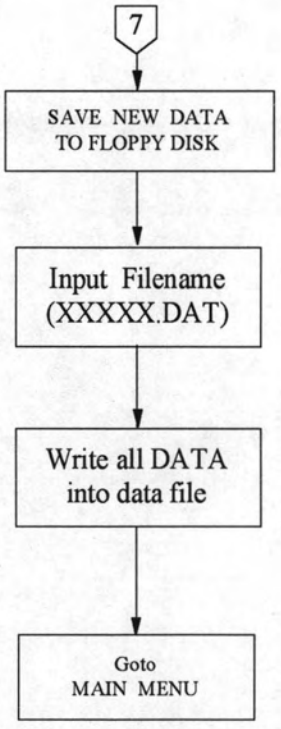
4) Feed Data



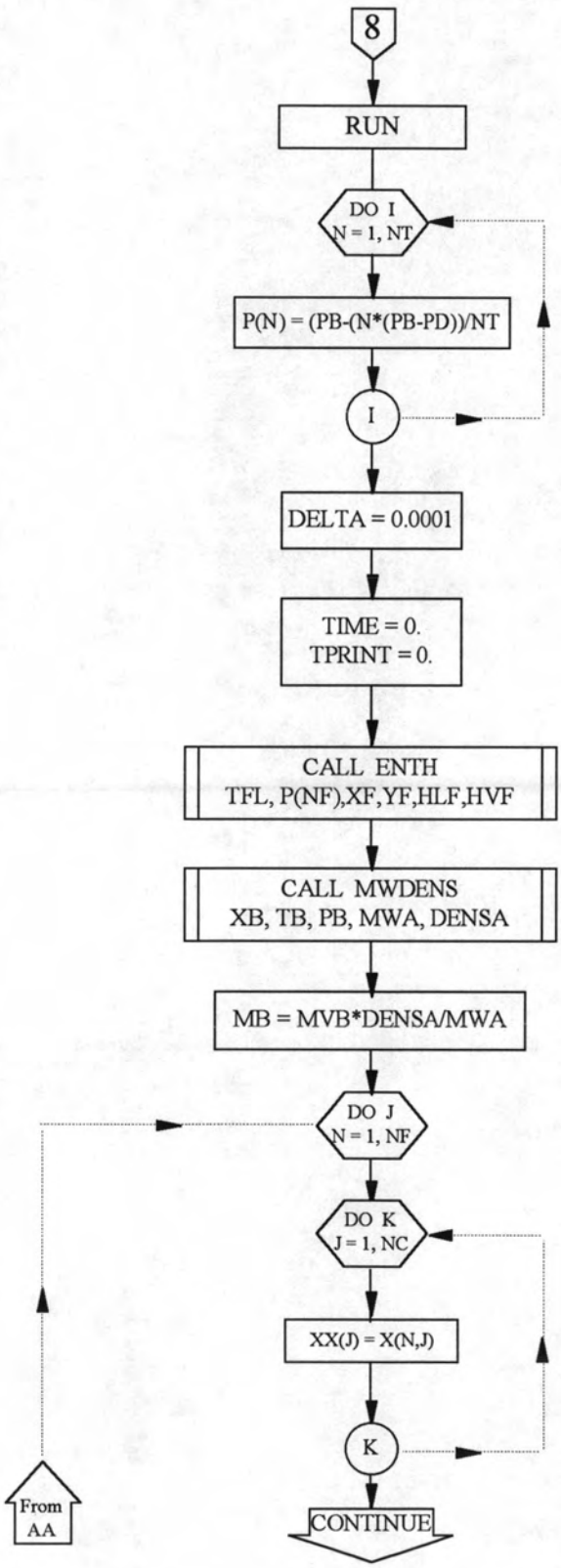
5) Initial Conditions



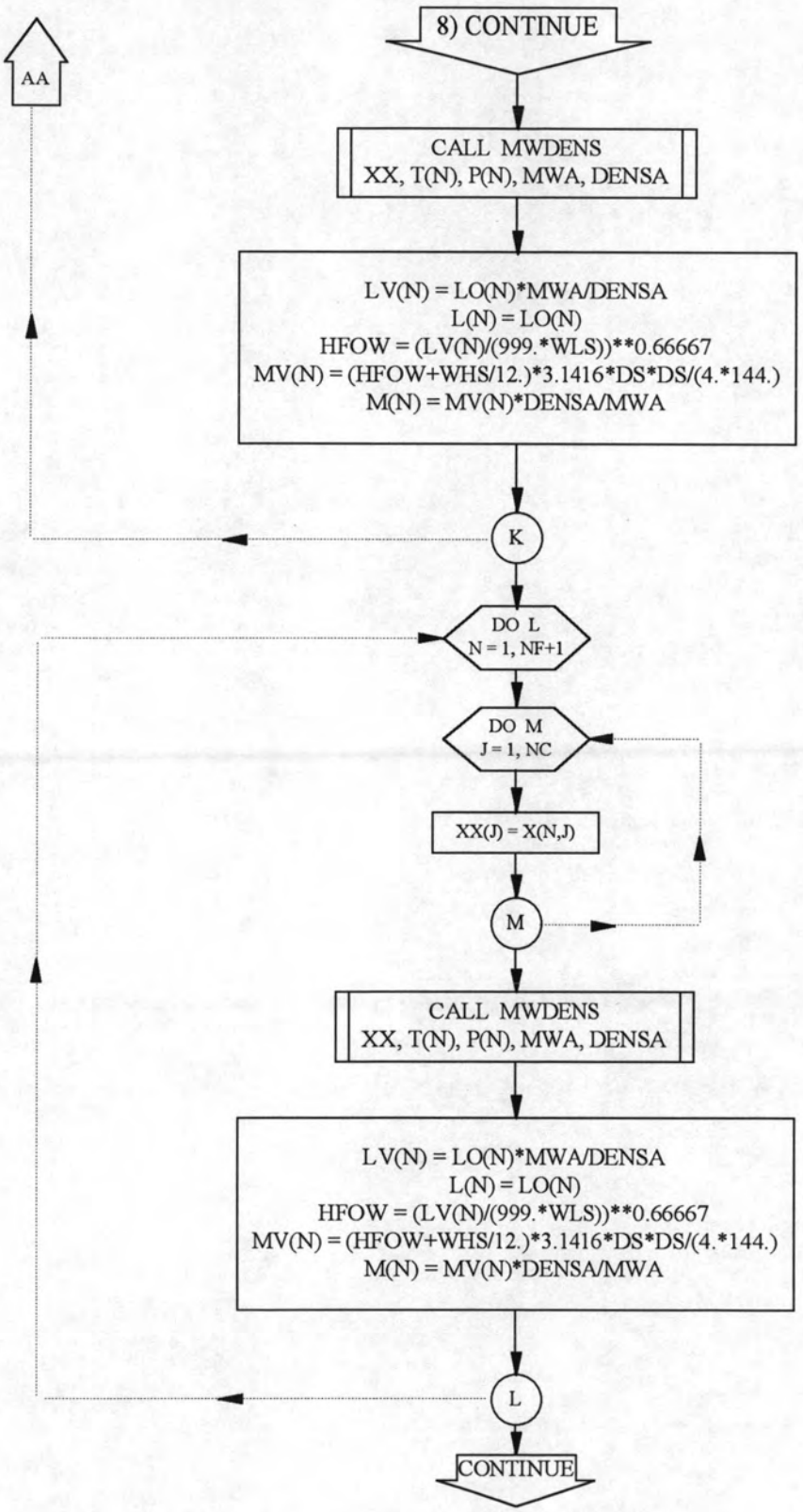
6) Edit Input Data



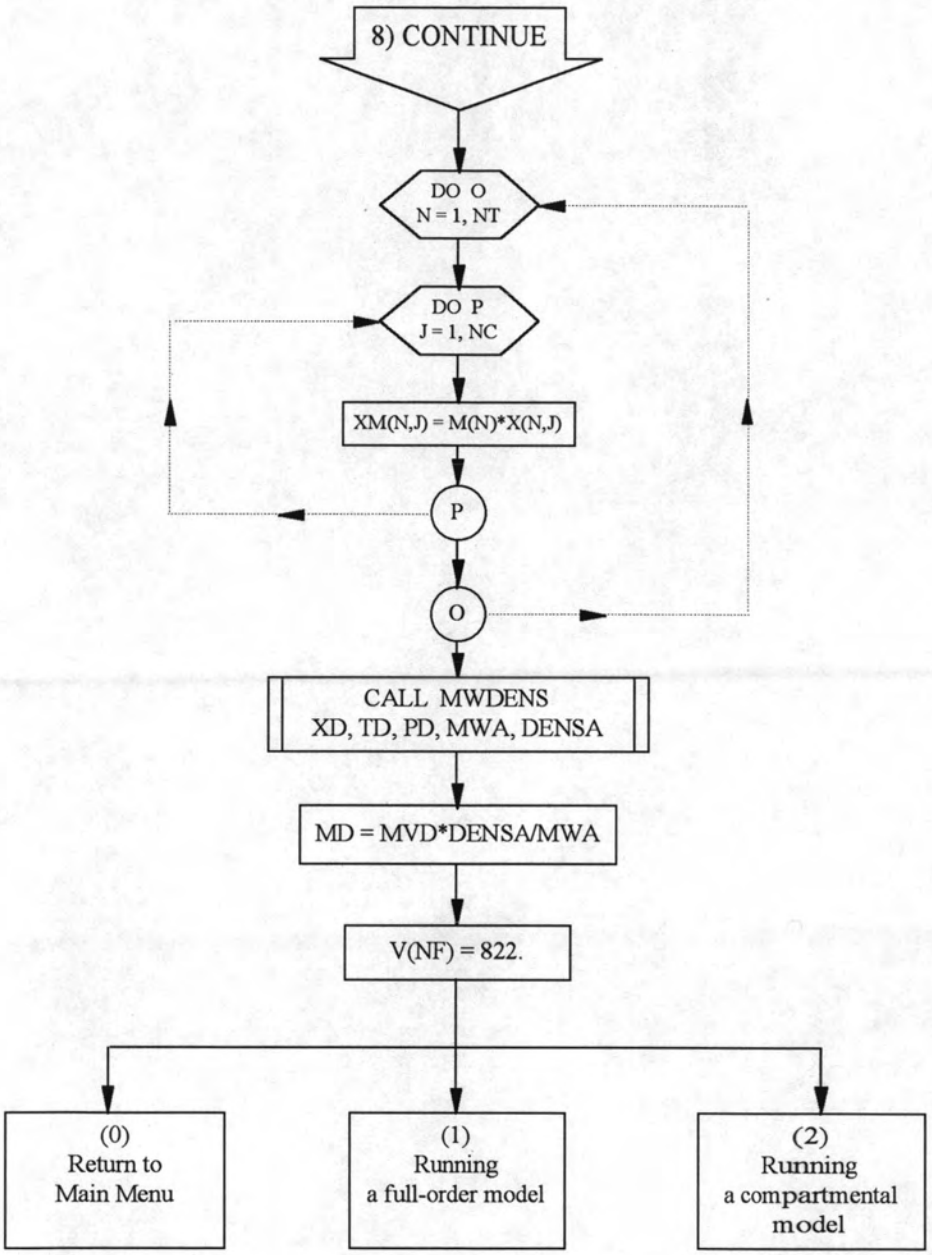
7) Save Input Data


8
RUN
DO I
N = 1, NT
P(N) = (PB-(N*(PB-PD))/NT
I
DELTA = 0.0001
TIME = 0.
TPRINT = 0.
CALL ENTH
TFL, P(NF),XF,YF,HLF,HVF
CALL MWDENS
XB, TB, PB, MWA, DENSA
MB = MVB*DENSA/MWA
DO J
N = 1, NF
DO K
J = 1, NC
XX(J) = X(N,J)
K
CONTINUE
From
AA

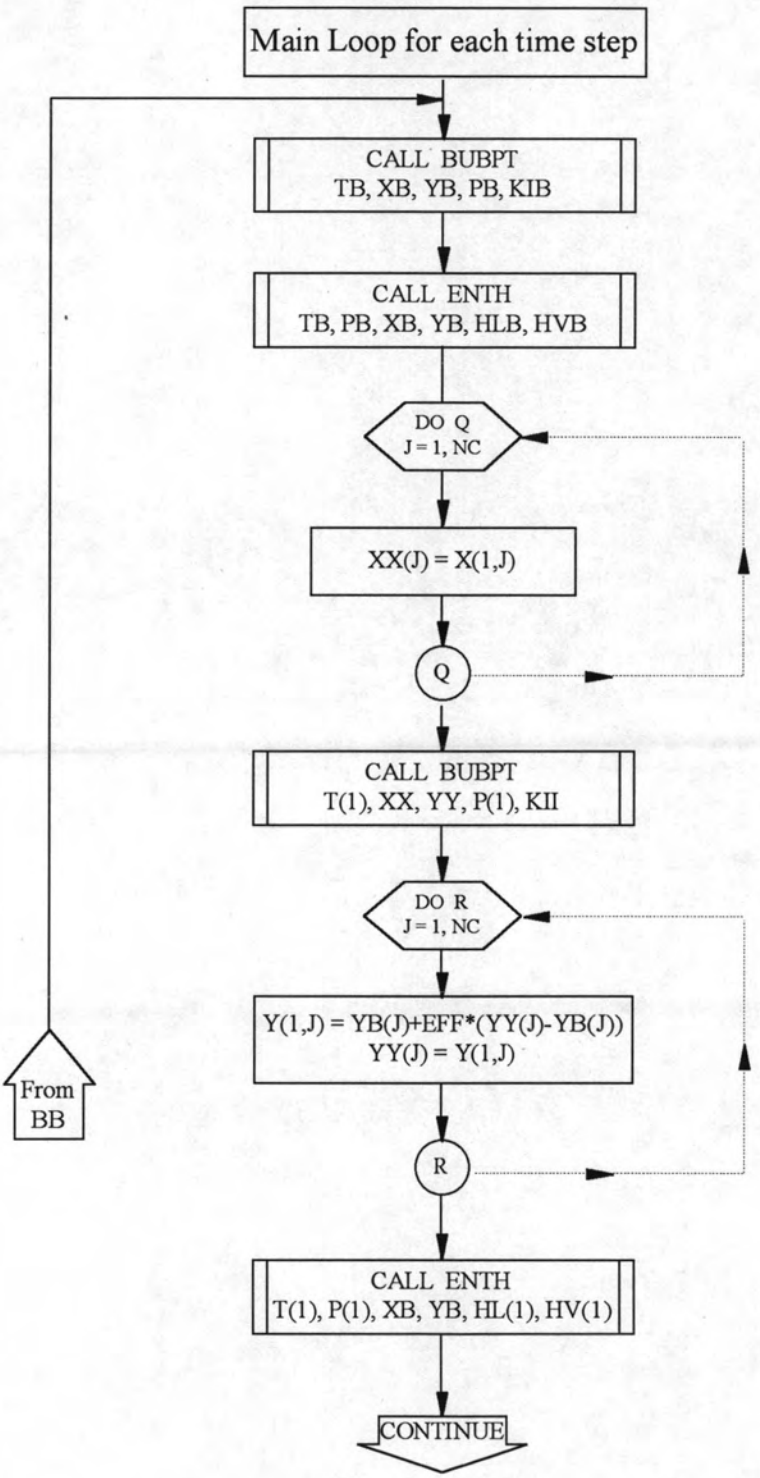
8) Run



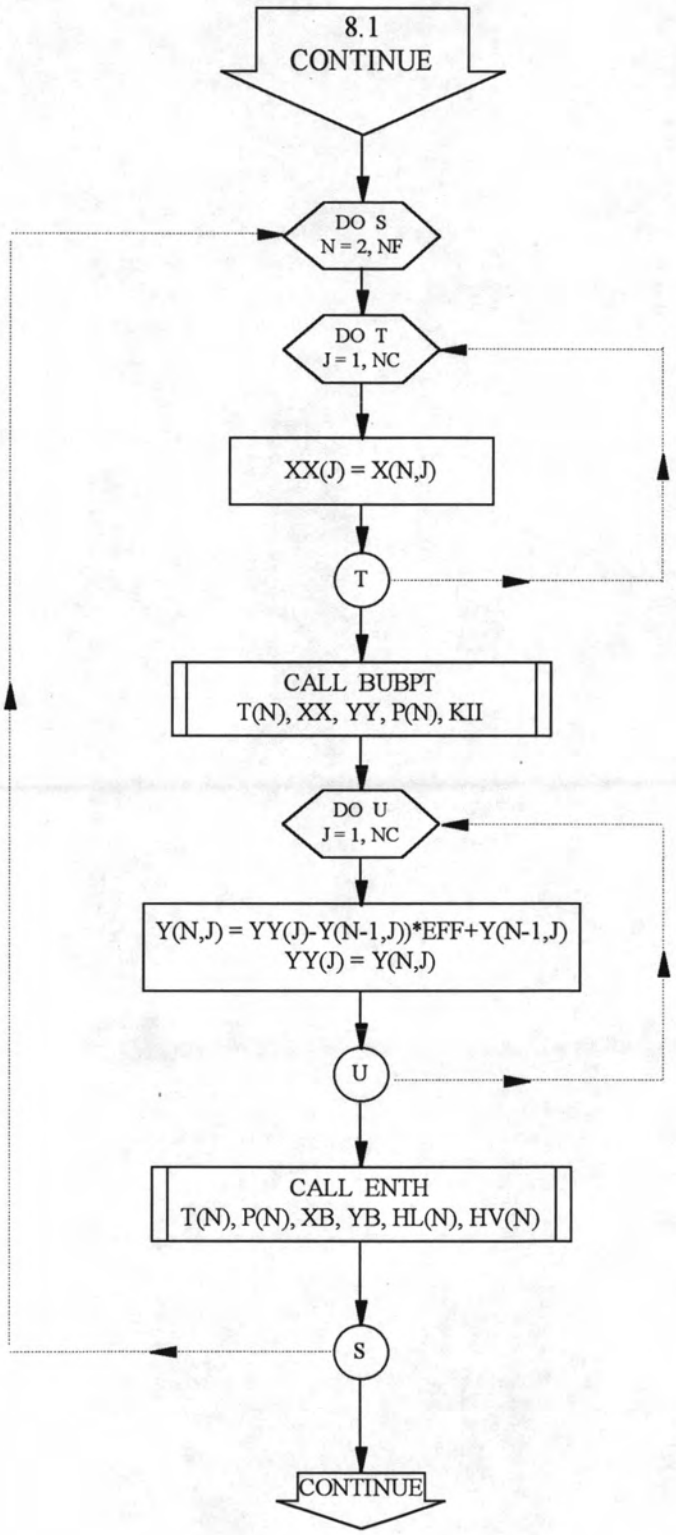
8) Run (Continue)



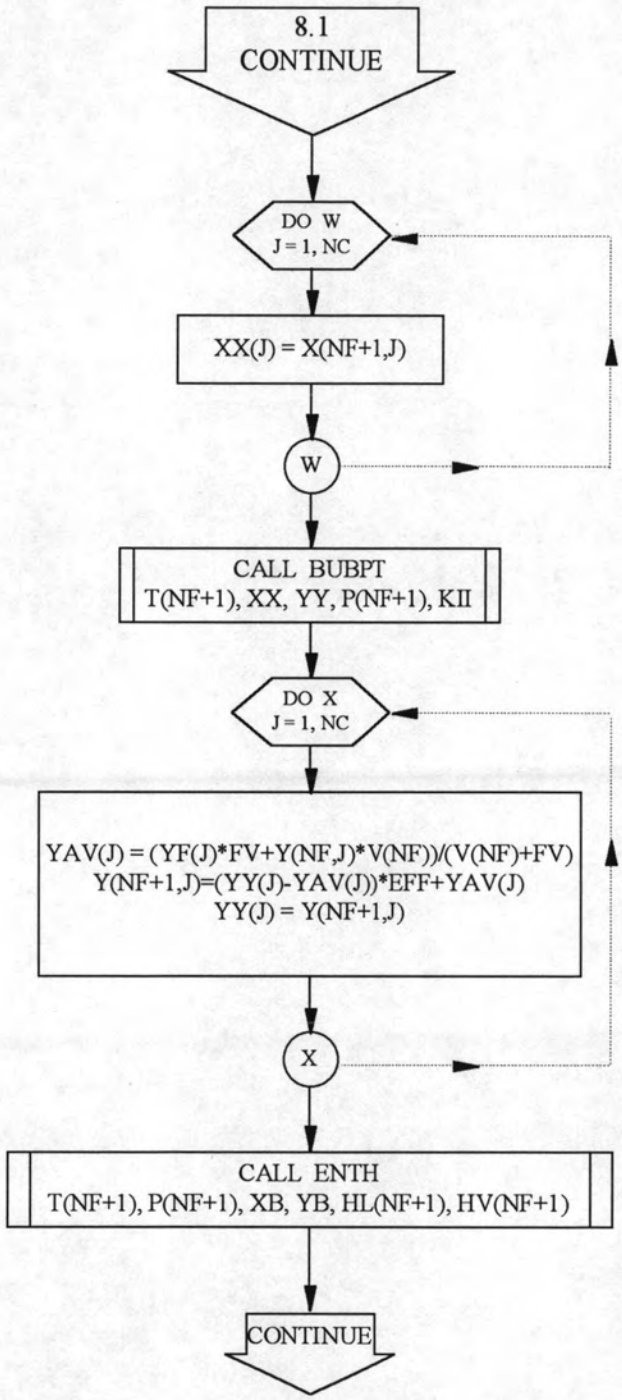
8) Run (Continue)



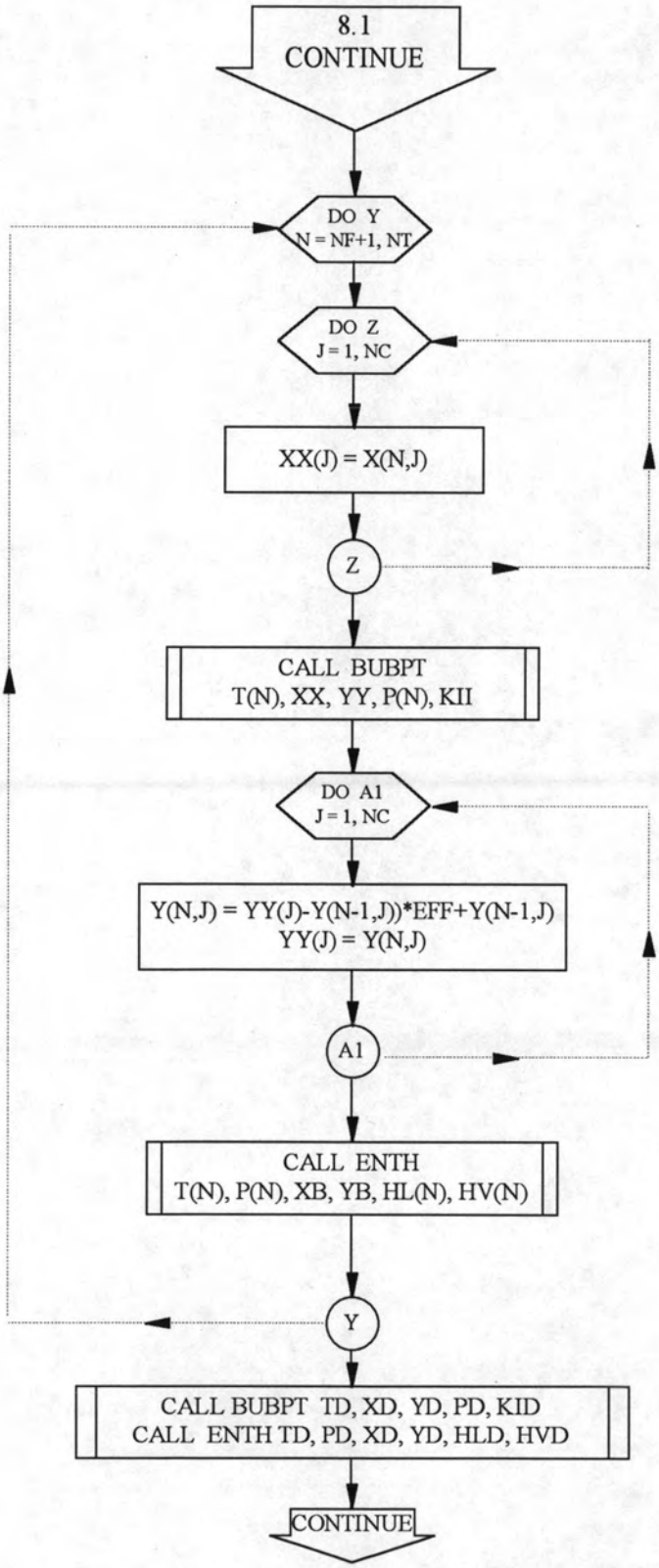
8.1) Running a full-order model



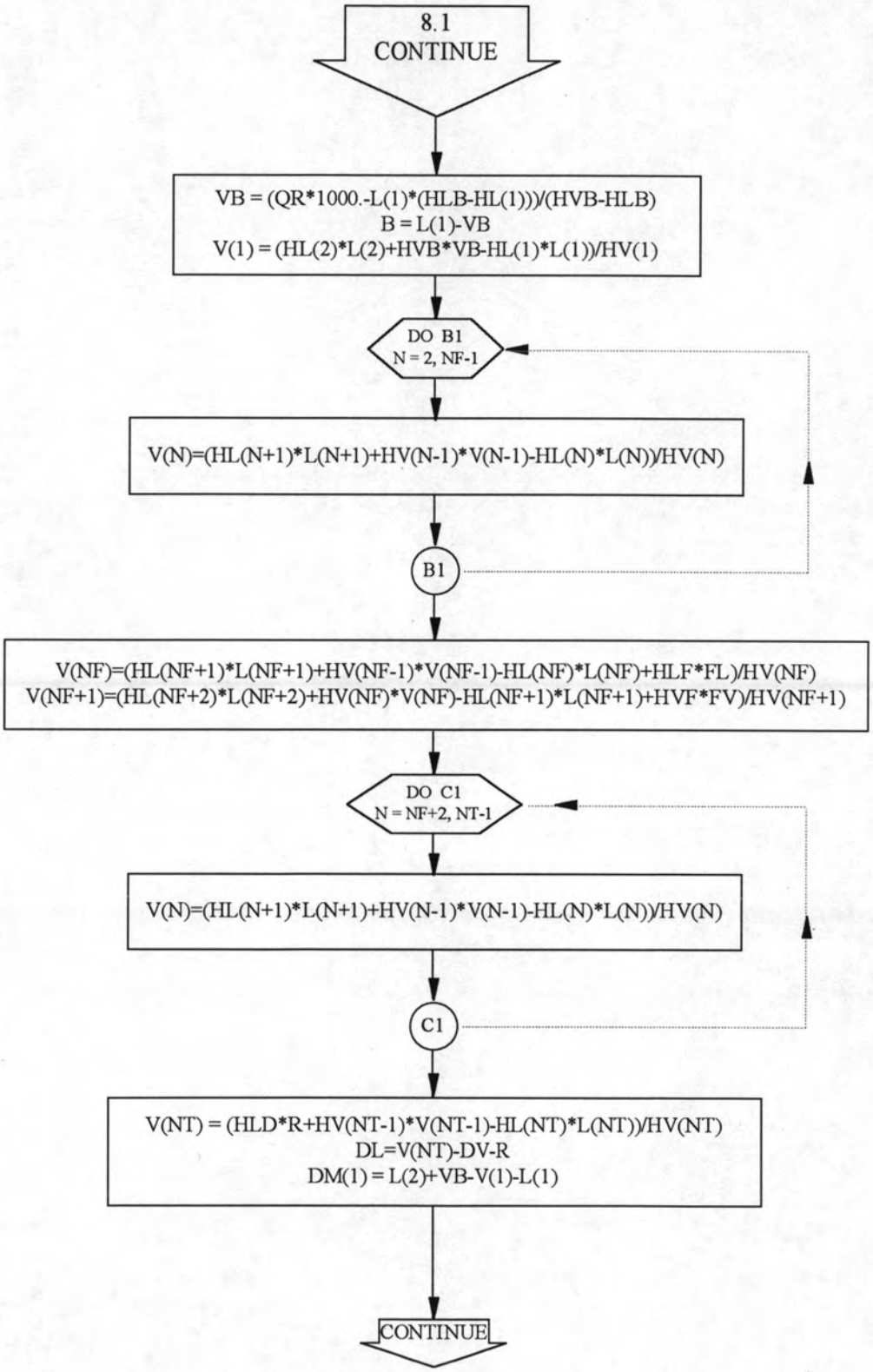
8.1) Running a full-order model (Continue)



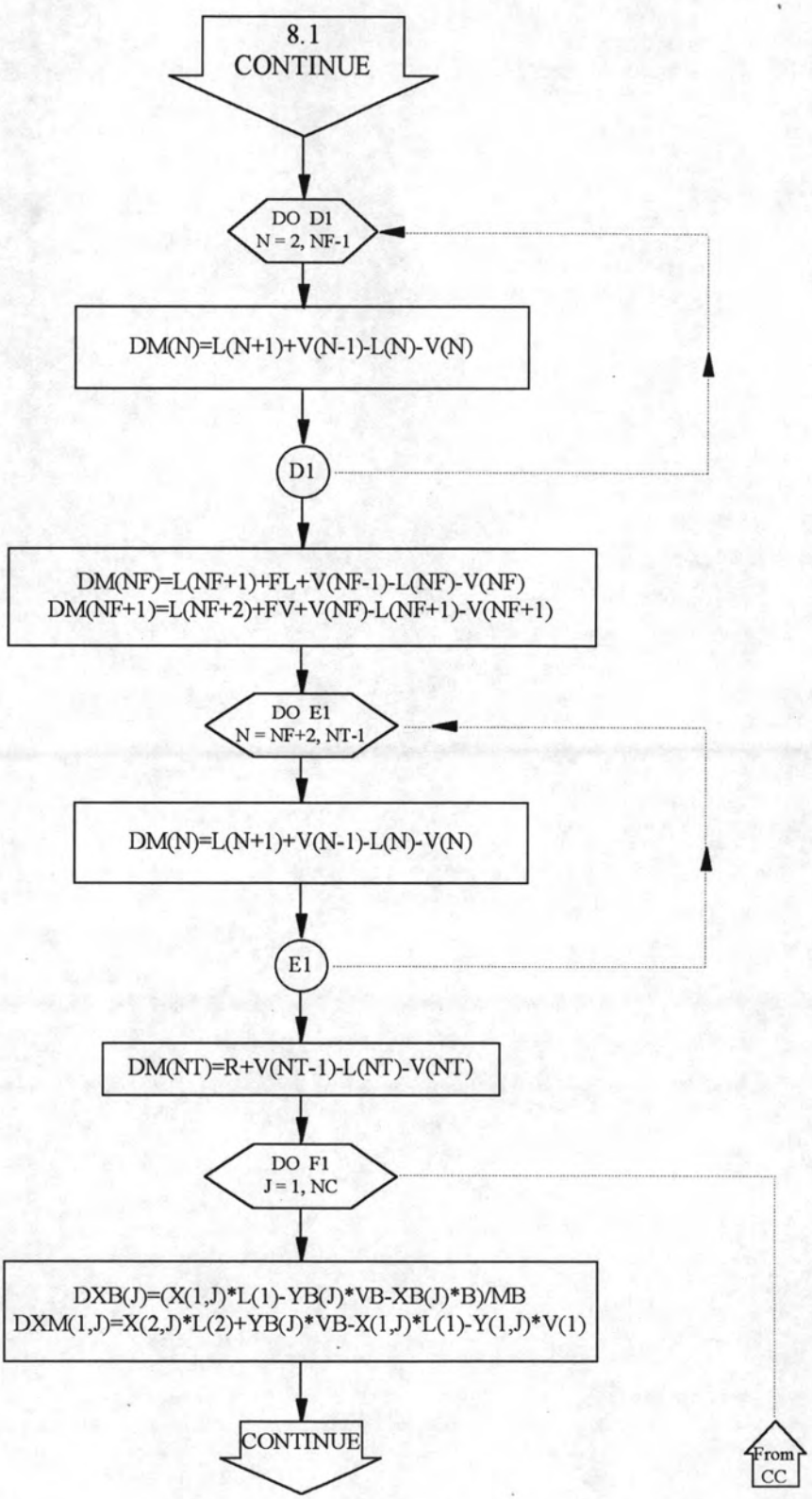
8.1) Running a full-order model (Continue)



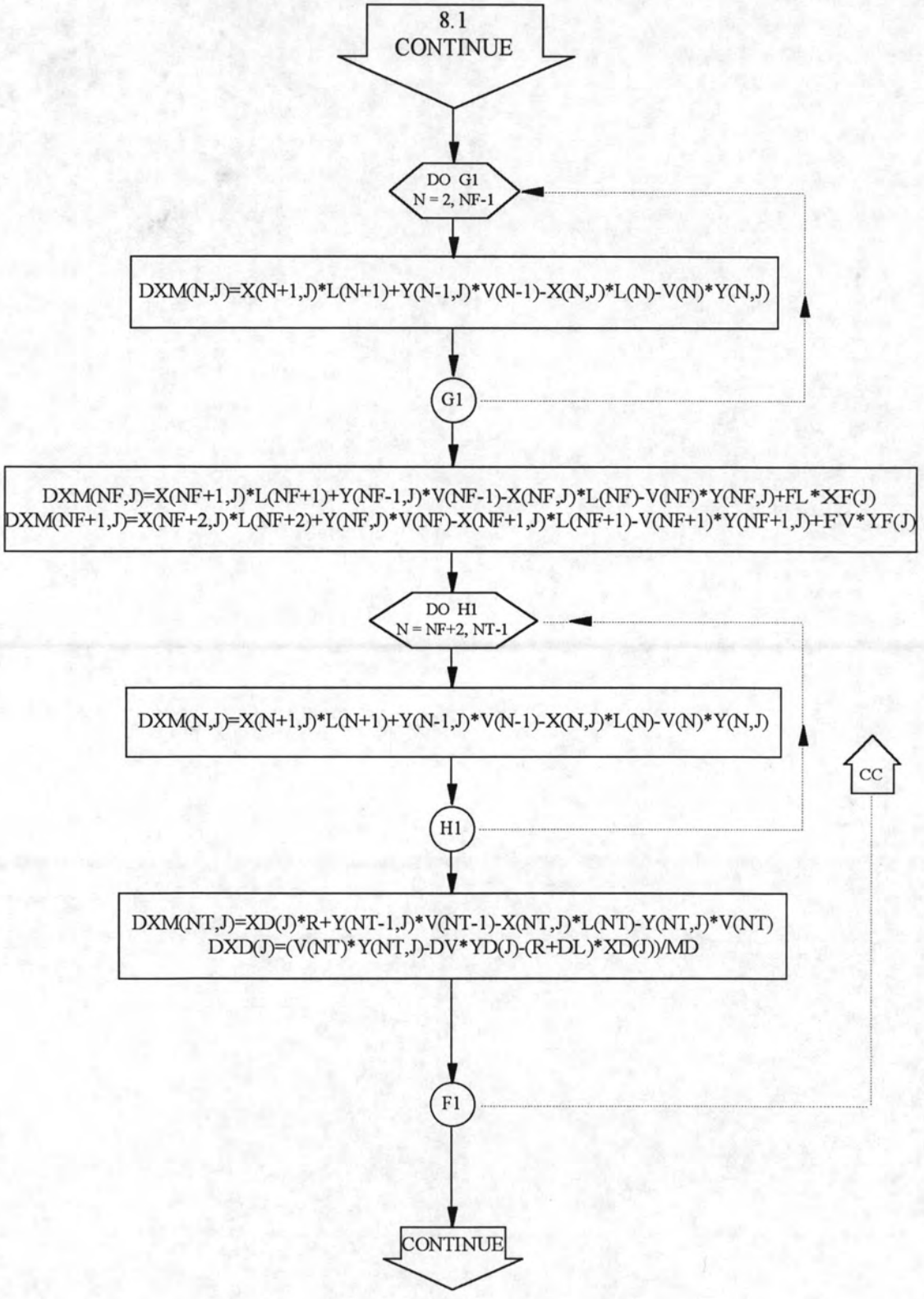
8.1) Running a full-order model (Continue)



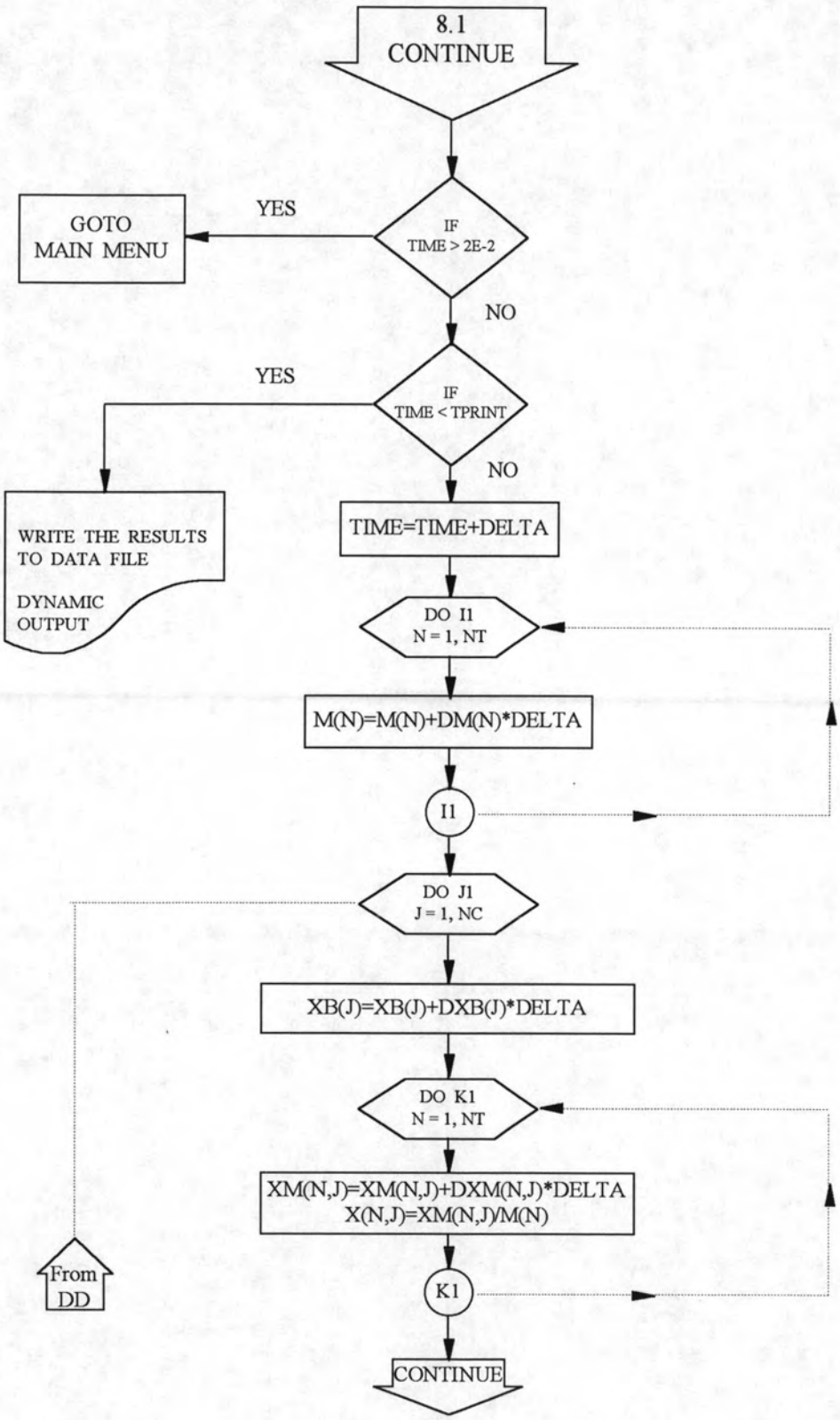
8.1) Running a full-order model (Continue)



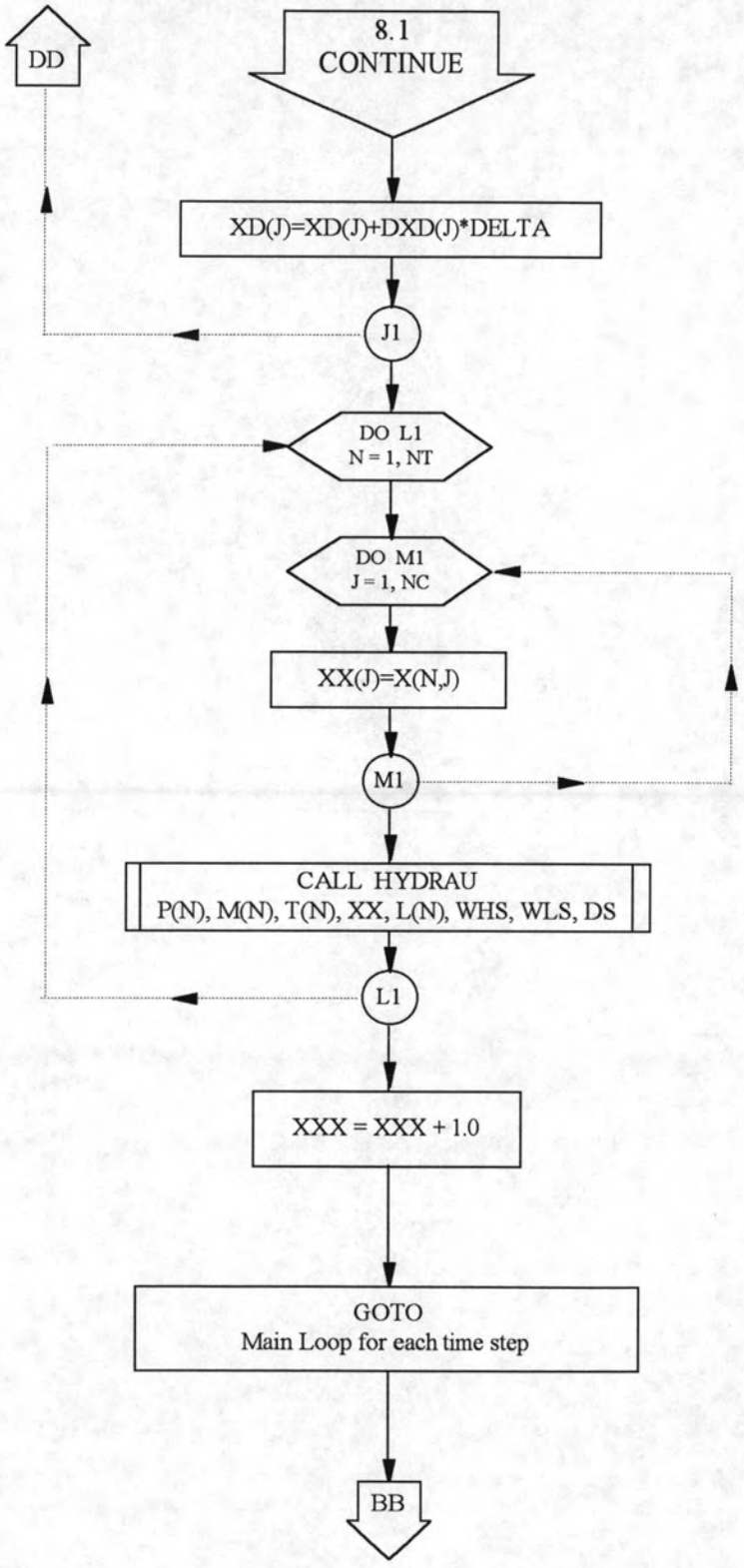
8.1) Running a full-order model (Continue)



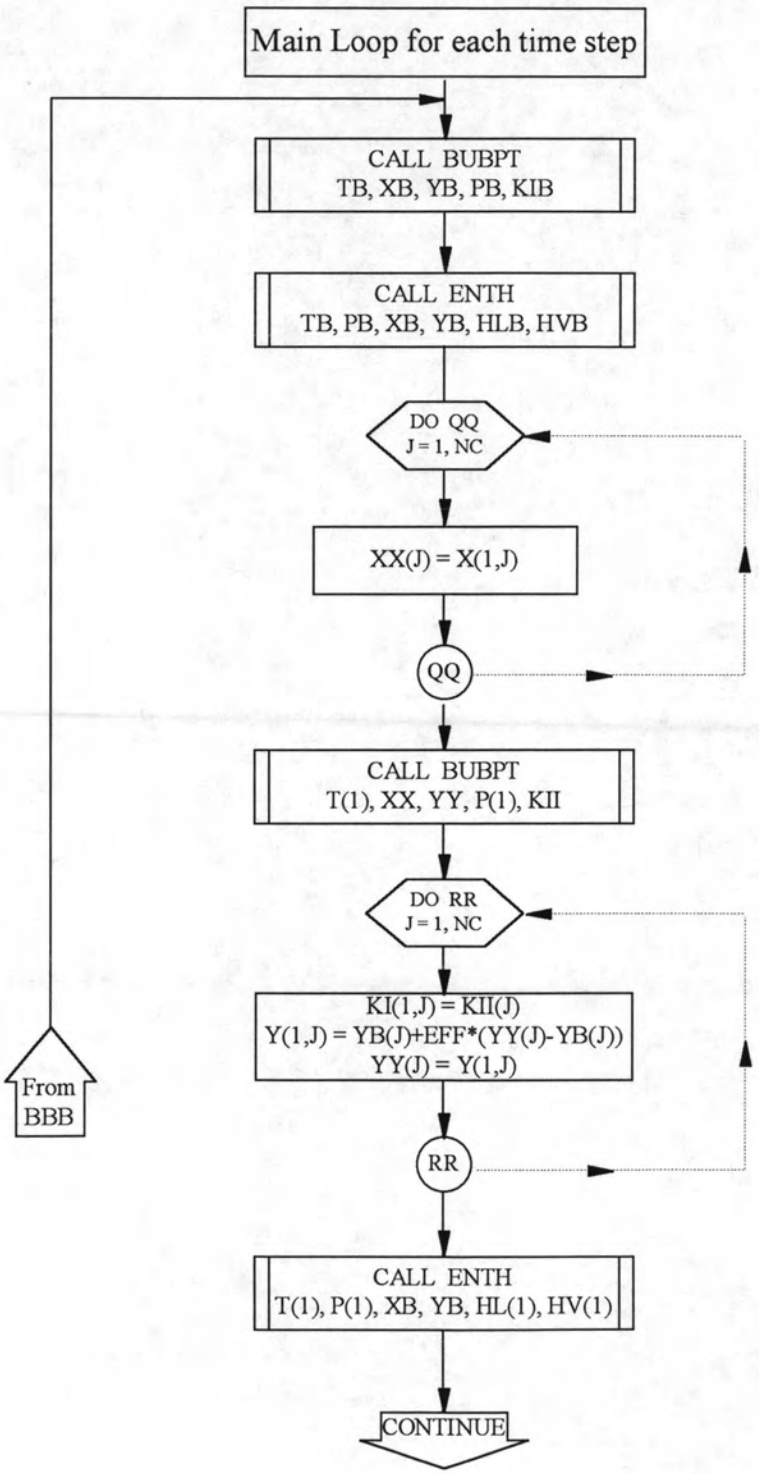
8.1) Running a full-order model (Continue)



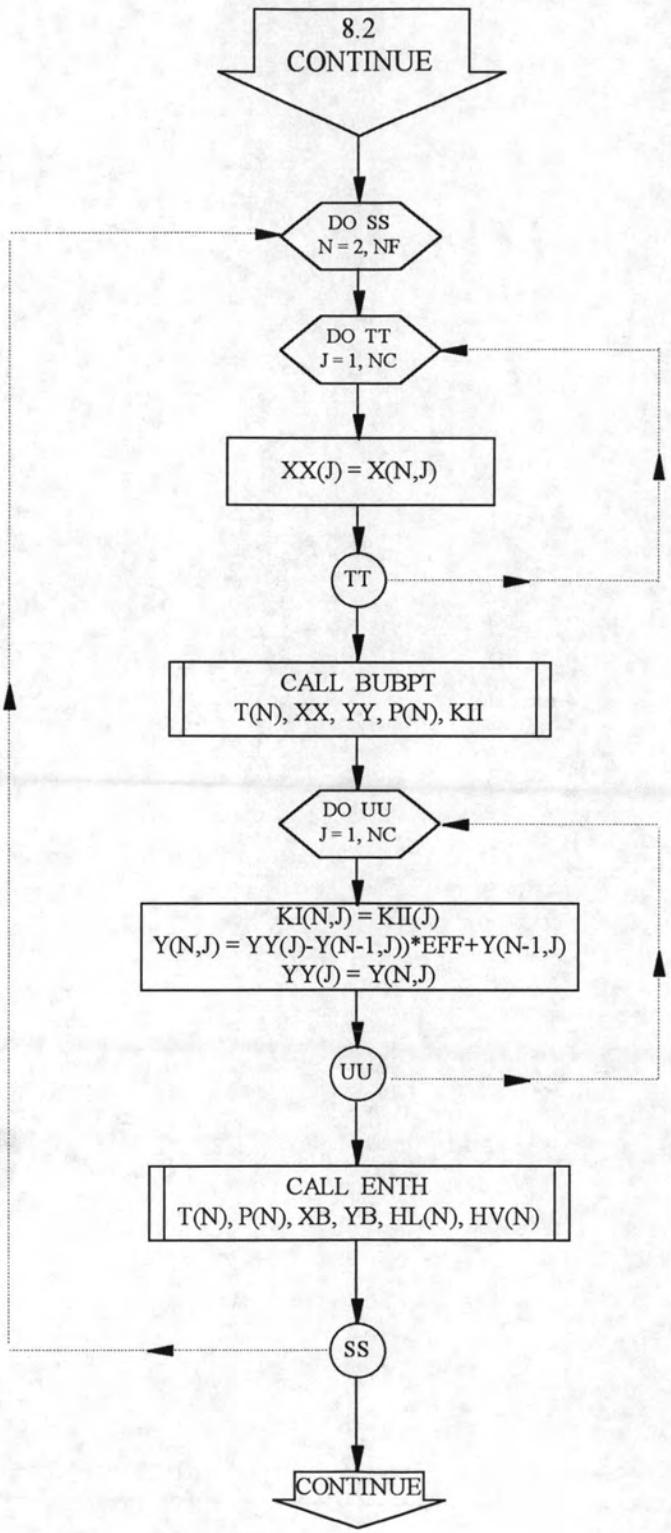
8.1) Running a full-order model (Continue)



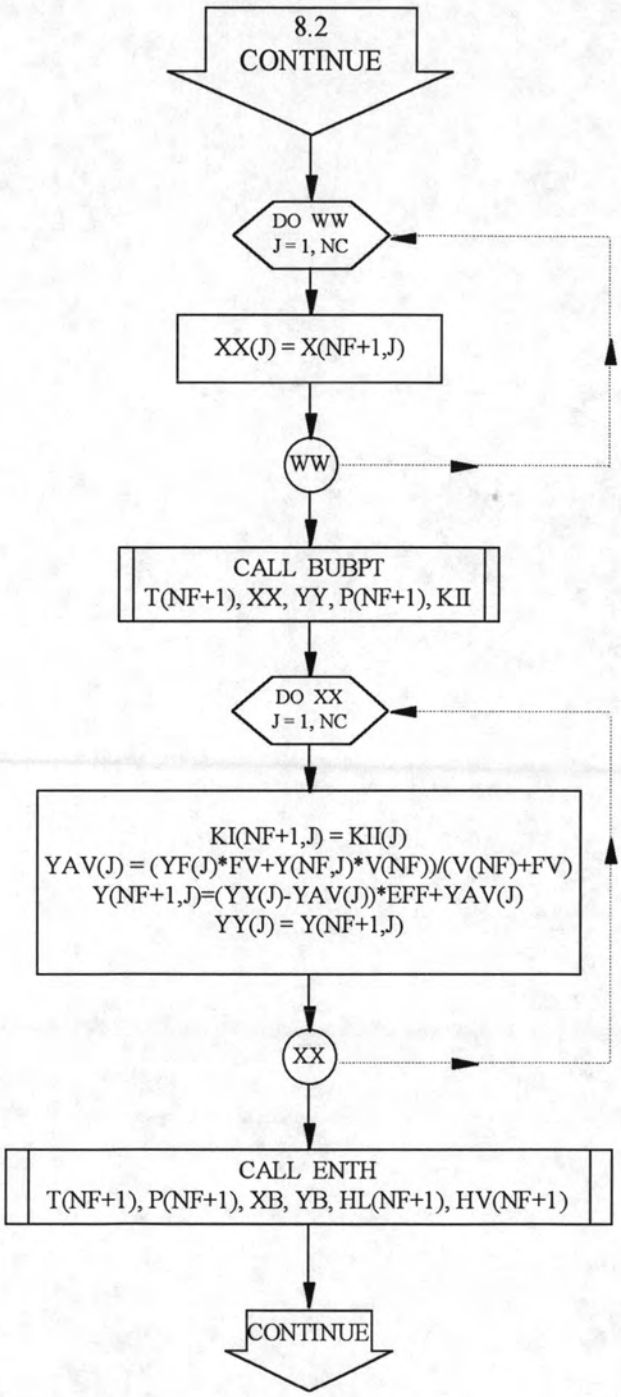
8.1) Running a full-order model (Continue)



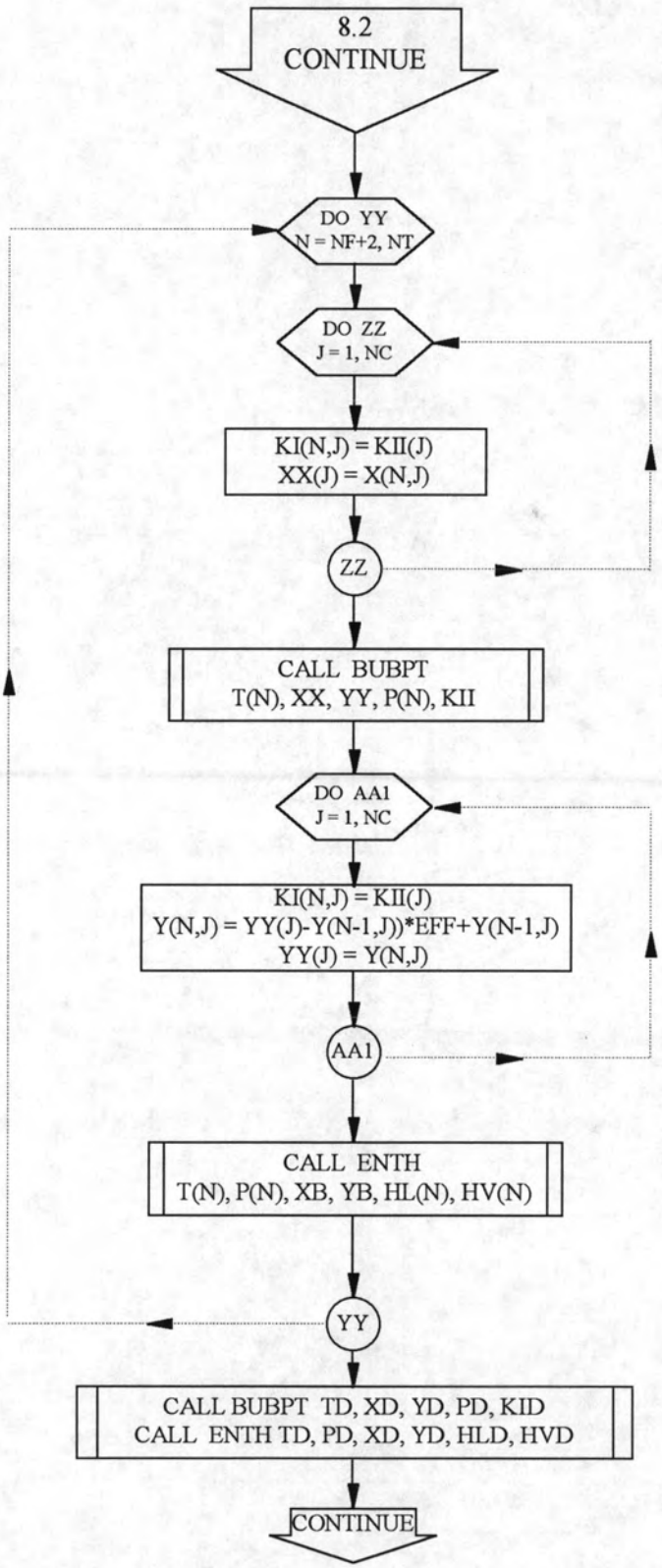
8.2) Running a compartmental model



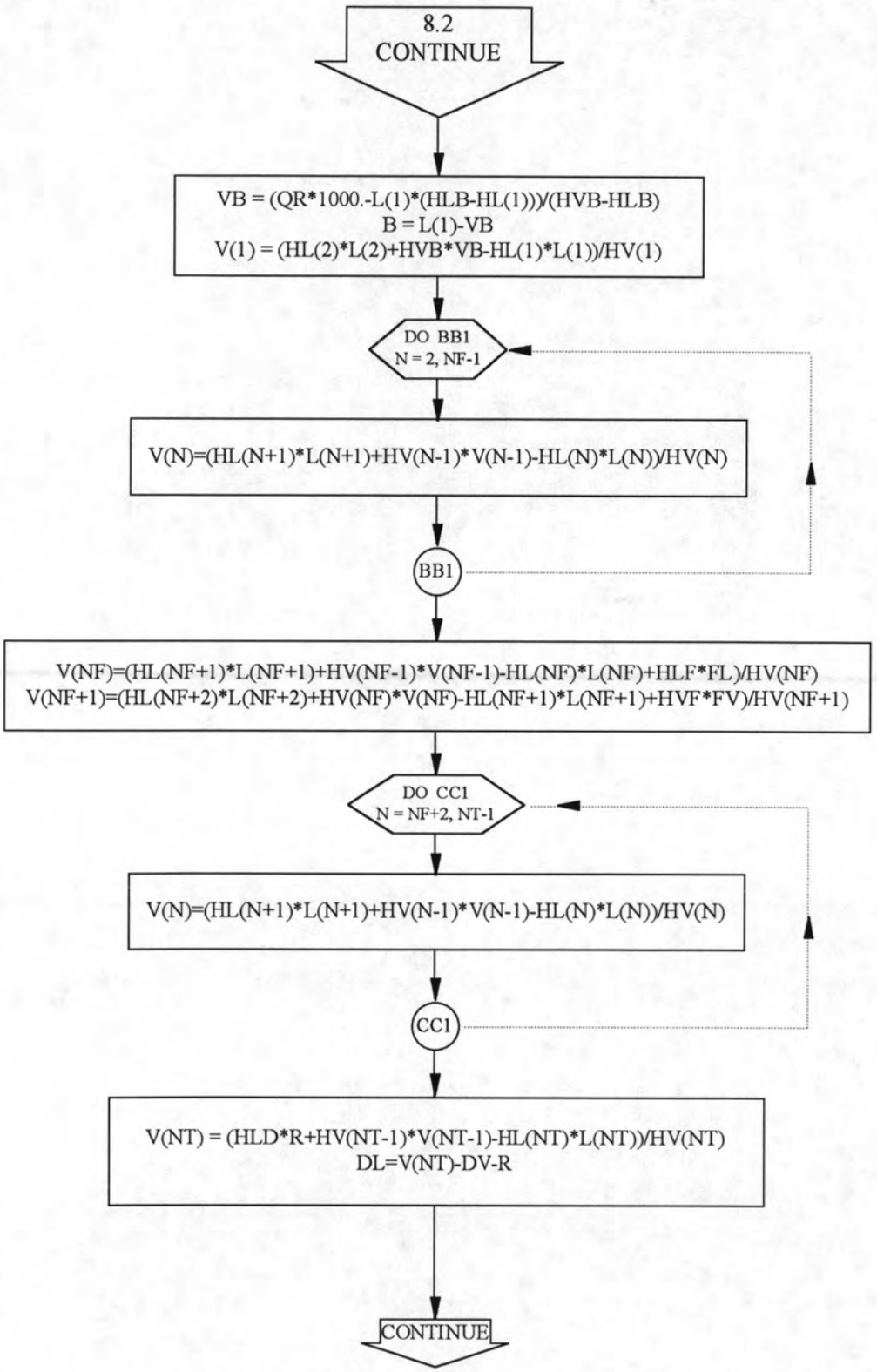
8.2) Running a compartmental model (Continue)



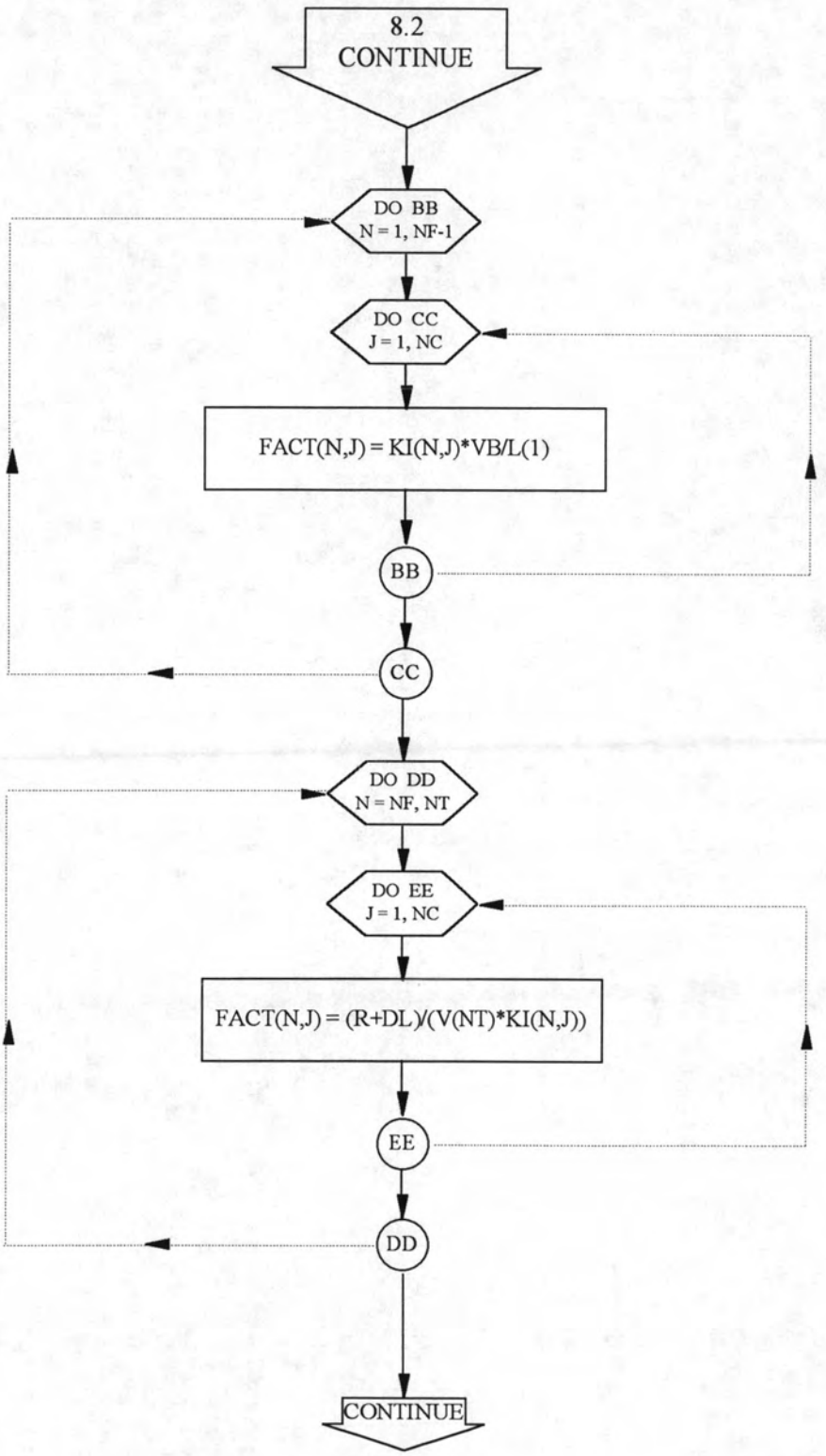
8.2) Running a compartmental model (Continue)



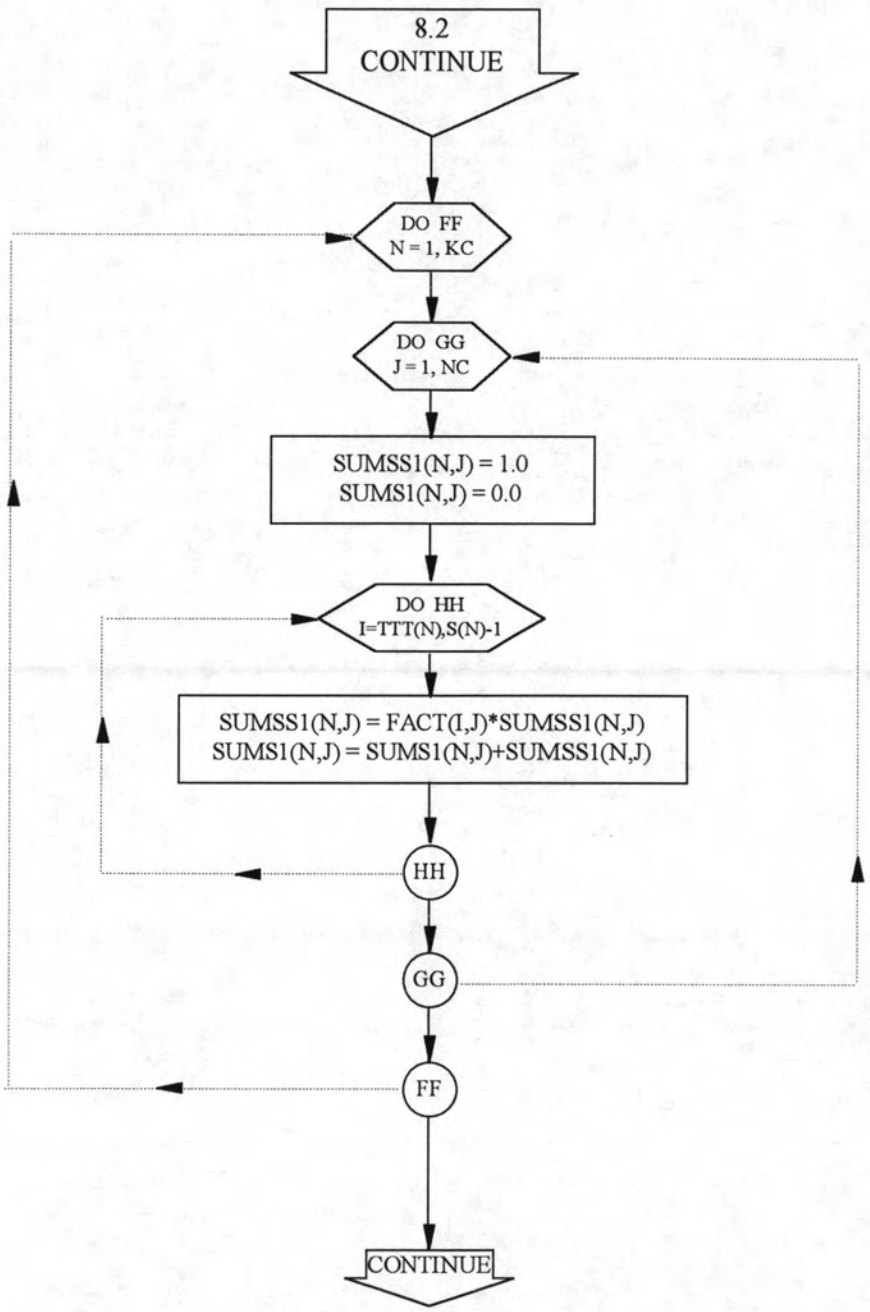
8.2) Running a compartmental model (Continue)



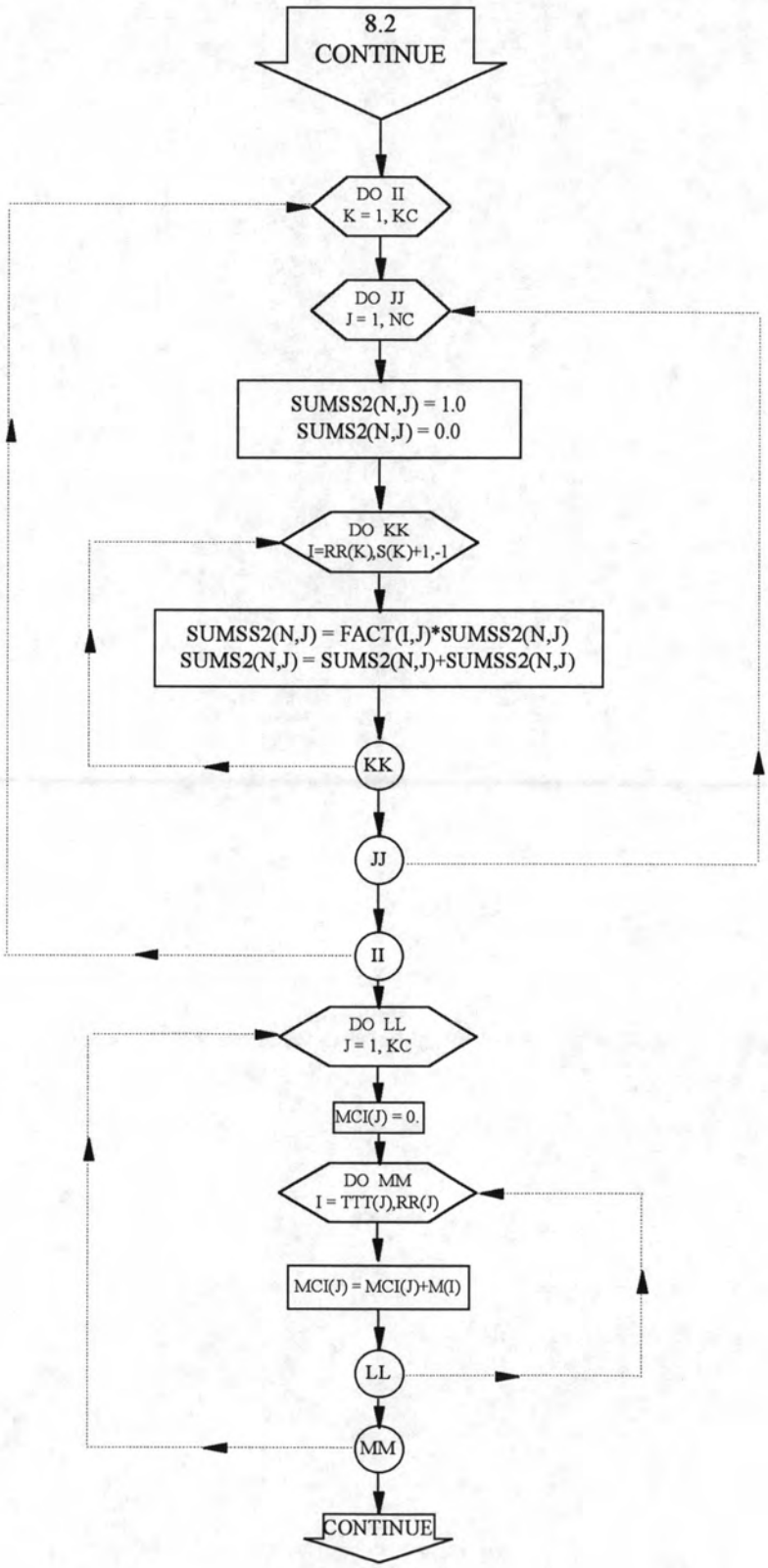
8.2) Running a compartmental model (Continue)



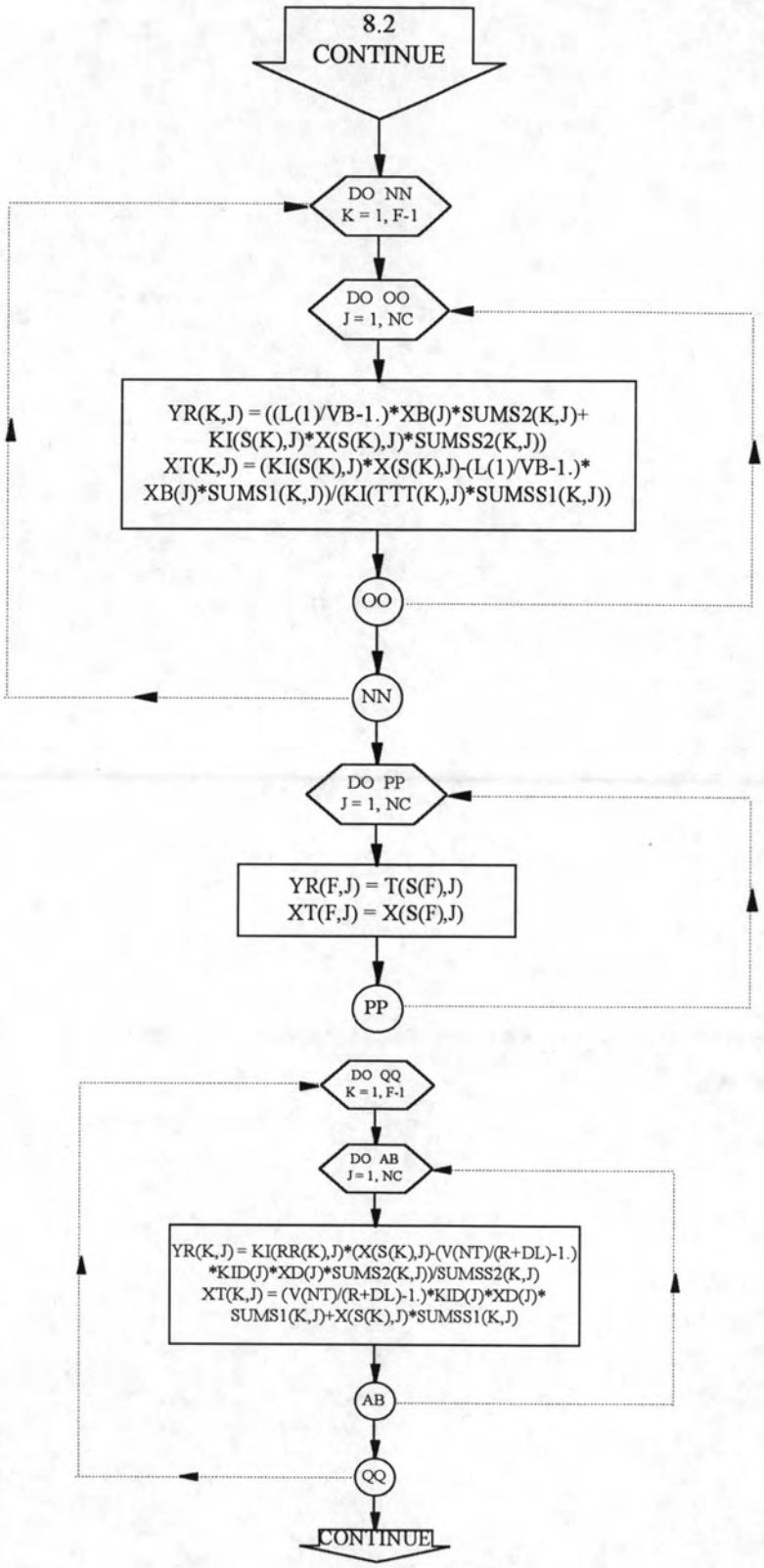
8.2) Running a compartmental model (Continue)



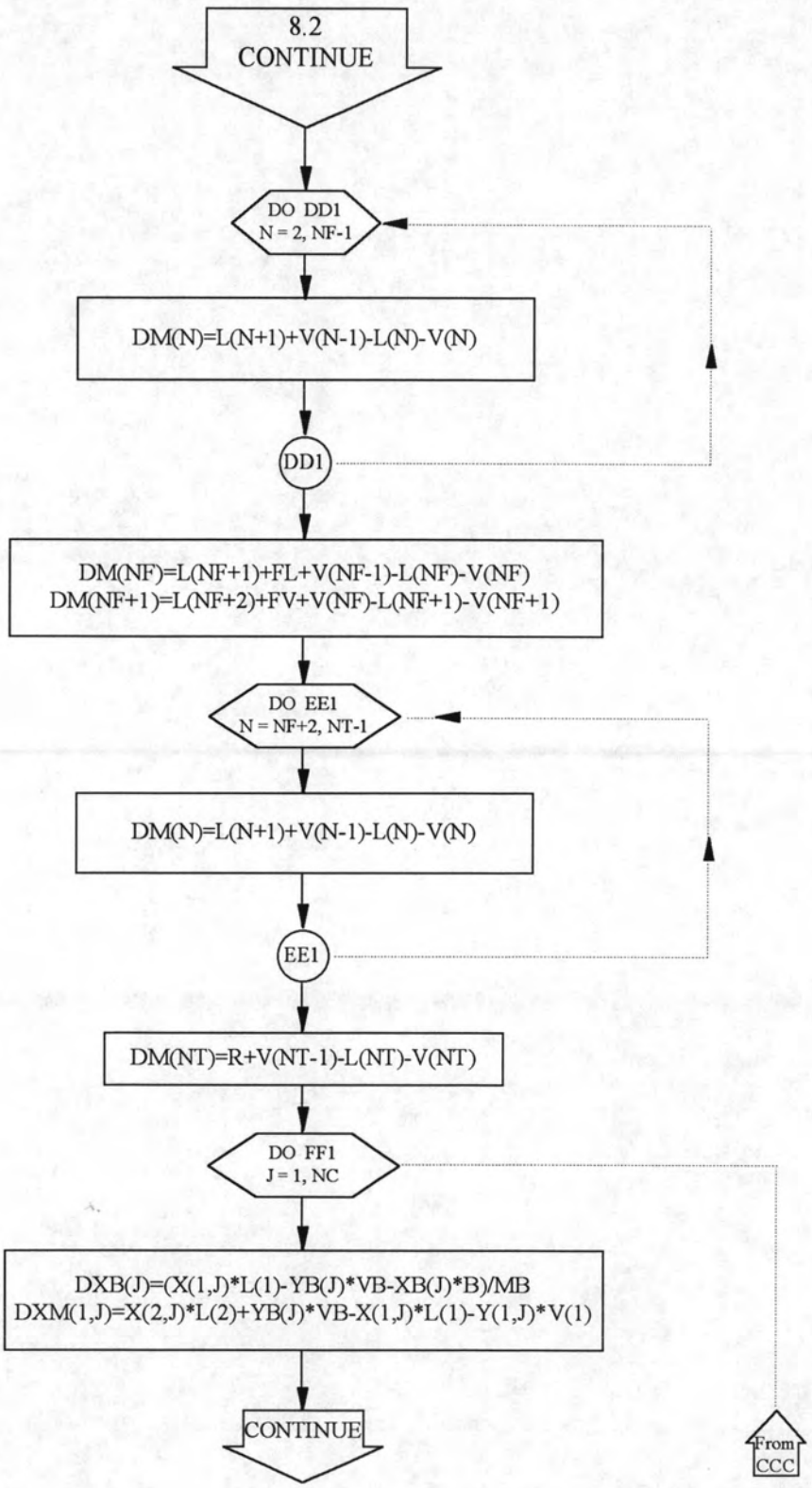
8.2) Running a compartmental model (Continue)



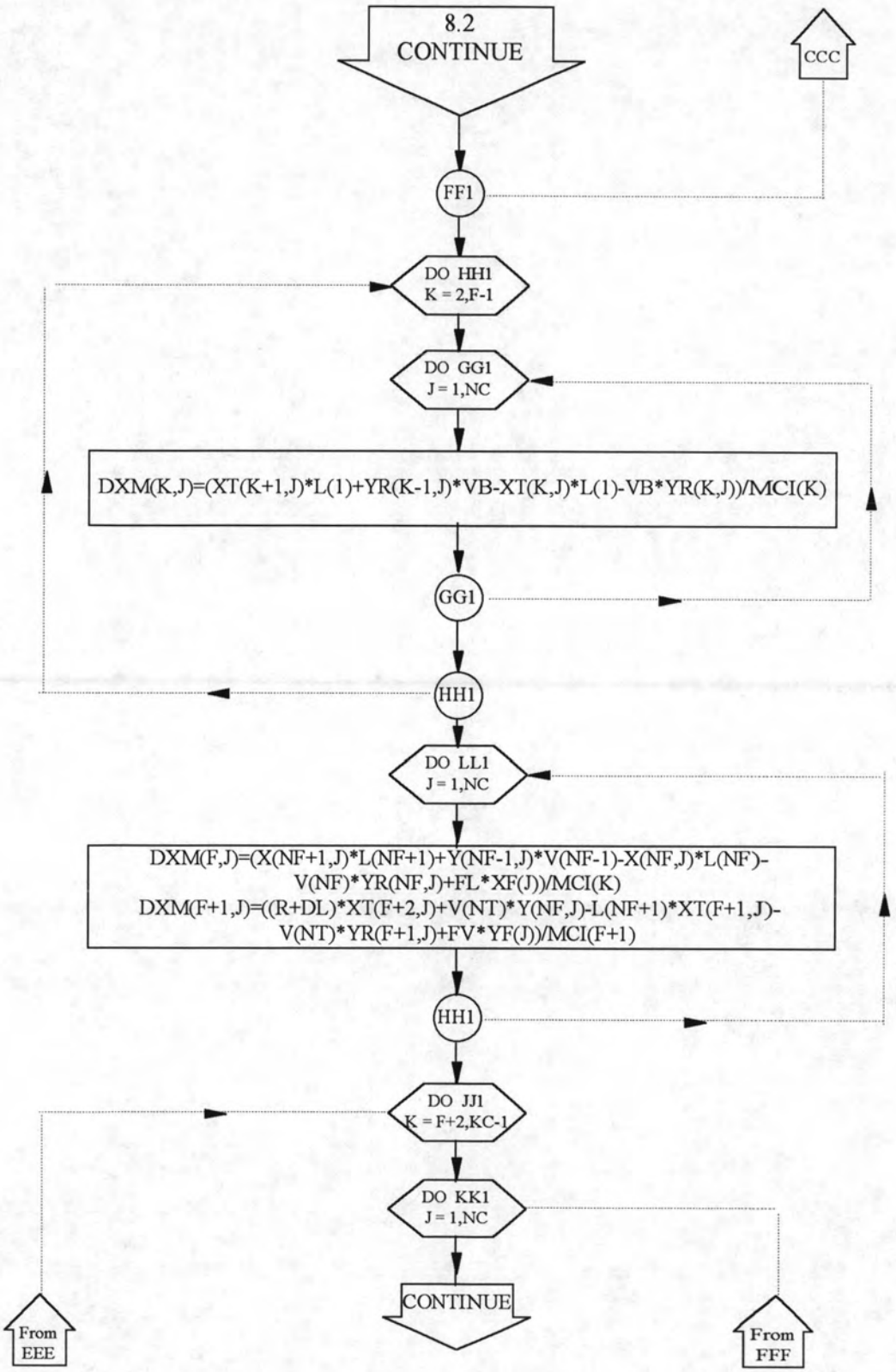
8.2) Running a compartmental model (Continue)



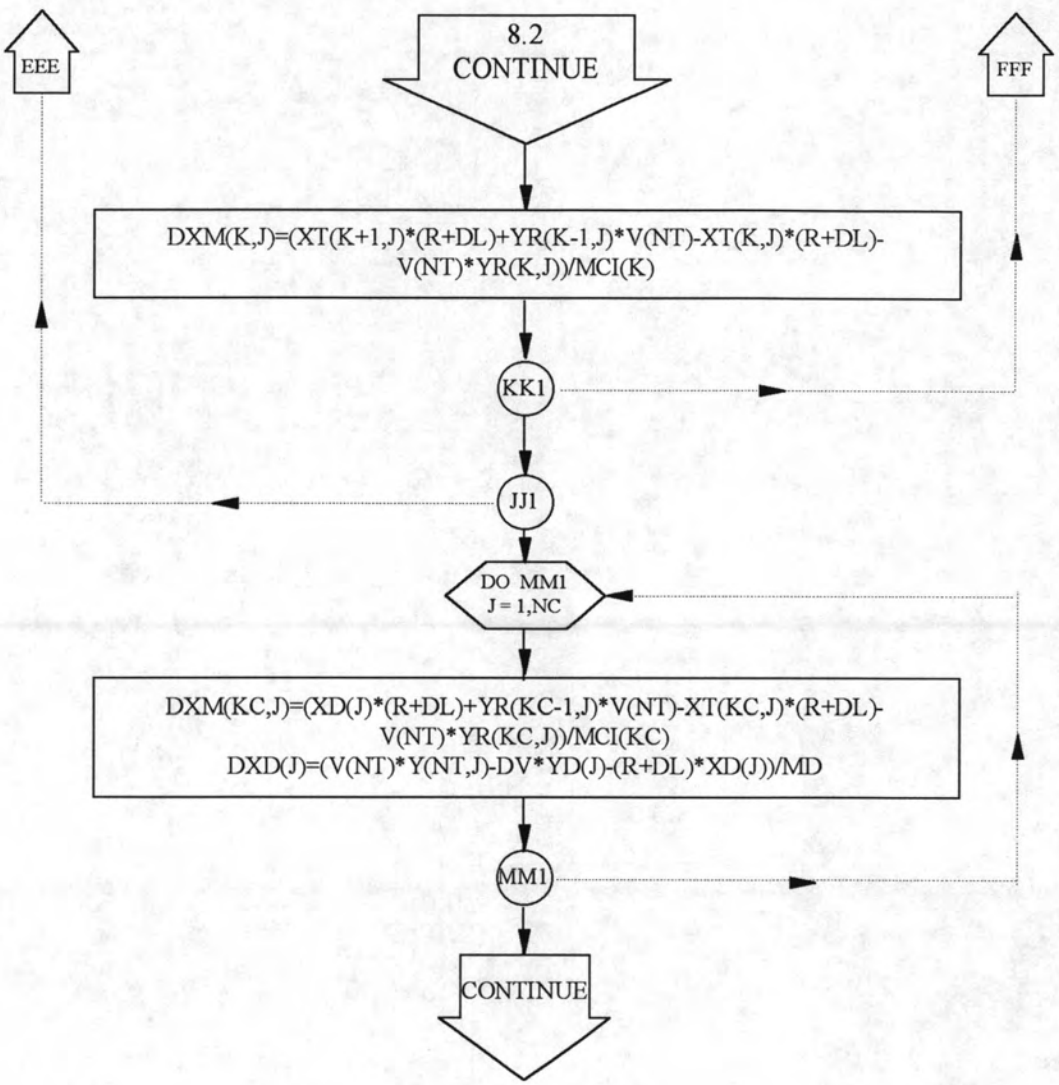
8.2) Running a compartmental model (Continue)



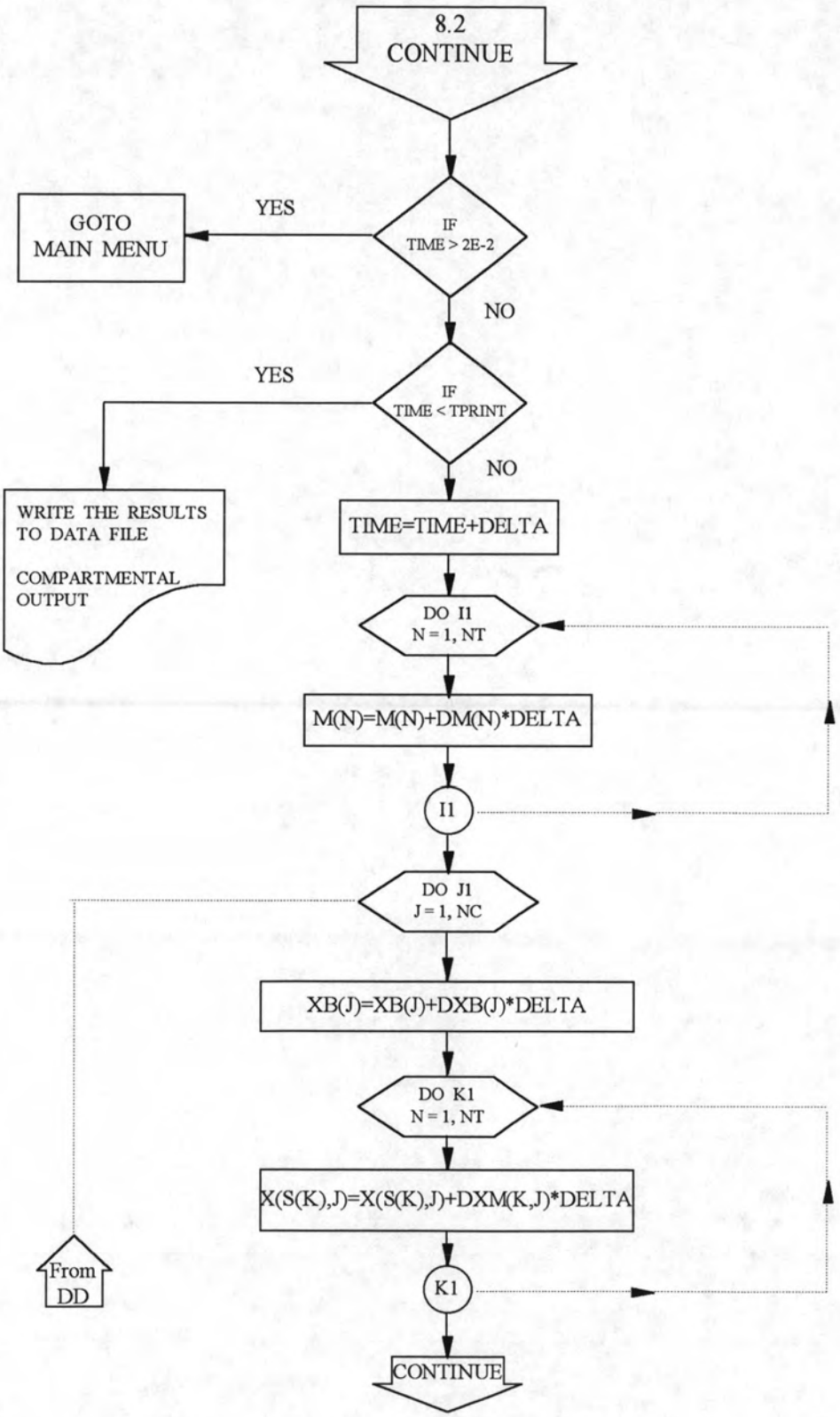
8.2) Running a compartmental model (Continue)



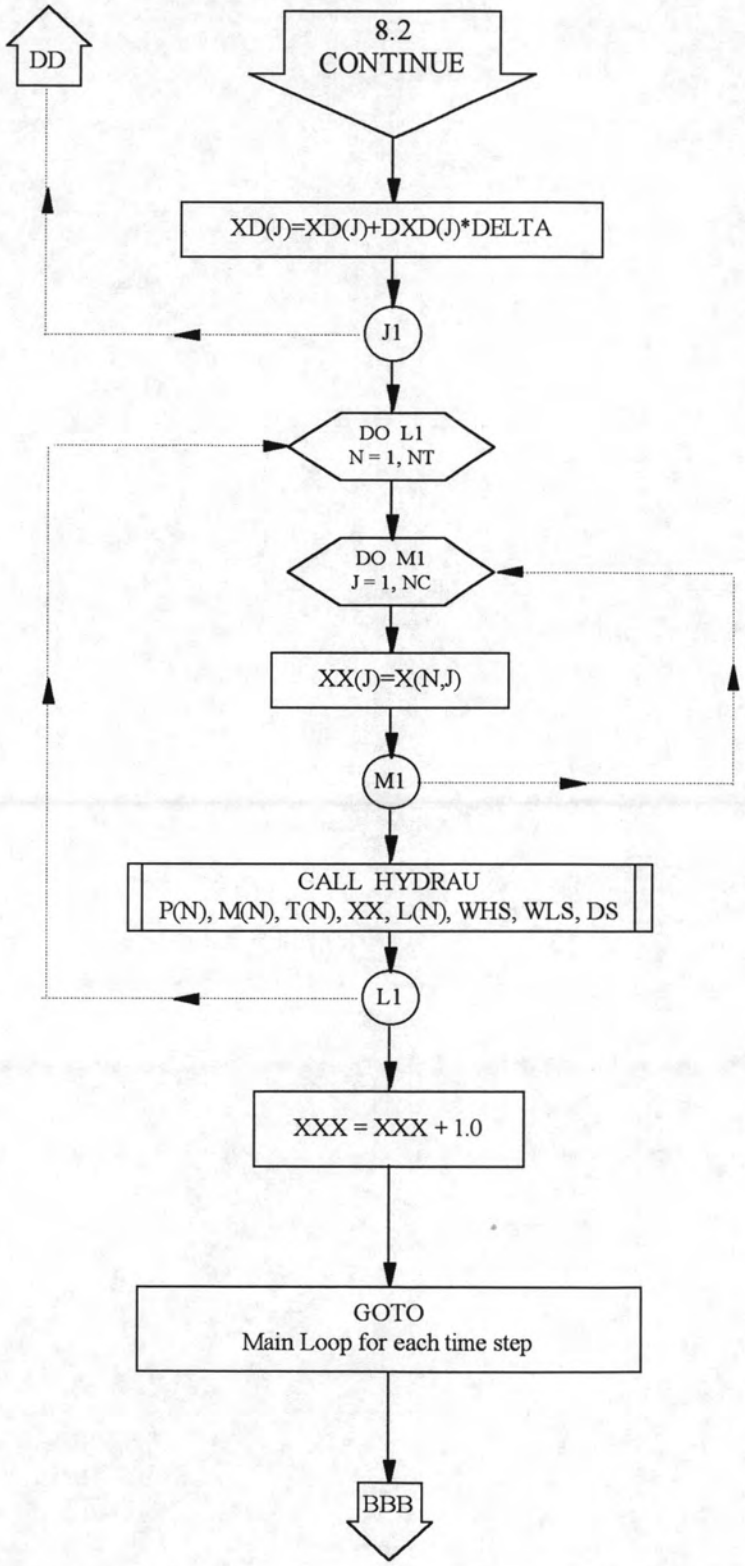
8.2) Running a compartmental model (Continue)



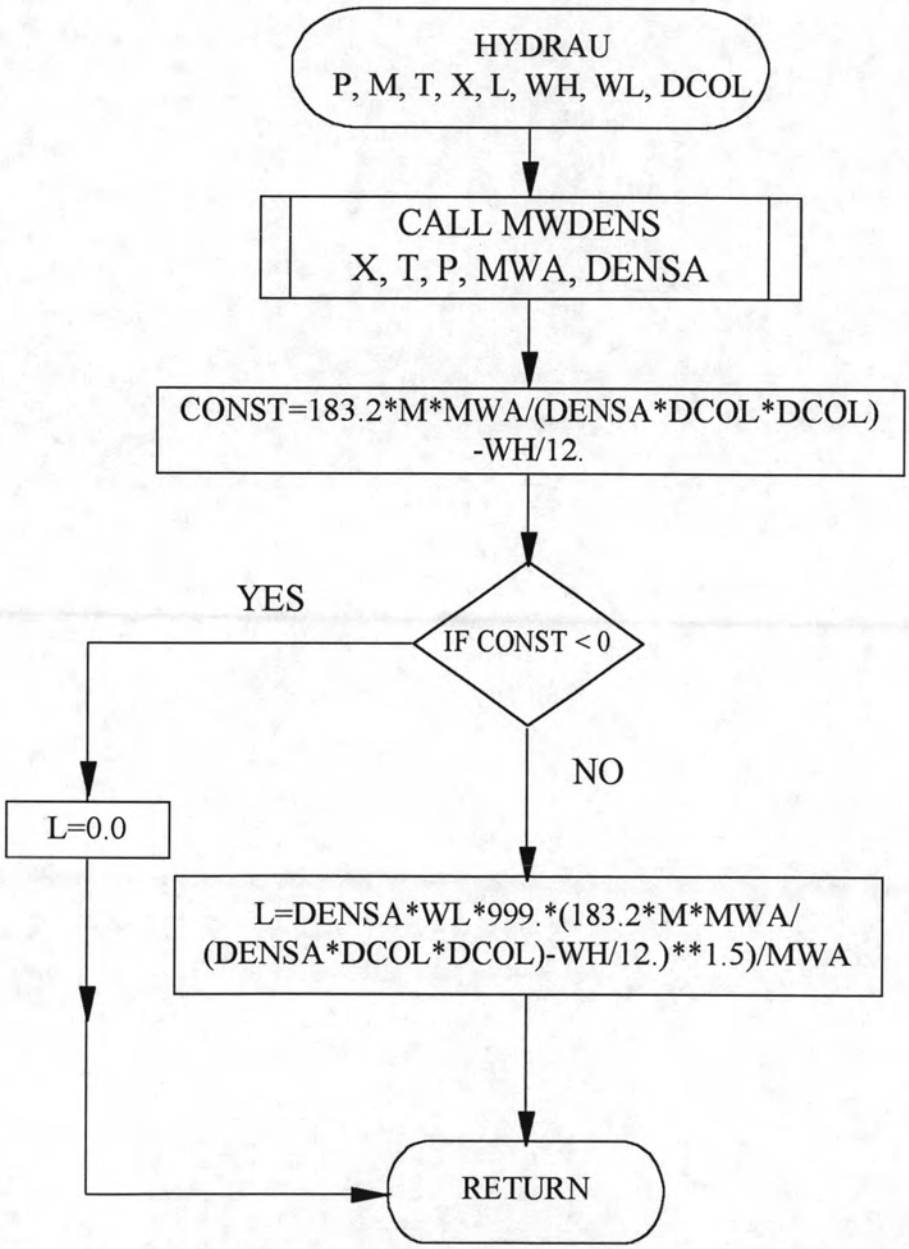
8.2) Running a compartmental model (Continue)



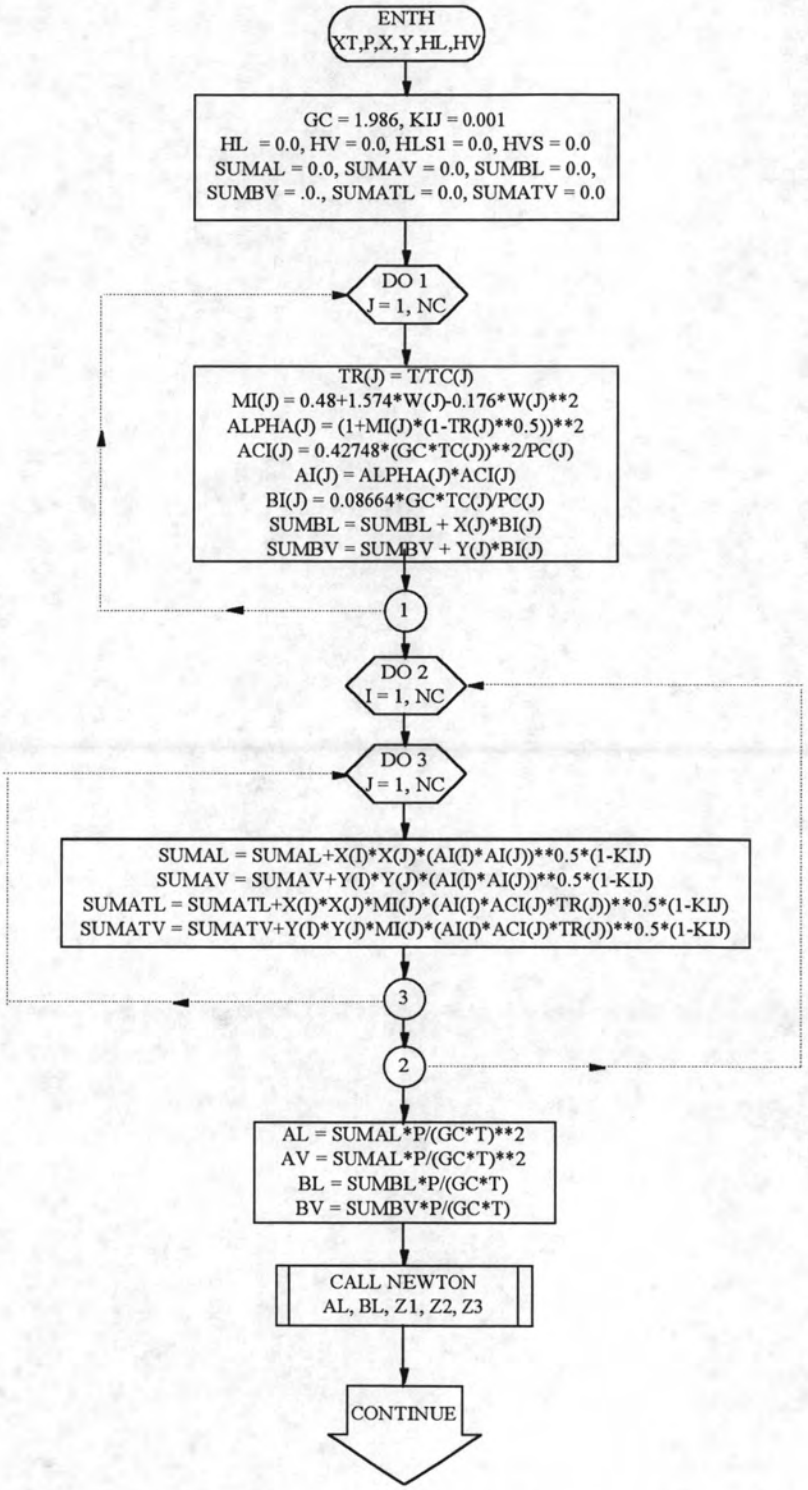
8.2) Running a compartmental model (Continue)



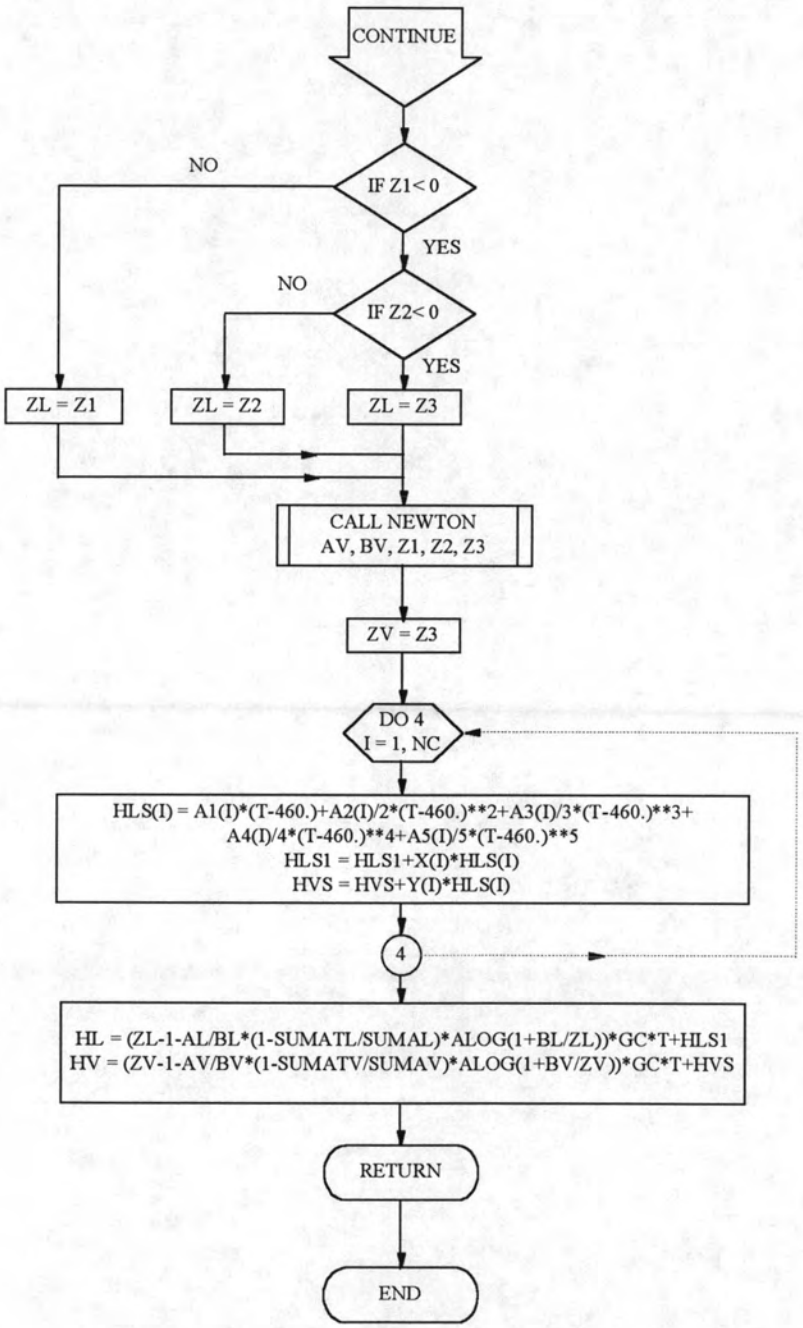
8.2) Running a compartmental model (Continue)



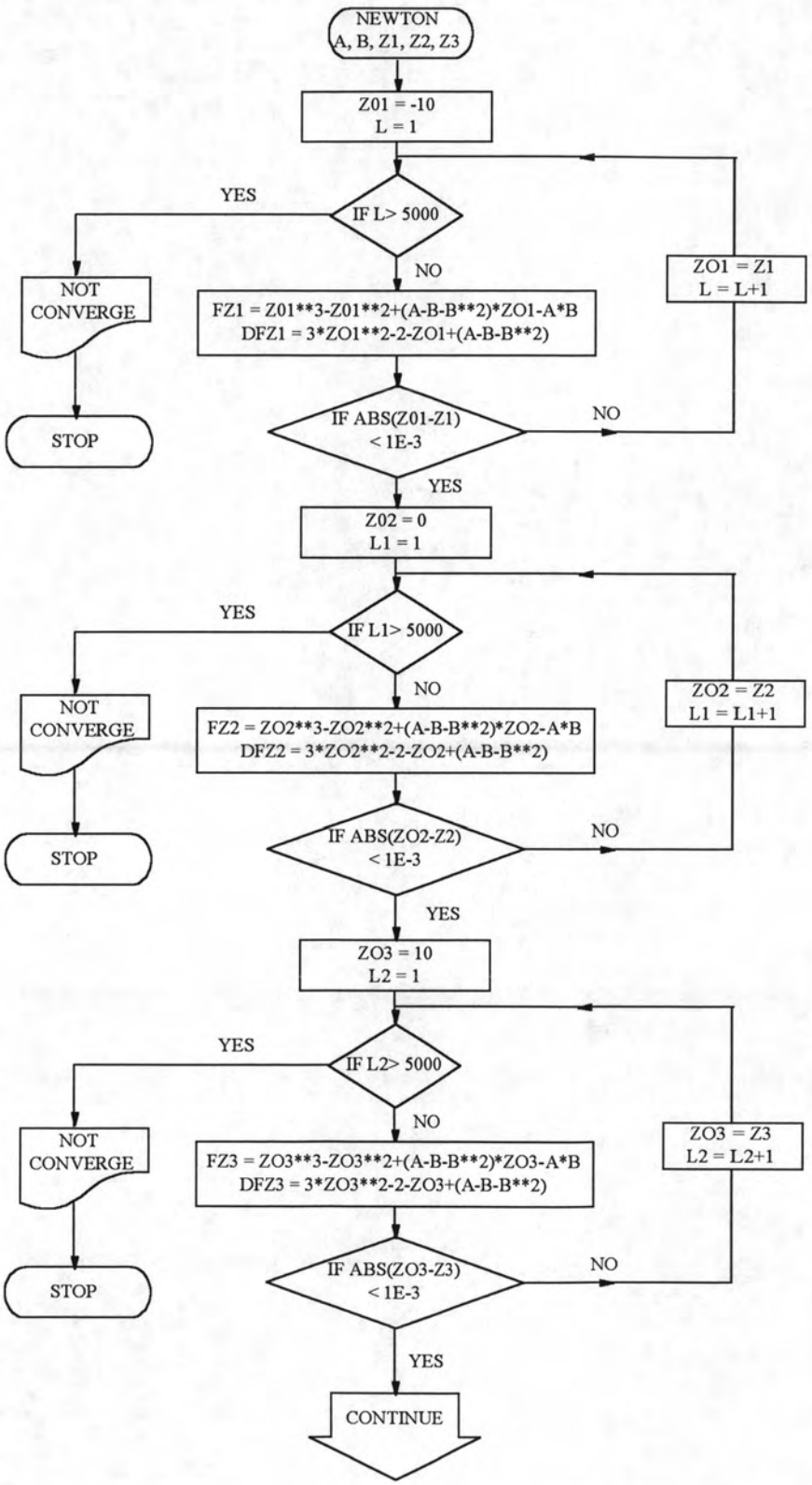
SUBPROGRAM HYDRAU



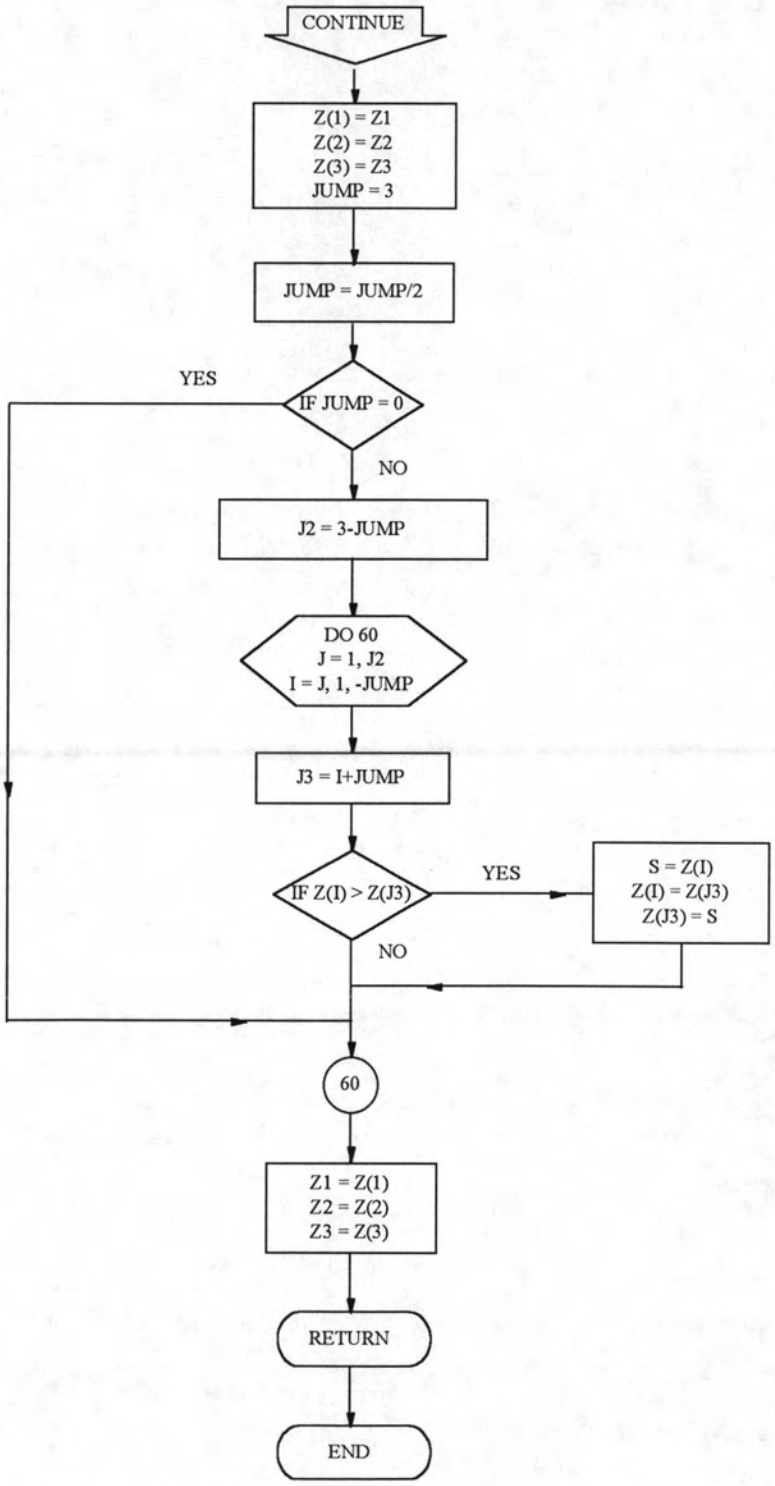
SUBROUTINE ENTH



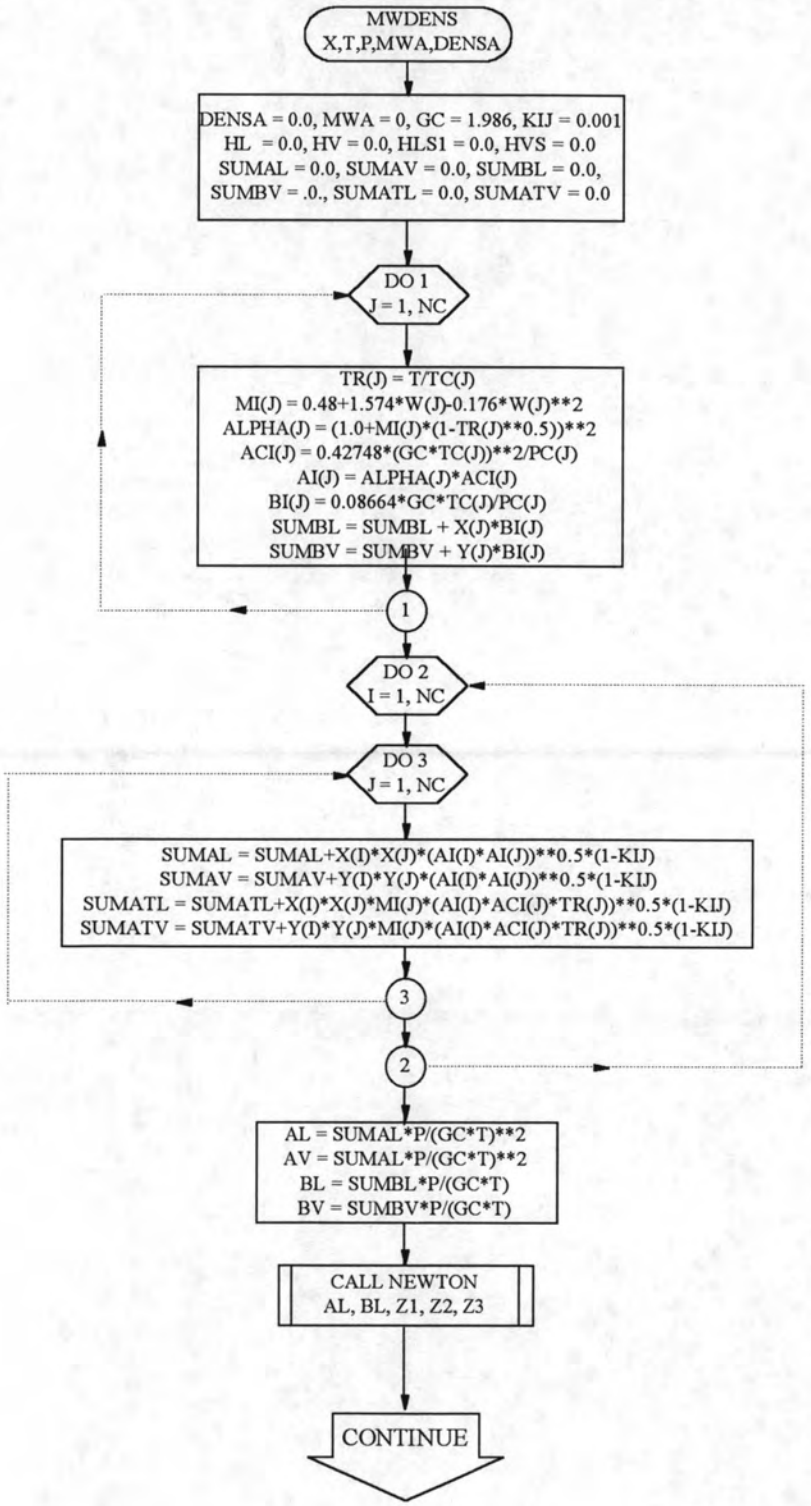
SUBROUTINE ENTH (Continue)



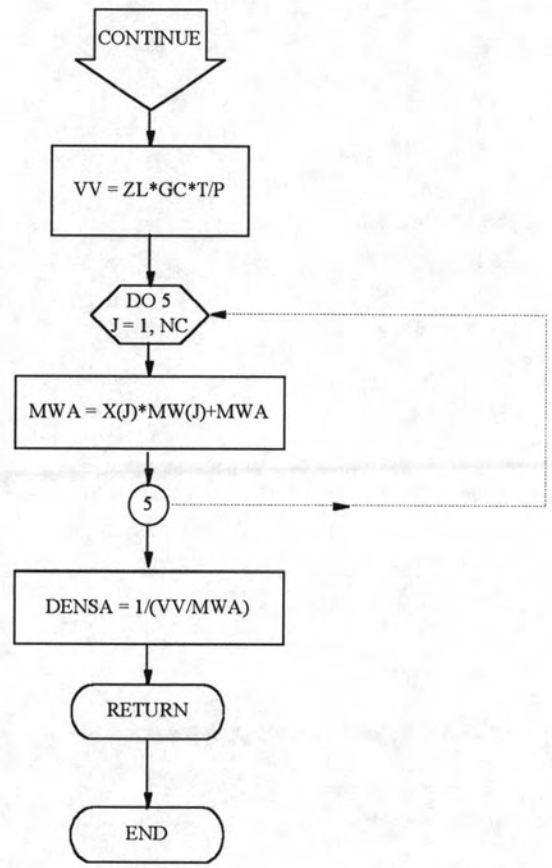
SUBROUTINE NEWTON



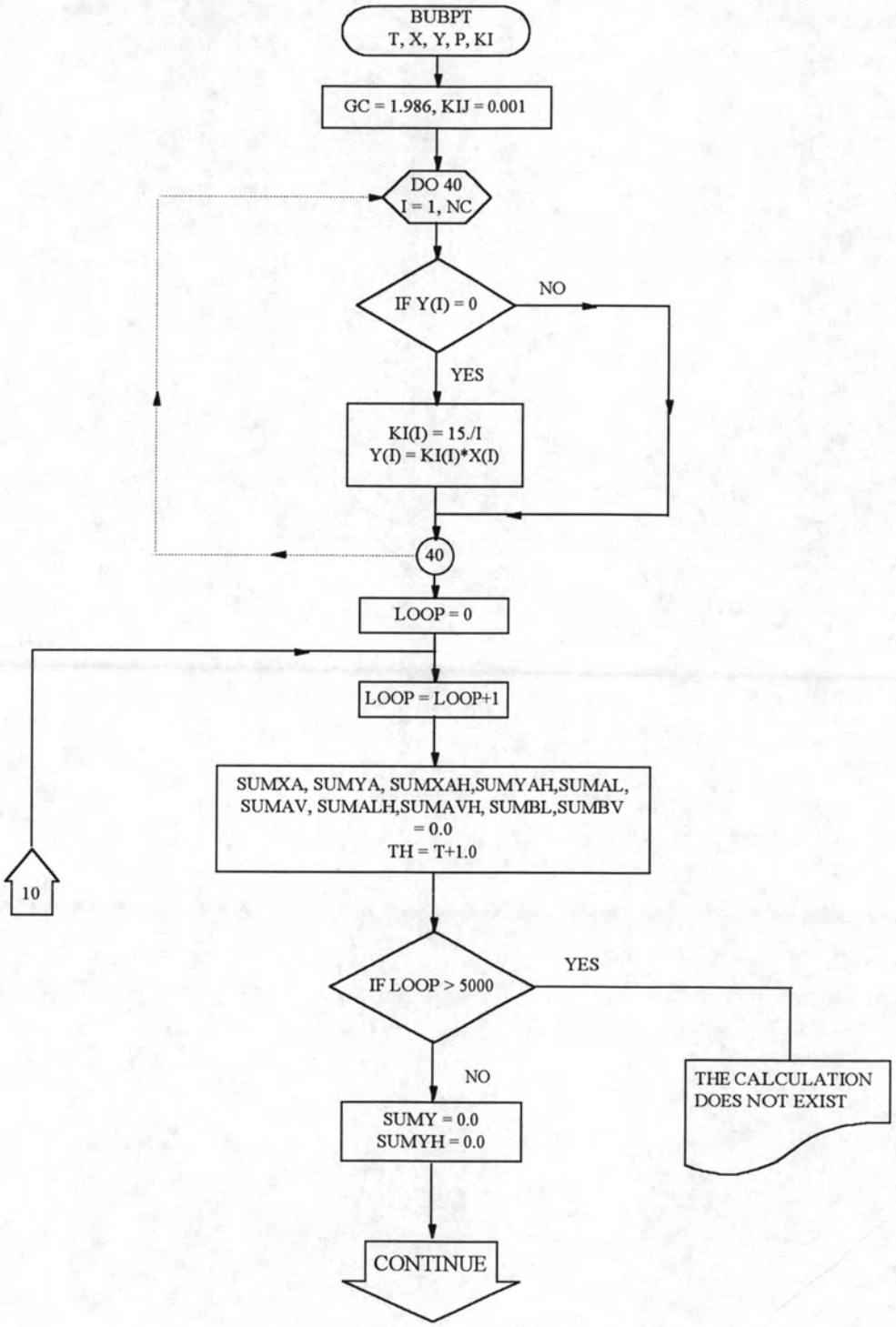
SUBROUTINE NEWTON (Continue)



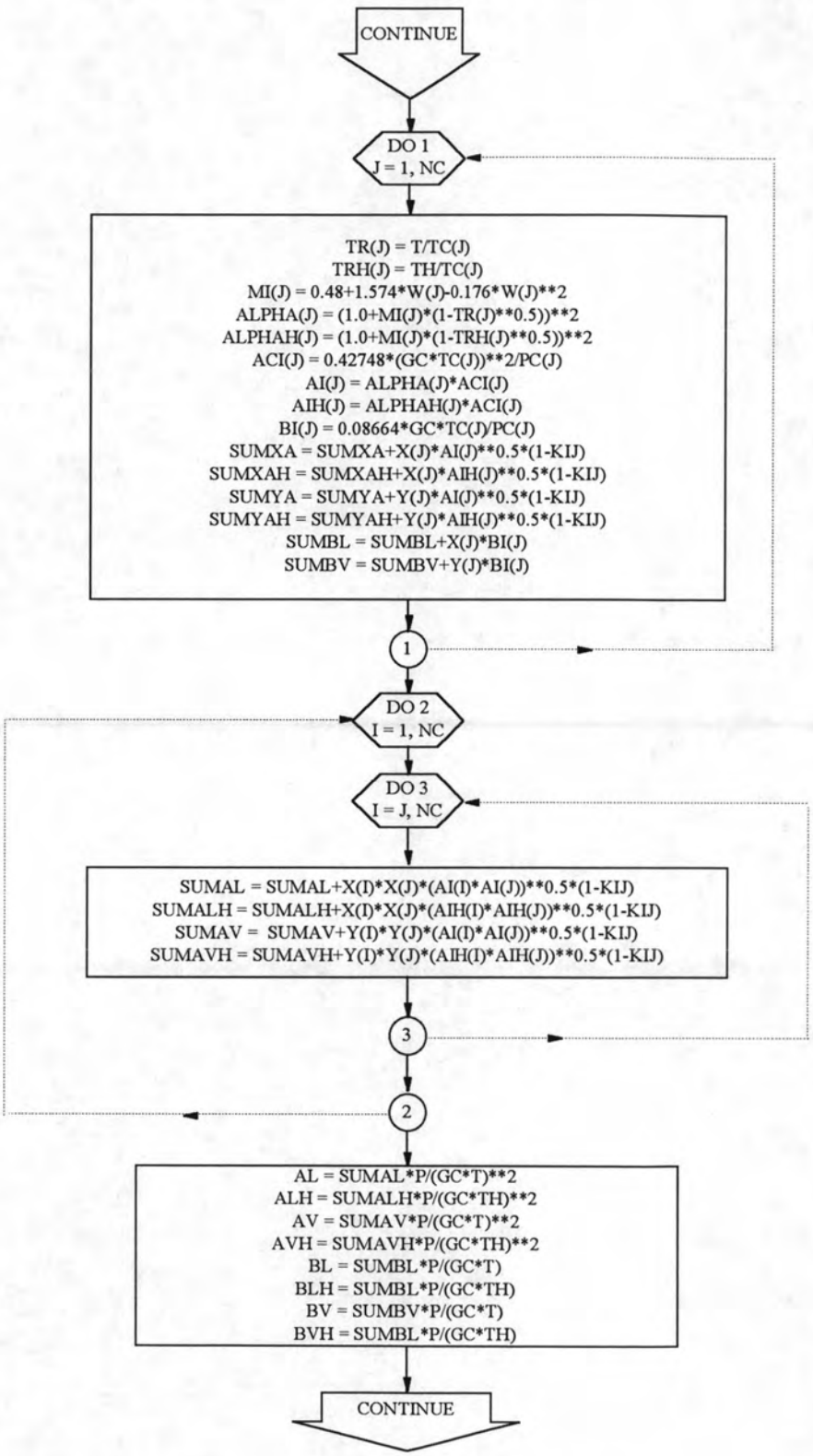
SUBROUTINE MWDENS



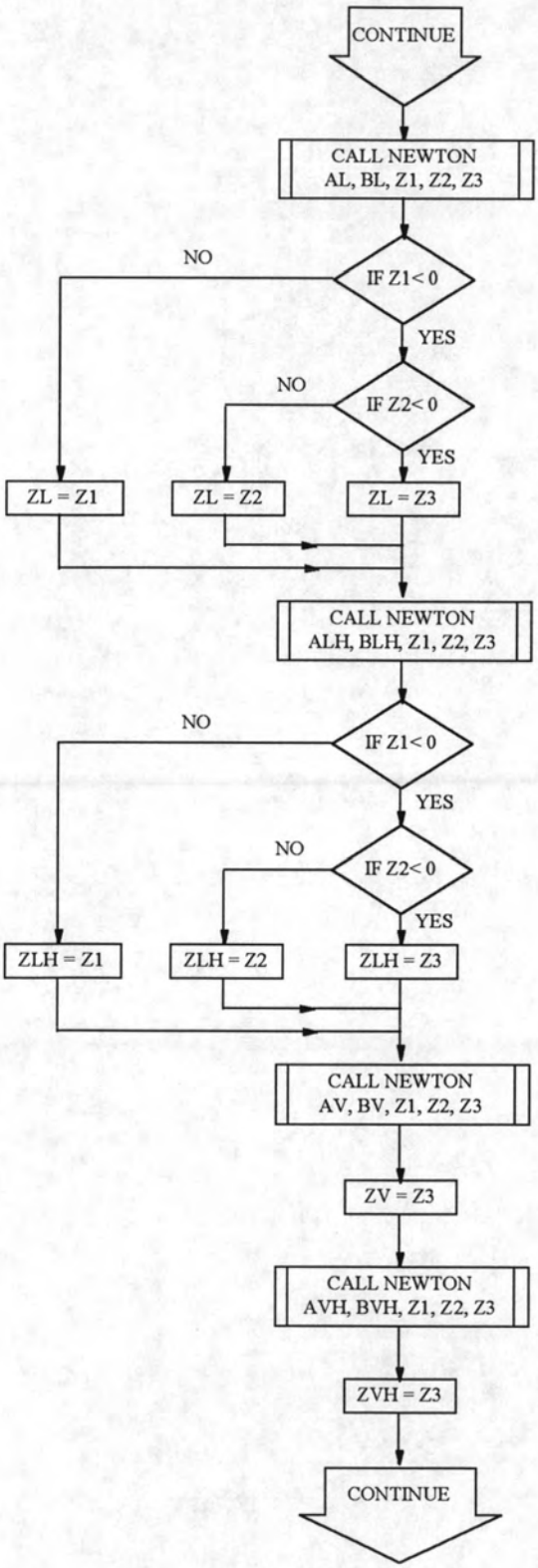
SUBROUTINE MWDENS (Continue)



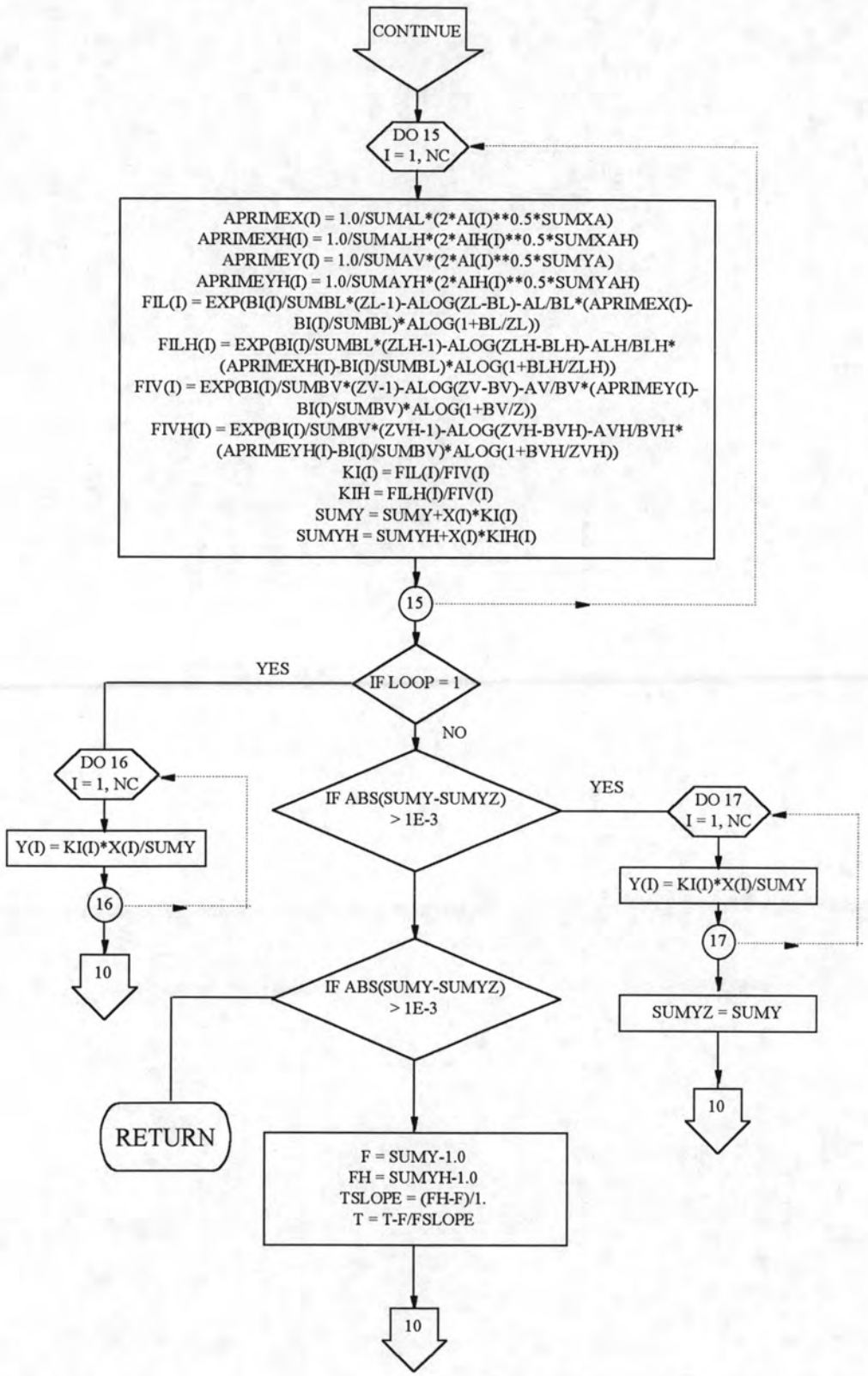
SUBROUTINE BUBPT



SUBROUTINE BUBPT (Continue)



SUBROUTINE BUBPT (Continue)



SUBROUTINE BUBPT (Continue)

Appendix B
List of Computer Program

```
CC    Compartmental Simulation Program for Multicomponent Distillation
CC    Created by Mr.Warin Iamteerapaiboon C 517339
CC    Chemical Engineering Department
CC    Chulalongkorn University @1994


      INCLUDE  'FGRAPH.FI'
      INCLUDE  'FGRAPH.FD'


CC
CC    Declare all variables
CC

CC
CC    INPUTS R, QR AND DV ARE FIXED
CC

      REAL MW,LO,MVB,MVD,MWA,MV,LV,M,L,MB,MD,MW1,TB,TC,PC,ZC,W,
     +A1,A2,A3,A4,A5,KID,KIB,KI,MCI,KII

      CHARACTER*15 NAME,NAMEX,name1
      CHARACTER   str*2,ans*1

      COMMON NC,MW(10),DENS(10),C1(10),C2(10),C3(10),BPT(10),AVP(10),
     +BVP(10),tc(10),pc(10),zc(10),w(10),a1(10),a2(10),a3(10),a4(10),
     +a5(10),rr(10),s(10),ttt(10),mci(10)

      DIMENSION LV(50),L(50),P(50),XF(10),YF(10),YAV(10),DXD(10),
     +YY(10),HL(50),HV(50),V(50),DM(50),DXM(50,10),XM(50,10),DXB(10)

      DIMENSION NAME(10),T(50),XB(10),X(50,10),Y(50,10),LO(50),XD(10),
     +YB(10),YD(10),XX(10),MV(50),M(50),KID(50),KIB(50),KI(50,10)

      DIMENSION FACT(50,10),YR(50,10),XT(50,10),SUMS1(50,10),
     +SUMS2(50,10),SUMSS1(50,10),SUMSS2(50,10),KII(10)

      INTEGER*2       dummy2, key, kc,rr,s,f,ttt
      EXTERNAL printmenu
      RECORD / rccoord / curpos

      OPEN( 1, FILE = 'physical.dat' )
      OPEN( 2, FILE = 'phytemp.dat' )
      OPEN( 5, FILE = 'result.dat')

CC
CC      Cover page
CC
```

```
      CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor(15)
      CALL settextposition( 3, 28, curpos )
      CALL outtext( 'Chulalongkorn  University' )
      CALL settextposition( 4, 25, curpos )
      CALL outtext( 'Chemical Engineering Department' )

      dummy2 = settextcolor( 14 )
      CALL settextposition( 11, 21, curpos )
      CALL outtext( 'Dynamics Compartmental Simulation Program' )
      CALL settextposition(13, 38, curpos )
      CALL outtext( 'for' )
      CALL settextposition(15, 27, curpos )
      CALL outtext( 'Multicomponent Distillation' )

      dummy2 = settextcolor( 15 )
      CALL settextposition(21, 35, curpos )
      CALL outtext( 'Created by' )
      CALL settextposition( 22, 24, curpos )
      CALL outtext( 'Mr.Warin Iamteerapaiboon  C 517339' )
      CALL settextposition( 23, 32, curpos )
      CALL outtext( 'M.Eng. Thesis @ 1994' )

      READ (*,*)
      CALL clearscreen( $VIEWPORT )

CC
CC   MAIN MENU
CC

 9000 key = -1
      DO WHILE( (key .LT. 0) .OR. (key .GT. 9) )
      CALL drawlines()
      CALL drawlines1()

      dummy2 = settextcolor( 14 )
      CALL settextposition( 4, 30, curpos )
      CALL outtext( '**** MAIN MENU ****' )
      dummy2 = settextcolor( 15 )
      CALL settextposition( 8, 25, curpos )
      CALL outtext( '0) Exit to Dos' )
      CALL settextposition( 9, 25, curpos )
      CALL outtext( '1) Components Database' )
      CALL settextposition( 10, 25, curpos )
      CALL outtext( '2) Characteristic of Column' )
      CALL settextposition( 11, 25, curpos )
      CALL outtext( '3) Operating Conditions' )
      CALL settextposition( 12, 25, curpos )
      CALL outtext( '4) Feed Data' )
      CALL settextposition( 13, 25, curpos )
      CALL outtext( '5) Initial Conditions')
      CALL settextposition( 14, 25, curpos )
      CALL outtext( '6) Edit Input Data' )
      CALL settextposition( 15, 25, curpos )
```

```
      CALL outtext( '7) Save Input Data' )
      CALL settextposition( 16, 25, curpos )
      CALL outtext( '8) Run' )
      CALL settextposition( 17, 25, curpos )
      CALL outtext( '9) Reporting & Reviewing the results' )
      dummy2 = settextcolor(14)
      CALL settextposition( 22, 25, curpos )
      CALL outtext ( 'Please ENTER your selection : ' )
      READ (*,*,ERR = 9000) key
      END DO
      dummy2 = setvideomode( $DEFAULTMODE )
      DO WHILE ( key .EQ. 0 )
            GOTO 400
      END DO

      DO WHILE ( key .EQ. 1 )
            GOTO 9100
      END DO

      DO WHILE ( key .EQ. 2 )
            GOTO 9200
      END DO

      DO WHILE ( key .EQ. 3 )
            GOTO 9300
      END DO

      DO WHILE ( key .EQ. 4 )
            GOTO 9400
      END DO

      DO WHILE ( key .EQ. 5 )
            GOTO 9500
      END DO

      DO WHILE ( key .EQ. 6 )
            GOTO 9600
      END DO

      DO WHILE ( key .EQ. 7 )
            GOTO 9700
      END DO

      DO WHILE ( key .EQ. 8 )
            GOTO 9800
      END DO

CC
CC    key = 1
CC

CC
CC    Component Database
CC
```

```
9100    keyc = -1
        DO WHILE( (keyc .LT. 0) .OR. (keyc .GT. 3) )
        CALL drawlines()
        CALL drawlines1()

        dummy2 = settextcolor( 14 )
        CALL settextposition( 4, 30, curpos )
        CALL outtext( '**** COMPONENT MENU ****' )
        dummy2 = settextcolor( 15 )
        CALL settextposition( 10, 25, curpos )
        CALL outtext( '0) Return to Main Menu' )
        CALL settextposition( 12, 25, curpos )
        CALL outtext( '1) List for All Components Database' )
        CALL settextposition( 14, 25, curpos )
        CALL outtext( '2) Select Component in your system ' )
        CALL settextposition( 16, 25, curpos )
        CALL outtext( '3) Append New Component Record' )
        dummy2 = settextcolor(14)
        CALL settextposition( 22, 25, curpos )
        CALL outtext ( 'Please ENTER your selection : ' )
        READ (*,*,ERR = 9100) keyc
        END DO
        dummy2 = setvideomode( $DEFAULTMODE )

        DO WHILE ( keyc .EQ. 0 )
                GOTO 9000
        END DO

        DO WHILE ( keyc .EQ. 1 )
                GOTO 9101
        END DO

        DO WHILE ( keyc .EQ. 2 )
                GOTO 9102
        END DO

        DO WHILE ( keyc .EQ. 3 )
                GOTO 9103
        END DO

CC
CC      keyc = 1
CC

CC
CC      1) List for All Component
CC

9101    CALL drawlines()
        CALL drawlines3()
        REWIND( UNIT = 1 )
9111    kk = 0
        dummy2 = settextcolor( 14 )
        CALL settextposition( 3, 27, curpos )
        CALL outtext( '*** Component Library ***' )
```

```
      dummy2 = settextcolor( 15 )
      kk1 = 0
9105  READ( 1, 9110, END = 9107 ) NAME1
      CALL settextposition( 6+kk, 10+kk1, curpos )
      CALL outtext( name1 )
      kk1 = kk1+16
      IF ( kk .GE. 16 ) THEN
      dummy2 = settextcolor( 14 )
      CALL settextposition( 23, 4, curpos )
      CALL outtext( ' Press any key to continue ...' )
      READ(*,*)
      CALL drawlines()
      GOTO 9111
      END IF
      IF ( kk1 .GE. 50 ) THEN
      kk  = kk + 1
      kk1 = 0
      END IF
      GOTO 9105
9110  FORMAT(3X,A15)
9120  FORMAT(A15)

9107  dummy2 = settextcolor( 14 )
      CALL settextposition( 23, 4, curpos )
      CALL outtext( ' Press any key to continue ...' )
      READ(*,*)
      GOTO 9100

CC
CC    keyc = 2
CC

CC
CC    2) Select Component
CC

9102  CALL drawlines()
      CALL drawlines1()
      dummy2 = settextcolor( 14 )
      CALL settextposition( 4, 27, curpos )
      CALL outtext( '*** Component Selection ***' )
      dummy2 = settextcolor( 15 )
      CALL settextposition( 5, 20, curpos )
      CALL outtext( 'The name must be typed in CAPITAL LETTER' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 9, 18, curpos )
      CALL outtext( '  Total number of component ( NC ) = ' )
      READ(*,*) NC
2220  DO 9130 j = 1, NC
      CALL settextposition( 10+j, 22, curpos )
      WRITE( str, '(I2)' ) j
      CALL outtext( 'Component Name no.'// str // ' =  ' )
      READ(*,9120) name(j)
      REWIND(UNIT = 1)
2200  READ( 1, 2070, END = 2210 ) NAME1
```

```
      IF ( name1 .EQ. name(j) ) THEN
      BACKSPACE( UNIT = 1)
      READ( 1, 2080 ) mw1,tb1,tc1,pc1,zc1,w1,aa1,aa2,aa3,aa4,aa5
      mw(j)   = mw1
      bpt(j)  = tb1
      tc(j)   = tc1
      pc(j)   = pc1
      zc(j)   = zc1
      w(j)    = w1
      a1(j)   = aa1
      a2(j)   = aa2
      a3(j)   = aa3
      a4(j)   = aa4
      a5(j)   = aa5
      GOTO 9130
      END IF
      GOTO 2200
2210  CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Component not exist !! ... Press ENTER' )
      READ(*,*)
      CALL drawlines()
      CALL drawlines1()
      dummy2 = settextcolor( 14 )
      CALL settextposition( 4, 27, curpos )
      CALL outtext( '*** Component Selection ***' )
      dummy2 = settextcolor( 15 )
      CALL settextposition( 5, 20, curpos )
      CALL outtext( 'The name must be typed in CAPITAL LETTER' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 9, 18, curpos )
      WRITE( str, '(I2)' ) NC
      CALL outtext( '  Total number of component ( NC ) = '// str )
      GOTO 2220
9130  CONTINUE
      CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)
2095  kk2 = 0
      CALL drawlines()
      CALL drawlines3()
      dummy2 = settextcolor( 14 )
      CALL settextposition( 3, 10, curpos )
      WRITE( str,'(I2)' ) NC
      CALL outtext( 'Your system has '//str//' components : ' )
      dummy2 = settextcolor( 15 )
      kk3 = 0
      DO 2090 j = 1,NC
      CALL settextposition( 6+kk2, 10+kk3, curpos )
      namex = name(j)
      CALL outtext( namex )
      kk3 = kk3+16
      IF ( kk2 .GE. 16 ) THEN
      dummy2 = settextcolor( 14 )
      CALL settextposition( 23, 4, curpos )
      CALL outtext( ' Press any key to continue ...' )
```

```
      READ(*,*)
      CALL drawlines()
      GOTO 2095
      END IF
      IF ( kk3 .GE. 50 ) THEN
      kk2  = kk2 + 1
      kk3 = 0
      END IF
2090  CONTINUE
      dummy2 = settextcolor( 14 )
      CALL settextposition( 23, 4, curpos )
      CALL outtext( ' Press any key to continue ...' )
      READ(*,*)
      GOTO 9100
2070  FORMAT(3X,A15)
2080  FORMAT(18X,F8.3,3F7.1,F6.3,F8.4,F10.6,4E16.7)

CC
CC    keyc = 3
CC

CC
CC    3) Append New Component Record
CC

9103  REWIND(UNIT = 1)
3001  READ( 1, 3070, END = 3000 ) ID,NAME1,MW1,TB1,TC1,PC1,ZC1,W1,AA1,
      +AA2,AA3,AA4,AA5
      WRITE(2,3070) ID,NAME1,MW1,TB1,TC1,PC1,ZC1,W1,AA1,AA2,AA3,AA4,AA5
      GOTO 3001
3000  CALL drawlines()
      dummy2 = settextcolor( 14 )
      CALL settextposition( 4, 22, curpos )
      CALL outtext( '**** APPEND NEW COMPONENT RECORD ****' )
      dummy2 = settextcolor( 15 )
      CALL settextposition( 6, 4, curpos )
      CALL outtext( 'Physical Property' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 10, 4, curpos )
      CALL outtext( 'ID no. ( 0 to terminate ) = ' )
      READ(*,3080) ID
      IF ( id .EQ. 0 ) THEN
            GOTO 3040
      END IF
      CALL settextposition( 12, 6, curpos )
      CALL outtext( 'Component Name      = ' )
      READ(*,3087) NAME1
      CALL settextposition( 13, 6, curpos )
      CALL outtext( 'Molecular Weight    = ' )
      READ(*,*) MW1
      CALL settextposition( 14, 6, curpos )
      CALL outtext( 'Boiling Point ( R )  = ' )
      READ(*,*) TB1
      CALL settextposition( 15, 6, curpos )
      CALL outtext( 'Critical Temp.( R )  = ' )
```

```
      READ(*,*) TC1
      CALL settextposition( 16, 6, curpos )
      CALL outtext( 'Critical Press.(psia) = ' )
      READ(*,*) PC1
      CALL settextposition( 17, 6, curpos )
      CALL outtext( 'Critical Z-factor    = ' )
      READ(*,*) ZC1
      CALL settextposition( 18, 6, curpos )
      CALL outtext( 'Acentric Factor      = ' )
      READ(*,*) W1

      dummy2 = settextcolor( 15 )
      CALL settextposition( 6, 45, curpos )
      CALL outtext( 'Heat Capacity Coefficients' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 12, 47, curpos )
      CALL outtext( ' a1  = ' )
      READ(*,*) AA1
      CALL settextposition( 13, 47, curpos )
      CALL outtext( ' a2  = ' )
      READ(*,*) AA2
      CALL settextposition( 14, 47, curpos )
      CALL outtext( ' a3  = ' )
      READ(*,*) AA3
      CALL settextposition( 15, 47, curpos )
      CALL outtext( ' a4  = ' )
      READ(*,*) AA4
      CALL settextposition( 16, 47, curpos )
      CALL outtext( ' a5  = ' )
      READ(*,*) AA5
      WRITE(2,3070) ID,NAME1,MW1,TB1,TC1,PC1,ZC1,W1,AA1,AA2,AA3,AA4,AA5
      GOTO 3000
3040  END FILE(UNIT = 2)
3070  FORMAT(I3,A15,F8.3,3F7.1,F6.3,F8.4,F10.6,4E16.7)
3080  FORMAT(I3)
3087  FORMAT(A15)
3090  FORMAT(F4.1)
3095  FORMAT(F5.3)
3097  FORMAT(F5.4)
      GOTO 9100

CC
CC    key = 2
CC

CC
CC  READ COLUMN DATA
CC

9200  CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 23, curpos )
      CALL outtext( '**** Characteristic of Column ****' )
2000  dummy2 = settextcolor( 14 )
```

```
      CALL settextposition( 8, 14, curpos )
      CALL outtext( 'Total number of plates  (NT)  =  ' )
      READ(*,*) NT
      CALL settextposition( 10, 14, curpos )
      CALL outtext( 'Number of trays in stripping section  (NF) = ' )
      READ(*,*) NF
      CALL settextposition( 11, 14, curpos )
      CALL outtext( 'Weir height in stripping section     (WHS) = ' )
      READ(*,*) WHS
      CALL settextposition( 12, 14, curpos )
      CALL outtext( 'Weir height in rectifying section    (WHR) = ' )
      READ(*,*) WHR
      CALL settextposition( 13, 14, curpos )
      CALL outtext( 'Column diameter in stripping section  (DS) = ' )
      READ(*,*) DS
      CALL settextposition( 14, 14, curpos )
      CALL outtext( 'Column diameter in rectifying section (DR) = ' )
      READ(*,*) DR
      CALL settextposition( 15, 14, curpos )
      CALL outtext( 'Weir length in stripping section     (WLS) = ' )
      READ(*,*) WLS
      CALL settextposition( 16, 14, curpos )
      CALL outtext( 'Weir length in rectifying section    (WLR) = ' )
      READ(*,*) WLR
      CALL settextposition( 17, 14, curpos )
      CALL outtext( 'Volumetric holdup in column base     (MVB) = ' )
      READ(*,*) MVB
      CALL settextposition( 18, 14, curpos )
      CALL outtext( 'Volumetric holdup in reflux drum     (MVD) = ' )
      READ(*,*) MVD
301   FORMAT(A\)
 13   FORMAT( 3I3 )
 14   FORMAT( 8F6.2 )
      CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Do you need to input a Characteristic of compartment ? (Y/N)  : ' )
      CALL settextposition( 24, 68, curpos )
      READ(*,11) ans
 11   FORMAT(A)
      IF ( ans .EQ. 'Y' .or. ans .EQ. 'y' ) THEN
      CALL settextposition( 24, 5, curpos )
      CALL outtext( '                                                                  ' )
      CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)

      CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 20, curpos )
      CALL outtext( '**** Characteristic of Compartment ****' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 8, 24, curpos )
      CALL outtext( 'Number of Compartment, k = ' )
      READ(*,*) kc
      CALL settextposition( 9, 24, curpos )
```

```
      CALL outtext( '    Feed Compartment, f = ' )
      READ(*,*) f
      DO 2250 k = 1,kc
      CALL settextposition( 10+k, 24, curpos )
      WRITE( str,'(I2)' ) k
      CALL outtext( 'r'//str//' = ' )
      READ(*,*) rr(k)
      CALL settextposition( 10+k, 34, curpos )
      CALL outtext( 's'//str//' = ' )
      READ(*,*) s(k)
      CALL settextposition( 10+k, 44, curpos )
      CALL outtext( 't'//str//' = ' )
      READ(*,*) ttt(k)
2250  CONTINUE
      END IF
      CALL settextposition( 24, 5, curpos )
      CALL outtext( '                                                    ' )
      CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)
      GOTO 9000

CC
CC    key = 3
CC

CC
CC  READ CONDITIONS
CC

9300  CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 25, curpos )
      CALL outtext( '**** Operating Conditions ****' )
      dummy2 = settextcolor( 14 )
      CALL settextposition(  8, 14, curpos )
      CALL outtext( 'Pressure in top of column    PD, (psia)  = ' )
      READ(*,*) PD
      CALL settextposition( 10, 14, curpos )
      CALL outtext( 'Pressure in bottom of column PB, (psia)  = ' )
      READ(*,*) PB
      CALL settextposition( 12, 14, curpos )
      CALL outtext( 'Reboiler heat-duty  QR, (x 1,000 Btu/hr) = ')
      READ(*,*) QR
      CALL settextposition( 14, 14, curpos )
      CALL outtext( 'Reflux rate  R, (moles/hr) = ' )
      READ(*,*) R
      CALL settextposition( 16, 14, curpos )
      CALL outtext( 'Vapor product from reflux drum DV, (moles/hr) = ')
      READ(*,*) DV
      CALL settextposition( 18, 14, curpos )
      CALL outtext( 'Murphree vapor-phase tray efficiency     EFF  = ')
      READ(*,*) EFF
      CALL settextposition( 24, 5, curpos )
```

```
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)
      GOTO 9000

CC
CC    key = 4
CC

CC
CC  READ FEED
CC

9400  CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 29, curpos )
      CALL outtext( '**** Feed Data ****' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 8, 14, curpos )
      CALL outtext( 'Liquid Feed flow rate (moles/hr) = ' )
      READ(*,*) FL
      CALL settextposition( 9, 14, curpos )
      CALL outtext( 'Liquid Feed temperature    (F) = ' )
      READ(*,*) TFL
      CALL settextposition( 11, 14, curpos )
      CALL outtext( 'Composition (mole fraction) : ' )
      DO 310 J = 1,NC
      CALL settextposition( 11+J, 17, curpos )
      namex = name(j)
      CALL outtext( namex // ' = ' )
      READ(*,*) XF(J)
310   CONTINUE
      CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 29, curpos )
      CALL outtext( '**** Feed Data ****' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 8, 14, curpos )
      CALL outtext( 'Vapor Feed flow rate (moles/hr) = ' )
      READ(*,*) FV
      CALL settextposition( 9, 14, curpos )
      CALL outtext( 'Vapor Feed temperature    (F) = ' )
      READ(*,*) TFV
      CALL settextposition( 11, 14, curpos )
      CALL outtext( 'Composition (mole fraction) : ' )
      DO 320 J = 1,NC
      CALL settextposition( 11+J, 17, curpos )
      namex = name(j)
      CALL outtext( namex // ' = '        )
      READ(*,*) YF(J)
320   CONTINUE
  8   FORMAT(1X,2F8.2,10E10.2)
      CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Press ENTER to continue ...' )
```

```
      READ(*,*)
      GOTO 9000

CC
CC    key = 5
CC
CC
CC  READ INITIAL CONDITIONS
CC

9500  CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 25, curpos )
      CALL outtext( '**** Initial Conditions ****' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 8, 14, curpos )
      CALL outtext( 'Temperature in column base TB, (F)  = ' )
      READ(*,*) TB
      CALL settextposition( 10, 14, curpos )
      CALL outtext( 'Composition in Column base  :' )
      DO 510 J = 1,NC
      CALL settextposition( 11+J, 17, curpos )
      namex = name(j)
      CALL outtext( namex // ' =  ' )
      READ(*,*) XB(J)
510   CONTINUE
      DO 15 N = 1,NT
      CALL drawlines()
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 25, curpos )
      CALL outtext( '**** Initial Conditions ****' )
      dummy2 = settextcolor( 14 )
      WRITE( str, '(I2)' ) N
      CALL settextposition( 8, 14, curpos )
      CALL outtext( 'Temperature in tray no.'//str//' (F) = ' )
      READ(*,*) T(N)
      CALL settextposition( 9, 14, curpos )
      CALL outtext( 'Liquid flow rate in tray no.'//str//' (moles/hr) = ' )
      READ(*,*) LO(N)
      DO 520 J = 1,NC
      CALL settextposition( 10, 14, curpos )
      CALL outtext( 'Composition in tray no.'//str//' :' )
      CALL settextposition( 11+J, 17, curpos )
      namex = name(j)
      CALL outtext( namex // ' =  ' )
      READ(*,*) X(N,J)
520   CONTINUE
      BLANK=0.
      CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)
 15   CONTINUE
      CALL drawlines()
```

```
      CALL drawlines2()
      dummy2 = settextcolor( 15 )
      CALL settextposition( 4, 25, curpos )
      CALL outtext( '**** Initial Conditions ****' )
      dummy2 = settextcolor( 14 )
      CALL settextposition( 8, 14, curpos )
      CALL outtext( 'Temperature in reflux drum TD, (F) = ' )
      READ(*,*) TD
      CALL settextposition( 10, 14, curpos )
      CALL outtext( 'Composition in reflux drum :' )
      DO 530 J = 1,NC
      CALL settextposition( 11+J, 17, curpos )
      namex = name(j)
      CALL outtext( namex // ' = ' )
      READ(*,*) XD(J)
  530 CONTINUE
      CALL settextposition( 24, 5, curpos )
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)
      GOTO 9000

CC
CC    Read old data from floppy disk
CC

CC
CC    key = 6
CC

 9600 CALL old()
      REWIND(UNIT = 3)
      READ(3,9610) NC
      DO 9615 j = 1,NC
      READ(3,9625) name(j),mw(j),bpt(j),tc(j),pc(j),zc(j),w(j),a1(j),a2(j),a3(j),a4(j),a5(j)
 9615 CONTINUE
      READ(3,9630) NT,NF,WHS,WHR,DS,DR,WLS,WLR,MVB,MVD
      READ(3,9670) kc,f
      READ(3,9670) (rr(j),s(j),ttt(j), j = 1,kc)
      READ(3,9640) PD,PB,QR,R,DV,EFF
      READ(3,9645) FL,TFL,(XF(J), J = 1,NC)
      READ(3,9645) FV,TFV,(YF(J), J = 1,NC)
      BLANK = 0.
      READ(3,9650) TB,BLANK,(XB(J), J = 1,NC)
      DO 9660 N = 1,NT
      NN = N
      READ(3,9655) NN,T(N),LO(N),(X(N,J),J=1,NC)
 9660 CONTINUE
      READ(3,9650) TB,R,(XD(J), J = 1,NC)
 9610 FORMAT(I3)
 9625 FORMAT(A15,F8.3,3F7.1,F6.3,F8.4,F10.6,4E16.7)
 9630 FORMAT(2I3,8F6.2)
 9640 FORMAT(6F8.2)
 9645 FORMAT(2F12.2,20E16.7)
 9650 FORMAT(5X,2F8.2,20E16.7)
 9655 FORMAT(1X,I3,1X,2F8.2,20E16.7)
```

```
 9670   FORMAT(1X,6I4)
        GOTO 9000

CC
CC      Save data into floppy disk
CC
CC
CC      key = 7
CC

 9700   CALL save()
        WRITE(4,9610) NC
        DO 9715 j = 1,NC
        WRITE(4,9625) name(j),mw(j),bpt(j),tc(j),pc(j),zc(j),w(j),a1(j),a2(j),a3(j),a4(j),a5(j)
 9715   CONTINUE
        WRITE(4,9630) NT,NF,WHS,WHR,DS,DR,WLS,WLR,MVB,MVD
        WRITE(4,9670) kc,f
        WRITE(4,9670) (rr(j),s(j),ttt(j), j = 1,kc)
        WRITE(4,9640) PD,PB,QR,R,DV,EFF
        WRITE(4,9645) FL,TFL,(XF(J), J = 1,NC)
        WRITE(4,9645) FV,TFV,(YF(J), J = 1,NC)
        WRITE(4,9650) TB,BLANK,(XB(J), J = 1,NC)
        DO 9760 N = 1,NT
        NN = N
        WRITE(4,9655) NN,T(N),LO(N),(X(N,J),J=1,NC)
 9760   CONTINUE
        WRITE(4,9650) TB,R,(XD(J), J = 1,NC)
        GOTO 9000

CC      Run Program

CC
CC      key = 8
CC

CC
CC      Assign temperature in Degree Rangin
CC

 9800   TFL = TFL + 460.
        TFV = TFV + 460.
        TB  = TB          + 460.
        TD  = TD          + 460.+125.0
        DO 18 N = 1,NT
        T(N) = T(N) + 460.
   18   CONTINUE

CC
CC    CALCULATE PRESSURE PROFILE
CC

        CALL drawlines()
        DO 35 N=1,NT
   35   P(N)=(PB-(N*(PB-PD))/NT)
        DELTA = 0.0001
```

```
      WRITE(*,37) DELTA
 37   FORMAT(1X,' DELTA = ', F8.5)
      TIME = 0.
      TPRINT = 0.
      CALL ENTH(TFL,P(NF),XF,YF,HLF,HVF)

CC
CC   CALL INTITIAL HOLDUPS
CC

      CALL MWDENS(XB,TB,PB,MWA,DENSA)
      MB=MVB*DENSA/MWA
      DO 20 N=1,NF
      DO 21 J=1,NC
 21   XX(J) = X(N,J)
      CALL MWDENS(XX,T(N),P(N),MWA,DENSA)
      LV(N) = LO(N)*MWA/DENSA
      L(N) = LO(N)
      HFOW = (LV(N)/(999.*WLS))**.66667
      MV(N) = (HFOW+WHS/12.)*3.1416*DS*DS/(4.*144.)
      M(N) = MV(N)*DENSA/MWA
 20   CONTINUE
      DO 25 N = NF+1,NT
      DO 26 J = 1,NC
 26   XX(J) = X(N,J)
      CALL MWDENS(XX,T(N),P(N),MWA,DENSA)
      LV(N) = LO(N)*MWA/DENSA
      L(N) = LO(N)
      HFOW = (LV(N)/(999.*WLR))**.66667
      MV(N) = (HFOW+WHR/12.)*3.1416*DR*DR/(4.*144.)
      M(N) = MV(N)*DENSA/MWA
 25   CONTINUE
      DO 30 N=1,NT
      DO 31 J=1,NC
      XM(N,J)=M(N)*X(N,J)
 31   CONTINUE
 30   CONTINUE
      CALL MWDENS(XD,TD,PD,MWA,DENSA)
      MD=MVD*DENSA/MWA

CC
CC   Initial Guess of V(5) for first efficiency calculation
CC

      V(NF) = 822.
CC
CC    Sub-munu for running program
CC

9850  keys = -1
      DO WHILE( (keys .LT. 0) .OR. (keys .GT. 2) )
      CALL drawlines()
      CALL drawlines1()

      dummy2 = settextcolor( 14 )
```

```
      CALL settextposition( 4, 30, curpos )
      CALL outtext( '**** RUN MENU ****' )
      dummy2 = settextcolor( 15 )
      CALL settextposition( 11, 25, curpos )
      CALL outtext( '0) Return to Main Menu' )
      CALL settextposition( 13, 25, curpos )
      CALL outtext( '1) Running a full-order model' )
      CALL settextposition( 15, 25, curpos )
      CALL outtext( '2) Running a compartmental model' )
      dummy2 = settextcolor(14)
      CALL settextposition( 22, 25, curpos )
      CALL outtext ( 'Please ENTER your selection : ' )
      READ (*,*,ERR = 9850) keys
      END DO
      dummy2 = setvideomode( $DEFAULTMODE )

      DO WHILE ( keys .EQ. 0 )
            GOTO 9000
      END DO

      DO WHILE ( keys .EQ. 1 )
            GOTO 600
      END DO

      DO WHILE ( keys .EQ. 2 )
            OPEN( 6, FILE = 'RESULTC.DAT' )
            GOTO 100
      END DO

CC
CC    Run a dynamics full-order model
CC

CC
CC  Main Loop for each time step
CC
      xxx=0

 600  CONTINUE
      write(*,*) xxx
      CALL BUBPT (TB,XB,YB,PB,KIB)
      CALL ENTH (TB,PB,XB,YB,HLB,HVB)
      DO 605 J=1,NC
 605  XX(J)=X(1,J)
      CALL BUBPT (T(1),XX,YY,P(1),KII)
      DO 606 J=1,NC
      Y(1,J)=YB(J)+EFF*(YY(J)-YB(J))
 606  YY(J)=Y(1,J)
      CALL ENTH(T(1),P(1),XX,YY,HL(1),HV(1))
      DO 610 N=2,NF
      DO 611 J=1,NC
 611  XX(J)=X(N,J)
      CALL BUBPT(T(N),XX,YY,P(N),KII)
      DO 612 J = 1,NC
      Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
```

```
612   YY(J)=Y(N,J)
      CALL ENTH(T(N),P(N),XX,YY,HL(N),HV(N))
610   CONTINUE
      DO 613 J=1,NC
613   XX(J)=X(NF+1,J)
      CALL BUBPT(T(NF+1),XX,YY,P(NF+1),KII)
      DO 614 J=1,NC
      YAV(J)=(YF(J)*FV+Y(NF,J)*V(NF))/(V(NF)+FV)
      Y(NF+1,J)=(YY(J)-YAV(J))*EFF+YAV(J)
614   YY(J)=Y(NF+1,J)
      CALL ENTH(T(NF+1),P(NF+1),XX,YY,HL(NF+1),HV(NF+1))
      DO 615 N=NF+2,NT
      DO 616 J=1,NC
616   XX(J)=X(N,J)
      CALL BUBPT(T(N),XX,YY,P(N),KII)
      DO 617 J=1,NC
      Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
617   YY(J)=Y(N,J)
      CALL ENTH (T(N),P(N),XX,YY,HL(N),HV(N))
615   CONTINUE
      CALL BUBPT (TD,XD,YD,PD,KII)
      CALL ENTH(TD,PD,XD,YD,HLD,HVD)

CC
CC    CALCULATE VAPOR RATES
CC

      VB=(QR*1000.-L(1)*(HLB-HL(1)))/(HVB-HLB)
      B = L(1)-VB
      V(1)=(HL(2)*L(2)+HVB*VB-HL(1)*L(1))/HV(1)
      DO 620 N=2,NF-1
      V(N)=(HL(N+1)*L(N+1)+HV(N-1)*V(N-1)-HL(N)*L(N))/HV(N)
620   CONTINUE
      V(NF)=(HL(NF+1)*L(NF+1)+HV(NF-1)*V(NF-1)-HL(NF)*L(NF)+HLF*FL)/HV(NF)
      V(NF+1)=(HL(NF+2)*L(NF+2)+HV(NF)*V(NF)+HVF*FV-HL(NF+1)*L(NF+1))/
      +HV(NF+1)
      DO 630 N=NF+2,NT-1
630   V(N)=(HL(N+1)*L(N+1)+HV(N-1)*V(N-1)-HL(N)*L(N))/HV(N)
      V(NT)=(HLD*R+HV(NT-1)*V(NT-1)-HL(NT)*L(NT))/HV(NT)
      DL=V(NT)-DV-R

CC
CC    EVALUATE DERIVATIVES
CC

      DM(1)=L(2)+VB-V(1)-L(1)
      DO 640 N=2,NF-1
640   DM(N)=L(N+1)+V(N-1)-L(N)-V(N)
      DM(NF)=L(NF+1)+FL+V(NF-1)-L(NF)-V(NF)
      DM(NF+1)=L(NF+2)+FV+V(NF)-L(NF+1)-V(NF+1)
      DO 650 N=NF+2,NT-1
650   DM(N)=L(N+1)+V(N-1)-L(N)-V(N)
      DM(NT)=R+V(NT-1)-L(NT)-V(NT)
      DO 660 J=1,NC
      DXB(J)=(X(1,J)*L(1)-YB(J)*VB-XB(J)*B)/MB
```

```
      DXM(1,J)=X(2,J)*L(2)+YB(J)*VB-X(1,J)*L(1)-Y(1,J)*V(1)
      DO 665 N=2,NF-1
665   DXM(N,J)=X(N+1,J)*L(N+1)+Y(N-1,J)*V(N-1)-X(N,J)*L(N)-V(N)*Y(N,J)
      DXM(NF,J)=X(NF+1,J)*L(NF+1)+Y(NF-1,J)*V(NF-1)-X(NF,J)*L(NF)-
      +V(NF)*Y(NF,J)+FL*XF(J)
      DXM(NF+1,J)=X(NF+2,J)*L(NF+2)+Y(NF,J)*V(NF)-X(NF+1,J)*L(NF+1)
      +-V(NF+1)*Y(NF+1,J)+FV*YF(J)
      DO 670 N=NF+2,NT-1
670   DXM(N,J)=X(N+1,J)*L(N+1)+Y(N-1,J)*V(N-1)-X(N,J)*L(N)-V(N)*Y(N,J)
      DXM(NT,J)=XD(J)*R+Y(NT-1,J)*V(NT-1)-X(NT,J)*L(NT)-Y(NT,J)*V(NT)
      DXD(J)=(V(NT)*Y(NT,J)-DV*YD(J)-(R+DL)*XD(J))/MD
660   CONTINUE
      IF (TIME .GT. 1.41e-2) GOTO 9000
      IF (TIME .LT. TPRINT) GOTO 710

      CALL drawlines()
      WRITE(5,701)
701   FORMAT (5X,'TIME   T      X1     X2     X3     X4     X5     X6     L')
      WRITE(5,702) TIME,TB,(XB(J),J=1,NC),B
702   FORMAT (1X,F5.4,3X,F7.2,8F14.6,F10.1)
      DO 703 N=1,NT
703   WRITE(5,704) N,T(N),(X(N,J),J=1,NC),L(N)
704   FORMAT (3X,I3,3X,F7.2,8F14.6,F10.1)
      WRITE(5,705) TD,(XD(J),J=1,NC),R
705   FORMAT (9X,F7.2,8F14.6,F10.1)
      WRITE(5,706) (YD(J),J=1,NC),DL
706   FORMAT(16X,8F14.6,F10.1)
      TPRINT = TPRINT + .001

CC
CC    INTEGRATION ALA EULER
CC

710   TIME = TIME + DELTA
      DO 715 N=1,NT
715   M(N)=M(N)+DM(N)*DELTA
      DO 720 J = 1,NC
      XB(J)=XB(J)+DXB(J)*DELTA
            IF (XB(J) .LT. 0.) XB(J) = 0.0
            IF (XB(J) .GT. 1.) XB(J) = 1.
      DO 725 N=1,NT
      XM(N,J)=XM(N,J)+DXM(N,J)*DELTA
      X(N,J)=XM(N,J)/M(N)
            IF (X(N,J) .GT. 1.) X(N,J) = 1.
            IF (X(N,J) .LT. 0.) X(N,J) = 0.0
725   CONTINUE
      XD(J)=XD(J)+DXD(J)*DELTA
            IF (XD(J) .LT. 0.) XD(J)=0.
            IF (XD(J) .GT. 1.) XD(J)=1.
720   CONTINUE

CC
CC  CALCULATE NEW LIQUID RATES
CC
      DO 770 N=1,NF
```

```
      DO 771 J=1,NC
      XX(J)=X(N,J)
771   CONTINUE
      CALL HYDRAU(P(N),M(N),T(N),XX,L(N),WHS,WLS,DS)
770   CONTINUE
      DO 773 N=NF+1,NT
      DO 775 J=1,NC
775   XX(J)=X(N,J)
      CALL HYDRAU(P(N),M(N),T(N),XX,L(N),WHR,WLR,DR)
773   CONTINUE
      xxx=xxx+1.0
      GOTO 600

CC
CC    Run a dynamics compartmental model
CC

CC
CC  Main Loop for each time step
CC

100   CONTINUE
      WRITE(*,*) XXX
      IF (kc .EQ. 0) THEN
      CALL drawlines()
      CALL drawlines1()
      dummy2 = settextcolor( 14 )
      CALL settextposition( 4, 30, curpos )
      CALL outtext( '**** ERROR MESSAGE ****' )
      dummy2 = settextcolor( 15 )
      CALL settextposition( 10, 33, curpos )
      CALL outtext( 'Please input....' )
      CALL settextposition( 12, 27, curpos )
      CALL outtext( 'A CHARACTISTIC OF COMPARTMENT' )
      CALL settextposition( 14, 23, curpos )
      CALL outtext( 'before running a compartmental model !!' )
      CALL settextposition( 24, 5, curpos )
      dummy2 = settextcolor( 14 )
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)
      GOTO 9000
      END IF

      CALL BUBPT (TB,XB,YB,PB,KIB)
      CALL ENTH (TB,PB,XB,YB,HLB,HVB)

      DO 105 J=1,NC
105   XX(J) = X(1,J)
      CALL BUBPT (T(1),XX,YY,P(1),KII)
      DO 106 J=1,NC
      KI(1,J) = KII(J)
      Y(1,J)=YB(J)+EFF*(YY(J)-YB(J))
106   YY(J)=Y(1,J)
      CALL ENTH(T(1),P(1),XX,YY,HL(1),HV(1))
      DO 110 N=2,NF
```

```
      DO 111 J=1,NC
111   XX(J)=X(N,J)
      CALL BUBPT(T(N),XX,YY,P(N),KII)
      DO 112 J = 1,NC
      KI(N,J) = KII(J)
      Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
112   YY(J)=Y(N,J)
      CALL ENTH(T(N),P(N),XX,YY,HL(N),HV(N))
110   CONTINUE
      DO 113 J=1,NC
113   XX(J)=X(NF+1,J)
      CALL BUBPT(T(NF+1),XX,YY,P(NF+1),KII)
      DO 114 J=1,NC
      KI(NF+1,J) = KII(J)
      YAV(J)=(YF(J)*FV+Y(NF,J)*V(NF))/(V(NF)+FV)
      Y(NF+1,J)=(YY(J)-YAV(J))*EFF+YAV(J)
114   YY(J)=Y(NF+1,J)
      CALL ENTH(T(NF+1),P(NF+1),XX,YY,HL(NF+1),HV(NF+1))

      DO 115 N=NF+2,NT
      DO 116 J=1,NC
      KI(N,J) = KII(J)
116   XX(J)=X(N,J)
      CALL BUBPT(T(N),XX,YY,P(N),KII)

      DO 117 J=1,NC
      KI(N,J) = KII(J)
      Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
117   YY(J)=Y(N,J)
      CALL ENTH (T(N),P(N),XX,YY,HL(N),HV(N))
115   CONTINUE

      CALL BUBPT (TD,XD,YD,PD,KID)
      CALL ENTH(TD,PD,XD,YD,HLD,HVD)

CC
CC    CALCULATE VAPOR RATES
CC

      VB=(QR*1000.-L(1)*(HLB-HL(1)))/(HVB-HLB)
      B = L(1)-VB
      V(1)=(HL(2)*L(2)+HVB*VB-HL(1)*L(1))/HV(1)
      DO 129 N=2,NF-1
      V(N)=(HL(N+1)*L(N+1)+HV(N-1)*V(N-1)-HL(N)*L(N))/HV(N)
129   CONTINUE

      V(NF)=(HL(NF+1)*L(NF+1)+HV(NF-1)*V(NF-1)-HL(NF)*L(NF)+HLF*FL)/HV(NF)
      V(NF+1)=(HL(NF+2)*L(NF+2)+HV(NF)*V(NF)+HVF*FV-HL(NF+1)*L(NF+1))/
     +HV(NF+1)
      DO 130 N=NF+2,NT-1
130   V(N)=(HL(N+1)*L(N+1)+HV(N-1)*V(N-1)-HL(N)*L(N))/HV(N)
      V(NT)=(HLD*R+HV(NT-1)*V(NT-1)-HL(NT)*L(NT))/HV(NT)
      DL=V(NT)-DV-R

CC
```

```
CC      Calculate Absorption & Stripping factor
CC

        DO 135 N = 1,NF-1
        DO 136 J = 1,NC
        FACT(N,J) = KI(N,J)*VB/L(1)
 136    CONTINUE
 135    CONTINUE
        DO 133 N = NF,NT
        DO 134 J = 1,NC
        FACT(N,J) = (R+DL)/(V(NT)*KI(N,J))
 134    CONTINUE
 133    CONTINUE

        DO 150 N = 1,KC
        DO 152 J = 1,NC
        SUMSS1(N,J) = 1.0
        SUMS1(N,J)  = 0.0
        DO 151 I = TTT(N),S(N)-1
        SUMSS1(N,J) = FACT(I,J)*SUMSS1(N,J)
        SUMS1(N,J) = SUMS1(N,J)+SUMSS1(N,J)
 151    CONTINUE
 152    continue
 150    CONTINUE

        DO 153 K = 1,KC
        DO 155 J = 1,NC
        SUMSS2(K,J) = 1.0
        SUMS2(K,J)  = 0.0
        DO 154 I = RR(k),S(k)+1,-1
        SUMSS2(K,J) = FACT(I,J)*SUMSS2(K,J)
        SUMS2(K,J) = SUMS2(K,J)+SUMSS2(K,J)
 154    CONTINUE
 155    continue
 153    CONTINUE

CC
CC      Calculate Compartment Holdup
CC

        DO 40 j = 1,kc
        MCI(j) = 0.
        DO 50 i = ttt(j),rr(j)
 50     MCI(j) = MCI(j) + M(i)
 40     CONTINUE

        DO 139 K = 1,F-1
        DO 140 J = 1,NC
        YR(K,J) = ((L(1)/VB-1.)*XB(J)*SUMS2(K,J)+KI(S(K),J)*X(S(K),J)*SUMSS2(K,J))
        XT(K,J) = (KI(S(K),J)*X(S(K),J)-(L(1)/VB-1.)*XB(J)*SUMS1(K,J))/
       +(KI(TTT(K),J)*SUMSS1(K,J))
 140    CONTINUE
 139    CONTINUE

        DO 145 J = 1,NC
```

```
      YR(F,J) = Y(S(F),J)
      XT(F,J) = X(S(F),J)
145   CONTINUE

      DO 141 K = F+1,KC
      DO 142 J = 1,NC
      YR(K,J) = KI(RR(K),J)*(X(S(K),J)-(V(NT)/(R+DL)-1.)*KID(J)*XD(J)*
     +SUMS2(K,J))/SUMSS2(K,J)
142   XT(K,J) = (V(NT)/(R+DL)-1.)*KID(J)*XD(J)*SUMS1(K,J)+X(S(K),J)*SUMSS1(K,J)
141   CONTINUE

CC
CC    EVALUATE DERIVATIVES
CC

      DM(1)=L(2)+VB-V(1)-L(1)
      DO 180 N=2,NF-1
180   DM(N)=L(N+1)+V(N-1)-L(N)-V(N)
      DM(NF)=L(NF+1)+FL+V(NF-1)-L(NF)-V(NF)
      DM(NF+1)=L(NF+2)+FV+V(NF)-L(NF+1)-V(NF+1)
      DO 182 N=NF+2,NT-1
182   DM(N)=L(N+1)+V(N-1)-L(N)-V(N)
      DM(NT)=R+V(NT-1)-L(NT)-V(NT)
      DO 160 J = 1,NC
      DXB(J) = (XT(1,J)*L(1)-YB(J)*VB-XB(J)*B)/MB
      DXM(1,J)=(XT(2,J)*L(1)+YB(J)*VB-XT(1,J)*L(1)-YR(1,J)*VB)/MCI(1)
160   CONTINUE
      DO 162 K = 2,F-1
      DO 164 J = 1,NC
164   DXM(K,J) = (L(1)*XT(K+1,J)+VB*YR(K-1,J)-L(1)*XT(K,J)-VB*YR(K,J))/MCI(K)
162   CONTINUE
      DO 165 J = 1,NC
      DXM(F,J) = (X(NF+1,J)*L(NF+1)+Y(NF-1,J)*V(NF-1)-X(NF,J)*L(NF)-
     +V(NF)*Y(NF,J)+FL*XF(J))
165   DXM(F+1,J) = ((R+DL)*XT(F+2,J)+V(NT)*Y(NF,J)-L(NF+1)*
     +XT(F+1,J)-V(NT)*YR(F+1,J)+FV*YF(J))/MCI(F+1)
      DO 166 K = F+2,KC-1
      DO 167 J = 1,NC
167   DXM(K,J) = ((R+DL)*XT(K+1,J)+V(NT)*YR(K-1,J)-(R+DL)*
     +XT(K,J)-V(NT)*YR(K,J))/MCI(K)
166   CONTINUE
      DO 168 J = 1,NC
      DXM(KC,J) = (XD(J)*(R+DL)+YR(KC-1,J)*V(NT)-XT(KC,J)*
     +(R+DL)-YR(KC,J)*V(NT))/MCI(KC)
168   DXD(J) = (V(NT)*YR(kc,J)-DV*YD(J)-(R+DL)*XD(J))/MD

      IF (TIME .GT. 1.41E-2) GOTO 9000
      IF (TIME .LT. TPRINT) GOTO 210

      CALL drawlines()
      WRITE(6,201)
201   FORMAT (5X,'TIME   T      X1     X2     X3     X4     X5     X6      L')
      WRITE(6,202) TIME,TB,(XB(J),J=1,NC),B
202   FORMAT (1X,F5.4,3X,F7.2,6F8.6,F8.1)
      DO 203 K=1,KC
```

```
      SI = S(K)
  203 WRITE(6,204) S(K),T(SI),(X(SI,J),J=1,NC),L(SI)
  204 FORMAT (3X,I3,3X,F7.2,6F8.6,F8.1)
      WRITE(6,205) TD,(XD(J),J=1,NC),R
  205 FORMAT (9X,F7.2,6F8.6,F8.1)
      WRITE(6,206) (YD(J),J=1,NC),DL
  206 FORMAT(16X,6F8.6,F8.1)
      TPRINT = TPRINT + .001

CC
CC    INTEGRATION ALA EULER
CC

  210 TIME = TIME + DELTA
      DO 215 N=1,NT
  215 M(N)=M(N)+DM(N)*DELTA

      DO 220 J = 1,NC
      XB(J)=XB(J)+DXB(J)*DELTA
            IF (XB(J) .LT. 0.) XB(J) = 0.0
            IF (XB(J) .GT. 1.) XB(J) = 1.
      DO 225 K = 1,F-1
      SI = S(K)
      X(SI,J)=X(SI,J)+DXM(K,J)*DELTA
            IF (X(SI,J) .GT. 1.) X(SI,J) = 1.
            IF (X(SI,J) .LT. 0.) X(SI,J) = 0.0
  225 CONTINUE
      XM(NF,J) = XM(NF,J)+DXM(F,J)*DELTA
      X(NF,J)  = XM(NF,J)/M(NF)
            IF (X(NF,J) .GT. 1.) X(NF,J) = 1.
            IF (X(NF,J) .LT. 0.) X(NF,J) = 0.0
      DO 226 K = F+1,KC
      SI = S(K)
      X(SI,J)=X(SI,J)+DXM(K,J)*DELTA
            IF (X(SI,J) .GT. 1.) X(SI,J) = 1.
            IF (X(SI,J) .LT. 0.) X(SI,J) = 0.0
  226 CONTINUE

      XD(J)=XD(J)+DXD(J)*DELTA
            IF (XD(J) .LT. 0.) XD(J)=0.
            IF (XD(J) .GT. 1.) XD(J)=1.
  220 CONTINUE

CC
CC  CALCULATE NEW LIQUID RATES
CC

      DO 270 N=1,NF
      DO 271 J=1,NC
      XX(J)=X(N,J)
  271 CONTINUE
      CALL HYDRAU(P(N),M(N),T(N),XX,L(N),WHS,WLS,DS)
  270 CONTINUE
      DO 273 N=NF+1,NT
      DO 275 J=1,NC
```

```
275   XX(J)=X(N,J)
      CALL HYDRAU(P(N),M(N),T(N),XX,L(N),WHR,WLR,DR)
273   CONTINUE
      XXX=XXX+1
      GOTO 100
400   STOP
      END

CC
CC    Calculate Liquid tray holdup by Francis Wier equation
CC

      SUBROUTINE  HYDRAU(P,M,T,X,L,WH,WL,DCOL)

      REAL M,L,MW,MWA

      COMMON NC,MW(10),DENS(10),C1(10),C2(10),C3(10),BPT(10),AVP(10),
     +BVP(10),tc(10),pc(10),zc(10),w(10),a1(10),a2(10),a3(10),a4(10),a5(10)

      DIMENSION X(10)

      CALL MWDENS(X,T,P,MWA,DENSA)
      CONST=183.2*M*MWA/(DENSA*DCOL*DCOL)-WH/12.
      IF (CONST .LE. 0.) GOTO 10
      L=DENSA*WL*999.*((183.2*M*MWA/(DENSA*DCOL*DCOL)-WH/12.)**1.5)/MWA
      RETURN
10    L=0.
      RETURN
      END

CC
CC    Enthalpy calculation
CC

      SUBROUTINE ENTH(T,P,X,Y,HL,HV)

      REAL GC,MI

      COMMON NC,MW(10),DENS(10),C1(10),C2(10),C3(10),BPT(10),AVP(10),
     +BVP(10),tc(10),pc(10),zc(10),w(10),a1(10),a2(10),a3(10),a4(10),a5(10)

      DIMENSION X(10),Y(10),TR(10),MI(10),ALPHA(10),ACI(10),AI(10),
     +BI(10),HLS(10)

CC
CC    Define constant value
CC

      GC = 1.986
      KIJ = 0.001

      HL = 0.0
      HV = 0.0
      HLS1 = 0.0
      HVS  = 0.0
```

```
      SUMAL  = 0.0
      SUMAV  = 0.0
      SUMBL  = 0.0
      SUMBV  = 0.0
      SUMATL = 0.0
      SUMATV = 0.0
      DO 1 J=1,NC
      TR(J) = T/TC(J)
      MI(J) = 0.48+1.574*W(J)-0.176*W(J)**2
      ALPHA(J) = (1.0+MI(J)*(1-TR(J)**(0.5)))**2
      ACI(J) = 0.42748*(GC*TC(J))**2/PC(J)
      AI(J) = ALPHA(J)*ACI(J)
      BI(J) = 0.08664*GC*TC(J)/PC(J)
      SUMBL = SUMBL + X(J)*BI(J)
      SUMBV = SUMBV + Y(J)*BI(J)
1     CONTINUE
      DO 2 I = 1,NC
      DO 3 J = 1,NC
      SUMAL = SUMAL+X(I)*X(J)*(AI(I)*AI(J))**0.5*(1-KIJ)
      SUMAV = SUMAV+Y(I)*Y(J)*(AI(I)*AI(J))**0.5*(1-KIJ)
      SUMATL = SUMATL+X(I)*X(J)*MI(J)*(AI(I)*ACI(J)*TR(J))**0.5*(1-KIJ)
      SUMATV = SUMATV+Y(I)*Y(J)*MI(J)*(AI(I)*ACI(J)*TR(J))**0.5*(1-KIJ)
3     CONTINUE
2     CONTINUE

      AL = SUMAL*P/(GC*T)**2
      AV = SUMAV*P/(GC*T)**2
      BL = SUMBL*P/(GC*T)
      BV = SUMBV*P/(GC*T)
      CALL NEWTON(AL,BL,Z1,Z2,Z3)
      IF ( Z1 .LE. 0 ) THEN
            IF ( Z2 .LE. 0 ) THEN
                  ZL = Z3
            ELSE
                  ZL = Z2
            END IF
      ELSE
            ZL = Z1
      END IF
      CALL NEWTON(AV,BV,Z1,Z2,Z3)
      ZV = Z3

      DO 4 I = 1,NC
      HLS(I) = A1(I)*(T-460.)+A2(I)/2*(T-460.)**2+A3(I)/3*(T-460.)**3+
      +A4(I)/4*(T-460.)**4+A5(I)/5*(T-460.)**5
      HLS1 =  HLS1+X(I)*HLS(I)
      HVS  =  HVS +Y(I)*HLS(I)
4     CONTINUE

      HL = (ZL-1-AL/BL*(1-SUMATL/SUMAL)*ALOG(1+BL/ZL))*GC*T+HLS1
      HV = (ZV-1-AV/BV*(1-SUMATV/SUMAV)*ALOG(1+BV/ZV))*GC*T+HVS

      RETURN
      END
```

```
CC
CC      Calculate the root of Z by newton's technique
CC

        SUBROUTINE NEWTON(A,B,Z1,Z2,Z3)

        DIMENSION Z(3)

        ZO1 = -10
        L = 1
 10     IF ( L .GT. 5000 ) THEN
                WRITE(*,*) '  ****** NOT CONVERGE !! ******'
                STOP
        END IF
        FZ1 = ZO1**3-ZO1**2+(A-B-B**2)*ZO1-A*B
        DFZ1 = 3*ZO1**2-2*ZO1+(A-B-B**2)
        Z1 = ZO1-FZ1/DFZ1
        IF (ABS(ZO1-Z1) .LT. 1E-3) THEN
        GOTO 20
        END IF
        ZO1 = Z1
        L = L+1
        GOTO 10

 20     ZO2 = 0
        L1 = 1
 25     IF ( L1 .GT. 5000 ) THEN
                WRITE(*,*) '  ****** NOT CONVERGE !! ******'
                STOP
        END IF
        FZ2 = ZO2**3-ZO2**2+(A-B-B**2)*ZO2-A*B
        DFZ2 = 3*ZO2**2-2*ZO2+(A-B-B**2)
        Z2 = ZO2-FZ2/DFZ2
        IF (ABS(ZO2-Z2) .LT. 1E-3) THEN
        GOTO 30
        END IF
        ZO2 = Z2
        L1 = L1+1
        GOTO 25

 30     ZO3 = 10
        L2 = 1
 35     IF ( L2 .GT. 5000 ) THEN
                WRITE(*,*) '  ****** NOT CONVERGE !! ******'
                STOP
        END IF
        FZ3 = ZO3**3-ZO3**2+(A-B-B**2)*ZO3-A*B
        DFZ3 = 3*ZO3**2-2*ZO3+(A-B-B**2)
        Z3 = ZO3-FZ3/DFZ3
        IF (ABS(ZO3-Z3) .LT. 1E-3) THEN
        GOTO 40
        END IF
        ZO3 = Z3
        L2 = L2+1
        GOTO 35
```

```
      Z(1) = Z1
      Z(2) = Z2
      Z(3) = Z3

      jump = 3
50    jump = jump/2
      IF ( jump .NE. 0 ) THEN
            j2 = 3-jump
            DO 60 j = 1,j2
            DO 60 i = j,1,-jump
            j3 = i+jump
            IF ( Z(i) .GT. Z(j3)) THEN
                  s = Z(i)
                  Z(i) = Z(j3)
                  Z(j3) = s
            END IF
60          CONTINUE
      GOTO 50
      END IF

      Z1 = Z(1)
      Z2 = Z(2)
      Z3 = Z(3)

40    RETURN
      END

CC
CC    Calculate average density
CC

      SUBROUTINE MWDENS(X,T,P,MWA,DENSA)

      COMMON NC,MW(10),DENS(10),C1(10),C2(10),C3(10),BPT(10),AVP(10),
     +BVP(10),tc(10),pc(10),zc(10),w(10),a1(10),a2(10),a3(10),a4(10),a5(10)

      DIMENSION X(10),TR(10),MI(10),ALPHA(10),ACI(10),AI(10),BI(10)

      REAL MW,MWA,MI,GC
      DENSA=0.0
      MWA=0.

CC
CC    Define constant value
CC

      GC = 10.731
      KIJ = 0.001

      SUMAL  = 0.0
      SUMBL  = 0.0
      SUMATL = 0.0

      DO 1 J=1,NC
```

```
      TR(J) = T/TC(J)
      MI(J) = 0.48+1.574*W(J)-0.176*W(J)**2
      ALPHA(J) = (1.0+MI(J)*(1-TR(J)**(0.5)))**2
      ACI(J) = 0.42748*(GC*TC(J))**2/PC(J)
      AI(J) = ALPHA(J)*ACI(J)
      BI(J) = 0.08664*GC*TC(J)/PC(J)
      SUMBL = SUMBL + X(J)*BI(J)
1     CONTINUE

      DO 2 I = 1,NC
      DO 3 J = 1,NC
      SUMAL = SUMAL+X(I)*X(J)*(AI(I)*AI(J))**0.5*(1-KIJ)
      SUMATL = SUMATL+X(I)*X(J)*MI(J)*(AI(I)*ACI(J)*TR(J))**0.5*(1-KIJ)
3     CONTINUE
2     CONTINUE

      AL = SUMAL*P/(GC*T)**2
      BL = SUMBL*P/(GC*T)

      CALL NEWTON(AL,BL,Z1,Z2,Z3)
      IF ( Z1 .LE. 0 ) THEN
            IF ( Z2 .LE. 0 ) THEN
                  ZL = Z3
            ELSE
                  ZL = Z2
            END IF
      ELSE
            ZL = Z1
      END IF

      VV = ZL*GC*T/P
      DO 5 J=1,NC
5     MWA=X(J)*MW(J)+MWA
      DENSA=1/(VV/MWA)

      RETURN
      END

CC
CC    Buble point Calculation
CC

      SUBROUTINE BUBPT(T,X,Y,P,KI)

      REAL GC,MI,KI, APRIMEX,APRIMEY,APRIMEXH,APRIMEYH,KIH,
     +FSLOPE,F,y

      COMMON NC,MW(10),DENS(10),C1(10),C2(10),C3(10),BPT(10),AVP(10),
     +BVP(10),tc(10),pc(10),zc(10),w(10),a1(10),a2(10),a3(10),a4(10),a5(10)

      DIMENSION X(10),Y(10),TR(10),MI(10),ALPHA(10),ACI(10),
     +AI(10),BI(10),FIL(10),FIV(10),KI(10),APRIMEX(10),APRIMEY(10)

      DIMENSION FILH(10),FIVH(10),APRIMEXH(10),APRIMEYH(10),KIH(10),
     +ALPHAH(10),AIH(10),TRH(10)
```

```
CC
CC      Define constant value
CC

        GC = 1.986
        KIJ = 0.001

        DO 40 I = 1,NC
        IF (Y(I) .EQ. 0.) THEN
                ki(i) = 15./I
                Y(I) = KI(I)*X(I)
        END IF
40      continue


        LOOP = 0
10      LOOP=LOOP+1

        SUMXA  = 0.0
        SUMYA  = 0.0
        SUMXAH = 0.0
        SUMYAH = 0.0
        SUMAL  = 0.0
        SUMAV  = 0.0
        SUMALH = 0.0
        SUMAVH = 0.0
        SUMBL  = 0.0
        SUMBV  = 0.0
        TH = T+1.0
        IF(LOOP .GT. 5000) GOTO 30
        SUMY=0.0
        SUMYH = 0.0

        DO 1 J=1,NC
        TR(J) = T/TC(J)
        TRH(J) = TH/TC(J)
        MI(J) = 0.48+1.574*W(J)-0.176*W(J)**2
        ALPHA(J) = (1.0+MI(J)*(1-TR(J)**(0.5)))**2
        ALPHAH(J) = (1.0+MI(J)*(1-TRH(J)**(0.5)))**2
        ACI(J) = 0.42748*(GC*TC(J))**2/PC(J)
        AI(J) = ALPHA(J)*ACI(J)
        AIH(J) = ALPHAH(J)*ACI(J)
        BI(J) = 0.08664*GC*TC(J)/PC(J)
        SUMXA = SUMXA+X(J)*AI(J)**0.5*(1-KIJ)
        SUMXAH = SUMXAH+X(J)*AIH(J)**0.5*(1-KIJ)
        SUMYA = SUMYA+Y(J)*AI(J)**0.5*(1-KIJ)
        SUMYAH = SUMYAH+Y(J)*AIH(J)**0.5*(1-KIJ)
        SUMBL = SUMBL + X(J)*BI(J)
        SUMBV = SUMBV + Y(J)*BI(J)
1       CONTINUE

        DO 2 I = 1,NC
        DO 3 J = 1,NC
        SUMAL = SUMAL+X(I)*X(J)*(AI(I)*AI(J))**0.5*(1-KIJ)
```

```
      SUMALH = SUMALH + X(I)*X(J)*(AIH(I)*AIH(J))**0.5*(1-KIJ)
      SUMAV = SUMAV+Y(I)*Y(J)*(AI(I)*AI(J))**0.5*(1-KIJ)
      SUMAVH = SUMAVH + Y(I)*Y(J)*(AIH(I)*AIH(J))**0.5*(1-KIJ)
3     CONTINUE
2     CONTINUE

      AL = SUMAL*P/(GC*T)**2
      ALH = SUMALH*P/(GC*TH)**2
      AV = SUMAV*P/(GC*T)**2
      AVH = SUMAVH*P/(GC*TH)**2
      BL = SUMBL*P/(GC*T)
      BLH = SUMBL*P/(GC*TH)
      BV  = SUMBV*P/(GC*T)
      BVH = SUMBL*P/(GC*TH)

      CALL NEWTON(AL,BL,Z1,Z2,Z3)
      IF ( Z1 .LE. 0 ) THEN
            IF ( Z2 .LE. 0 ) THEN
                  ZL = Z3
            ELSE
                  ZL = Z2
            END IF
      ELSE
            ZL = Z1
      END IF
      CALL NEWTON(ALH,BLH,Z1,Z2,Z3)
      IF ( Z1 .LE. 0 ) THEN
            IF ( Z2 .LE. 0 ) THEN
                  ZLH = Z3
            ELSE
                  ZLH = Z2
            END IF
      ELSE
            ZLH = Z1
      END IF
      CALL NEWTON(AV,BV,Z1,Z2,Z3)
      ZV = Z3
      CALL NEWTON(AVH,BVH,Z1,Z2,Z3)
      ZVH = Z3

      DO 15 I=1,NC
      APRIMEX(I) = 1.0/SUMAL*(2*AI(I)**0.5*SUMXA)
      APRIMEXH(I) = 1.0/SUMALH*(2*AIH(I)**0.5*SUMXAH)
      APRIMEY(I) = 1.0/SUMAV*(2*AI(I)**0.5*SUMYA)
      APRIMEYH(I) = 1.0/SUMAVH*(2*AIH(I)**0.5*SUMYAH)
      FIL(I) = EXP(BI(I)/SUMBL*(ZL-1)-ALOG(ZL-BL)-AL/BL*(APRIMEX(I)-
      +BI(I)/SUMBL)*ALOG(1+BL/ZL))
      FILH(I) = EXP(BI(I)/SUMBL*(ZLH-1)-ALOG(ZLH-BLH)-ALH/BLH*
      +(APRIMEXH(I)-BI(I)/SUMBL)*ALOG(1+BLH/ZLH))
      FIV(I) = EXP(BI(I)/SUMBV*(ZV-1)-ALOG(ZV-BV)-AV/BV*(APRIMEY(I)-
      +BI(I)/SUMBV)*ALOG(1+BV/ZV))
      FIVH(I) = EXP(BI(I)/SUMBV*(ZVH-1)-ALOG(ZVH-BVH)-AVH/BVH*
      +(APRIMEYH(I)-BI(I)/SUMBV)*ALOG(1+BVH/ZVH))
      KI(I) = FIL(I)/FIV(I)
      KIH(I) = FILH(I)/FIVH(I)
```

```
      SUMY = SUMY +X(I)*KI(I)
      SUMYH = SUMYH +X(I)*KIH(I)
15    CONTINUE

      IF(LOOP .EQ. 1) THEN
      DO 16 I = 1,NC
      Y(I) = KI(I)*X(I)/SUMY
16    CONTINUE
      GOTO 10
      END IF

      IF (ABS(SUMY-SUMYZ) .GE. 1E-3) THEN
      DO 17 I = 1,NC
      Y(I) = KI(I)*X(I)/SUMY
17    CONTINUE
      SUMYZ = SUMY
      GOTO 10
      END IF

      IF ( ABS(SUMY-1.) .LT. 1E-3) RETURN
      F=SUMY-1.0
      FH = SUMYH-1.0
      FSLOPE=(FH-F)/1.
      T=T-F/FSLOPE
      GOTO 10

30    WRITE(*,*) 'The calculation does not converge !!'
      STOP
      END

CC
CC    Draw Large Border lines
CC

      SUBROUTINE drawlines()

      INCLUDE  'FGRAPH.FD'
      RECORD / rccoord / curpos

      dummy = setvideomode( $ERESCOLOR )
      CALL clearscreen( $GCLEARSCREEN )
      dummy2 = setcolor( 3 )
      CALL    moveto( 5, 5, curpos )
      dummy2 = lineto( 5, 340 )
      dummy2 = lineto( 635,340 )
      dummy2 = lineto( 635,5 )
      dummy2 = lineto( 5, 5 )
      CALL   moveto( 7, 7, curpos )
      dummy2 = lineto( 7, 338)
      dummy2 = lineto( 633, 338)
      dummy2 = lineto( 633, 7 )
      dummy2 = lineto( 7, 7 )

      RETURN
      END
```

```
CC
CC      Draw Small Border lines
CC

        SUBROUTINE drawlines1()
        INCLUDE  'FGRAPH.FD'
        RECORD / rccoord / curpos

        dummy2 = setcolor( 4 )
        CALL    moveto( 120, 80, curpos )
        dummy2 = lineto( 120, 270 )
        dummy2 = lineto( 520, 270 )
        dummy2 = lineto( 520, 80 )
        dummy2 = lineto( 120,80 )
        CALL    moveto( 122, 82, curpos )
        dummy2 = lineto( 122, 268 )
        dummy2 = lineto( 518, 268 )
        dummy2 = lineto( 518, 82 )
        dummy2 = lineto( 122, 82 )

        RETURN
        END

CC
CC      Draw Middle Border lines
CC

        SUBROUTINE drawlines2()

        INCLUDE  'FGRAPH.FD'
        RECORD / rccoord / curpos

        dummy2 = setcolor( 4 )
        CALL    moveto( 80, 80, curpos )
        dummy2 = lineto( 80, 270 )
        dummy2 = lineto( 560, 270 )
        dummy2 = lineto( 560, 80 )
        dummy2 = lineto( 80,80 )
        CALL    moveto( 82, 82, curpos )
        dummy2 = lineto( 82, 268 )
        dummy2 = lineto( 558, 268 )
        dummy2 = lineto( 558, 82 )
        dummy2 = lineto( 82, 82 )

        RETURN
        END

CC
CC      Draw Component Border lines
CC

        SUBROUTINE drawlines3()

        INCLUDE  'FGRAPH.FD'
```

```
      RECORD / rccoord / curpos

      dummy2 = setcolor( 4 )
      CALL   moveto( 60, 60, curpos )
      dummy2 = lineto( 60, 290 )
      dummy2 = lineto( 580, 290 )
      dummy2 = lineto( 580, 60 )
      dummy2 = lineto( 60,60 )
      CALL   moveto( 62, 62, curpos )
      dummy2 = lineto( 62, 288 )
      dummy2 = lineto( 578, 288 )
      dummy2 = lineto( 578, 62 )
      dummy2 = lineto( 62, 62 )

      RETURN
      END

CC
CC    Edit old data
CC

      SUBROUTINE old()

      INCLUDE  'FGRAPH.FD'
      RECORD / rccoord / curpos
      CHARACTER*20 fname

 100  CALL drawlines()
      CALL drawlines1()
      dummy2 = settextcolor( 14 )
      CALL settextposition( 4, 28, curpos )
      CALL outtext( '*** Edit Old Data ***' )
      CALL settextposition( 13, 18, curpos )
      CALL outtext( 'Please type data filename :  ' )
      READ(*,120) fname
      OPEN( 3, FILE = fname, ERR = 100)
 120  FORMAT(A)
      RETURN
      END
CC
CC    Save data
CC

      SUBROUTINE save()

      INCLUDE  'FGRAPH.FD'
      RECORD / rccoord / curpos
      CHARACTER*20 filename

 100  CALL drawlines()
      CALL drawlines1()
      dummy2 = settextcolor( 14 )
      CALL settextposition( 4, 28, curpos )
      CALL outtext( '*** Save Data ***' )
      CALL settextposition( 13, 18, curpos )
```

```
      CALL outtext( 'Please type data filename :  ' )
      READ(*,120) filename
      OPEN( 4, FILE = filename, ERR = 100)
120   FORMAT(A)
      RETURN
      END
```

Appendix C
Physical Property Constants and Coefficients

This appendix is a physical property data bank for 176 chemicals that are divided into inorganic and organic groups. Within each group, the succession of elements is alphabetical in the empirical formula. However, organic chemicals begin with carbon and hydrogen according to the convention in the *Handbook of Chemistry and Physics.*

In Part A, the following physical property constants are listed:

M = molecular weight.
T_b = normal boiling point, $^\circ R$
T_C = critical temperature, $^\circ R$
P_C = critical pressure, *psia*
Z_C = critical compressibility factor
ω = Pitzer's acentric factor
δ = Hildebrand's solubility parameter at 25 $^\circ C, (cal/cm^3)^{1/2}$
v_L = Liquid molal volumn at superscripted temperature $(^\circ C), cm^3/gmole$; values in parentheses are for hypothetical liquid.

In Part B, physical property coefficients are listed for:

1. Ideal gas heat capacity.

$$C^\circ_{PV} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4, \qquad Btu/lbmole\ ^\circ F,$$

where $T = ^\circ F$

2. Antoine vapor pressure.

$$\ln \frac{P_i^s}{P_C} = A_1 - \frac{A_2}{T' + A_3}$$

where P_i^s = vapor pressure and $T' = ^\circ F$

Source : Henley and Seader, Equlibrium-Stage Separation Operations in Chemical Engineering, John Wiley & Sons Inc., New York, 1981.

Part A

Number	Empirical Formula	Name	M	T_b	T_c	P_c	Z_c	ω	δ	v_L
Inorganic Chemicals										
1	Ar	Argon	39.948	157.1	271.2	705.4	0.293	−0.0034	5.330	
2	Br_2	Bromine	159.808	597.5	1051.5	1499.0	0.298	0.1242	11.442	51.2[20]
3	CCl_4	Carbon tetrachloride	153.823	629.5	1001.5	661.3	0.277	0.1938	9.338	97.1[25]
4	CO	Carbon monoxide	28.010	147.0	239.3	507.4	0.289	0.048	3.1300	(35.2)[25]
5	$COCl_2$	Phosgene	98.916	505.3	819.3	823.0	0.279	0.203	8.4170	71.6[20]
6	CO_2	Carbon dioxide	44.011	350.4	547.6	1070.5	0.273	0.177	7.1200	(44.0)[25]
7	CS_2	Carbon disulfide	76.131	574.9	993.6	1146.3	0.285	−0.115	9.8640	58.9[20]
8	C_2OCl_4	Trichloroacetyl chloride	181.833	704.1	1061.4	594.6	0.275	0.359	12.0540	112.2[20]
9	ClH	Hydrogen chloride	36.461	338.6	584.2	1198.5	0.267	0.133	7.0110	30.6[-85]
10	Cl_2	Chlorine	70.906	430.4	750.9	1118.4	0.278	0.0743	8.708	45.4[-33]
11	HI	Hydrogen iodide	127.912	428.0	761.7	1190.4	0.305	0.0290	8.270	45.6[-50]
12	H_2	Hydrogen	2.016	36.7	59.7	190.8	0.321	0.0	0.0	(31.0)[25]
13	H_2O	Water	18.015	671.7	1165.1	3206.7	0.232	0.3477	18.0	18.1[20]
14	H_2S	Hydrogen sulfide	34.080	383.1	672.4	1306.5	0.283	0.0868	8.8	34.3[-85]
15	H_3N	Ammonia	17.031	431.5	730.2	1653.7	0.248	0.2582	12.408	26.7[20]
16	Ne	Neon	20.183	49.1	80.1	395.3	0.306	−0.0299	0.0	
17	NO	Nitric oxide	30.006	218.5	324.0	940.5	0.267	0.5877	0.0	
18	NO_2	Nitrogen dioxide	46.006	530.1	775.8	1469.6	0.247	0.8499	16.208	31.8[20]
19	N_2	Nitrogen	28.013	139.3	227.3	492.9	0.289	0.0206	4.440	(53.0)[25]
20	N_2O	Nitrous oxide	44.013	330.7	557.5	1053.7	0.277	0.1601	5.474	35.9[-89]
21	O_2	Oxygen	31.999	162.3	278.6	736.9	0.291	0.0250	4.0	(28.4)[25]
22	O_2S	Sulfur dioxide	64.063	473.7	775.2	1144.8	0.267	0.2402	6.0	44.0[-10]
23	O_3S	Sulfur trioxide	80.058	572.2	883.6	1196.8	0.252	0.4384	15.329	45.0[45]
Organic Chemicals										
24	$CHCl_3$	Chloroform	119.378	602.8	965.8	793.6	0.277	0.2117	9.236	80.2[20]
25	CHN	Hydrogen cyanide	27.026	538.0	822.0	718.6	0.172	0.3752	12.192	39.3[20]
26	CH_2O	Formaldehyde	30.026	457.1	747.3	984.6	0.222	0.2298	10.604	36.8[-20]
27	CH_3Cl	Methyl chloride	50.488	448.1	749.3	968.5	0.270	0.1530	8.585	55.2[20]
28	CH_3I	Methyl iodide	141.939	568.2	950.7	1061.1	0.283	0.1925	9.863	62.3[20]
29	CH_4	Methane	16.043	201.0	343.9	673.1	0.289	0.0	5.680	(52.0)[25]
30	CH_4O	Methanol	32.042	607.8	923.7	1153.6	0.228	0.5556	14.510	40.5[20]
31	CH_5N	Methylamine	31.058	480.1	774.1	1081.6	0.260	0.2852	10.479	44.2[-11]
32	C_2HCl_3	Trichloroethylene	131.389	648.1	979.5	727.5	0.278	0.4281	9.263	89.9[20]

Part A (cont'd)

Number	Empirical Formula	Name	M	T_b	T_c	P_c	Z_c	ω	δ	v_L
Organic Chemicals										
33	C_2HCl_3O	Dichloroacetyl chloride	147.388	685.2	1039.1	668.5	0.271	0.3645	12.679	96.2[18]
34	C_2H_2	Acetylene	26.038	339.1	555.0	890.3	0.267	0.1917	5.329	42.3[-84]
35	$C_2H_2Cl_2O$	Chloroacetyl chloride	112.943	687.9	1054.8	740.7	0.255	0.3194	13.856	79.5[20]
36	C_2H_3Cl	Vinyl chloride	62.499	467.0	776.8	774.5	0.266	0.0929	7.717	64.5[-14]
37	C_2H_3ClO	Acetyl chloride	78.498	583.3	914.3	832.7	0.270	0.3238	12.485	71.0[20]
38	$C_2H_3Cl_3$	1,1,2-Trichloroethane	113.405	969.5	1101.9	701.2	0.267	0.2273	9.628	92.6[20]
39	C_2H_3N	Acetonitrile	41.053	638.6	986.2	701.0	0.184	0.3234	12.049	52.5[20]
40	C_2H_4	Ethylene	28.054	305.0	509.5	742.2	0.284	0.0872	5.801	(61.0)[-25]
41	$C_2H_4Cl_2$	1,1-Dichloroethane	98.960	594.8	941.7	734.8	0.274	0.2450	8.913	84.7[25]
42	$C_2H_4Cl_2$	1,2-Dichloroethane	98.960	641.9	1010.8	778.9	0.267	0.3064	9.828	79.2[18]
43	C_2H_4O	Acetaldehyde	44.054	528.4	830.1	805.3	0.238	0.2882	9.844	56.6[20]
44	C_2H_4O	Ethylene oxide	44.054	510.6	842.7	1043.4	0.260	0.2121	10.271	49.0[0]
45	$C_2H_4O_2$	Acetic acid	60.052	705.0	1070.6	839.1	0.220	0.4536	10.051	57.2[20]
46	$C_2H_4O_2$	Methyl formate	60.052	548.9	876.9	870.7	0.259	0.2562	10.018	61.7[20]
47	C_2H_5Cl	Ethyl chloride	64.515	513.8	828.7	764.2	0.268	0.1918	8.471	75.1[20]
48	C_2H_6	Ethane	30.070	332.2	550.0	709.8	0.282	0.1064	6.050	(68.0)[-25]
49	C_2H_6O	Dimethyl ether	46.069	447.0	720.1	764.2	0.271	0.1960	7.608	69.1[20]
50	C_2H_6O	Ethanol	46.069	632.7	929.3	925.3	0.250	0.6341	12.915	58.4[20]
51	$C_2H_6O_2$	Ethylene glycol	62.069	847.1	1161.4	1091.9	0.242	0.1177	16.604	55.7[20]
52	C_2H_6S	Dimethyl sulfide	62.130	558.9	905.5	802.4	0.268	0.1951	9.045	73.3[20]
53	C_2H_6S	Ethyl mercaptan	62.130	554.7	898.5	796.5	0.271	0.1856	8.933	74.1[20]
54	C_2H_7N	Ethylamine	45.085	521.5	821.1	815.6	0.264	0.2861	9.427	66.0[20]
55	C_3H_3N	Acrylonitrile	53.064	630.8	934.5	512.9	0.186	0.3853	11.029	65.8[20]
56	C_3H_4	Methylacetylene	40.065	449.9	724.3	816.2	0.271	0.2150	8.010	56.7[-50]
57	C_3H_4	Propadiene	40.065	429.6	721.7	747.2	0.284	0.0631	6.854	61.6[25]
58	C_3H_6	Propylene	42.081	405.8	657.2	667.0	0.279	0.1421	6.208	79.0[25]
59	C_3H_6O	Acetone	58.080	592.7	917.0	693.7	0.247	0.3035	9.566	73.5[20]
60	$C_3H_6O_2$	Ethyl formate	74.080	589.5	915.3	680.4	0.258	0.2784	9.311	79.9[18]
61	$C_3H_6O_2$	Methyl acetate	74.080	594.7	912.4	680.9	0.256	0.3269	9.014	79.3[20]
62	$C_3H_6O_2$	Propionic acid	74.080	745.5	1102.8	778.9	0.249	0.5322	12.385	74.6[20]
63	C_3H_7NO	Dimethylformamide	73.095	767.1	1074.4	683.1	0.236	0.7458	11.775	77.0[20]
64	C_3H_8	Propane	44.097	416.0	665.9	617.4	0.278	0.1538	6.400	84.0[25]
65	C_3H_8O	Isopropanol	60.095	639.8	915.0	691.0	0.249	0.6614	11.572	76.5[20]
66	C_3H_8O	*n*-Propanol	60.096	666.7	966.4	737.1	0.250	0.6111	12.050	74.7[20]

67	C_3H_9N	Trimethylamine	59.112	496.9	779.9	590.8	0.272	0.2008	7.070	93.4[20]
68	C_4H_4	Vinylacetylene	52.076	501.7	821.3	704.8	0.264	0.0970	10.229	73.3[9]
69	C_4H_4S	Thiophene	84.136	643.3	1062.3	705.4	0.246	0.0670	9.654	78.6[16]
70	C_4H_5N	Methacrylonitrile	67.091	654.2	998.2	563.3	0.228	0.2823	8.576	83.3[20]
71	C_4H_6	Dimethylacetylene	54.092	540.4	879.7	737.4	0.270	0.1359	7.937	78.3[20]
72	C_4H_6	Ethylacetylene	54.092	506.3	834.7	683.2	0.269	0.0610	7.937	83.2[16]
73	C_4H_6	1,2-Butadiene	54.092	511.2	834.7	578.1	0.276	0.0987	7.950	83.7[25]
74	C_4H_6	1,3-Butadiene	54.092	483.8	765.0	628.0	0.272	0.2028	6.940	88.0[25]
75	C_4H_8	1-Butene	56.108	480.2	755.3	583.0	0.274	0.2085	6.766	95.6[25]
76	C_4H_8	*cis*-2-Butene	56.108	498.3	779.7	610.0	0.272	0.2575	6.760	91.2[25]
77	C_4H_8	Isobutene	56.108	479.3	752.2	580.0	0.274	0.1975	6.760	95.4[25]
78	C_4H_8	*trans*-2-Butene	56.108	493.3	770.7	595.0	0.273	0.2230	6.760	93.8[25]
79	C_4H_8O	Isobutyraldehyde	72.107	606.9	909.7	609.0	0.261	0.3800	9.199	91.4[20]
80	C_4H_8O	Methyl ethyl ketone	72.107	635.0	964.2	603.0	0.251	0.3188	9.199	89.6[20]
81	$C_4H_8O_2$	*n*-Butyric acid	88.107	785.6	1130.7	648.1	0.249	0.6030	11.861	92.0[20]
82	$C_4H_8O_2$	Ethyl acetate	88.107	630.5	941.9	556.0	0.254	0.3718	8.974	97.8[20]
83	$C_4H_8O_2$	Methyl propionate	88.107	635.6	955.1	578.0	0.256	0.3500	9.046	96.3[20]
84	$C_4H_8O_2$	Propyl formate	88.107	638.1	968.6	589.3	0.260	0.3154	9.024	96.7[16]
85	C_4H_9NO	Dimethyl acetamide	87.120	792.3	1182.0	583.7	0.230	0.3762	10.788	93.0[25]
86	C_4H_{10}	Isobutane	58.124	470.6	734.7	529.1	0.276	0.1825	6.730	105.5[25]
87	C_4H_{10}	*n*-Butane	58.124	490.8	765.3	550.7	0.274	0.1954	6.634	101.4[25]
88	$C_4H_{10}O$	Isobutanol	74.123	686.9	985.9	623.0	0.256	0.5917	10.949	92.4[20]
89	$C_4H_{10}O$	*n*-Butanol	74.123	703.6	1013.2	640.5	0.256	0.5903	11.440	91.5[20]
90	$C_4H_{10}O$	*t*-Butyl alcohol	74.123	640.0	912.0	576.1	0.255	0.6071	10.316	94.2[20]
91	$C_4H_{10}O$	Diethyl ether	74.123	553.9	840.2	523.2	0.264	0.2800	7.544	104.0[20]
92	$C_4H_{10}O_3$	Diethylene glycol	106.122	933.8	1225.9	668.0	0.244	1.1747	13.551	95.1[20]
93	$C_5H_4O_2$	Furfural	96.085	782.8	1182.8	714.2	0.243	0.4239	11.986	82.8[20]
94	C_5H_{10}	2-Methyl-1-butene	70.135	547.8	850.0	514.4	0.274	0.2000	7.055	108.7[25]
95	C_5H_{10}	2-Methyl-2-butene	70.135	561.1	870.0	527.6	0.273	0.2120	7.055	106.7[25]
96	C_5H_{10}	3-Methyl-1-butene	70.135	527.8	831.0	507.0	0.278	0.1490	7.055	112.8[25]
97	C_5H_{10}	Cyclopentane	70.135	580.4	921.2	655.0	0.274	0.1966	8.010	94.7[25]
98	C_5H_{10}	1-Pentene	70.135	545.6	853.0	586.0	0.273	0.2198	7.055	110.4[25]
99	C_5H_{10}	*cis*-2-Pentene	70.135	558.2	860.6	512.0	0.272	0.2060	7.055	107.8[25]
100	C_5H_{10}	*trans*-2-Pentene	70.135	557.1	857.0	508.4	0.272	0.2090	7.055	109.0[25]
101	$C_5H_{10}O$	Diethyl ketone	86.134	674.9	1009.7	542.3	0.256	0.3407	8.898	105.8[20]
102	$C_5H_{10}O_2$	*n*-Propyl acetate	102.134	674.5	988.9	483.6	0.253	0.3936	8.729	115.1[20]
103	C_5H_{12}	Isopentane	72.151	541.8	829.8	483.0	0.270	0.2104	7.020	117.4[25]
104	C_5H_{12}	*n*-Pentane	72.151	556.6	845.6	489.5	0.269	0.2387	7.020	116.1[25]
105	C_5H_{12}	Neopentane	72.151	508.8	780.8	464.0	0.276	0.1950	7.020	123.3[25]
106	$C_6H_3Cl_3$	1,2,4-Trichlorobenzene	181.449	876.0	1322.9	578.2	0.262	0.3358	9.956	124.8[20]

Part A (cont'd)

Number	Empirical Formula	Name	M	T_b	T_c	P_c	Z_c	ω	δ	V_L
Organic Chemicals										
107	$C_6H_4Cl_2$	*m*-Dichlorobenzene	147.004	803.1	1231.1	562.9	0.252	0.3073	9.554	114.1[20]
108	$C_6H_4Cl_2$	*o*-Dichlorobenzene	147.004	813.9	1255.1	595.3	0.256	0.2720	9.815	112.6[20]
109	$C_6H_4Cl_2$	*p*-Dichlorobenzene	147.004	804.7	1232.6	566.5	0.253	0.2822	9.645	117.8[15]
110	C_6H_5Br	Bromobenzene	157.010	772.9	1206.3	655.4	0.245	0.2508	9.753	105.0[25]
111	C_6H_5Cl	Chlorobenzene	112.559	729.7	1138.3	656.0	0.266	0.2545	9.623	101.8[20]
112	C_6H_5I	Iodobenzene	204.011	830.7	1298.1	655.8	0.266	0.2470	9.782	110.0[4]
113	C_6H_6	Benzene	78.114	635.9	1012.7	714.2	0.272	0.2116	9.158	89.4[25]
114	C_6H_6O	Phenol	94.113	819.0	1251.1	889.1	0.279	0.4201	12.106	88.9[40]
115	C_6H_7N	Aniline	93.129	823.1	1257.8	768.6	0.261	0.3830	11.461	91.1[20]
116	C_6H_{12}	Cyclohexane	84.162	637.0	995.3	591.5	0.272	0.2149	8.193	108.7[25]
117	C_6H_{12}	Methylcyclopentane	84.162	621.0	959.0	549.0	0.271	0.2316	7.847	113.1[25]
118	C_6H_{12}	1-Hexene	84.162	605.0	920.0	471.7	0.269	0.2463	7.400	125.8[25]
119	C_6H_{14}	2,2-Dimethylbutane	86.178	581.2	880.9	450.5	0.275	0.2317	6.712	122.7[25]
120	C_6H_{14}	2,3-Dimethylbutane	86.178	596.1	900.5	455.4	0.272	0.2447	6.967	131.2[25]
121	C_6H_{14}	*n*-Hexane	86.178	615.4	914.2	440.0	0.266	0.2972	7.266	131.6[25]
122	C_6H_{14}	2-Methylpentane	86.178	600.2	896.5	440.1	0.269	0.2771	7.018	132.0[25]
123	C_6H_{14}	3-Methylpentane	86.178	605.6	907.8	453.1	0.270	0.2745	7.132	129.8[25]
124	$C_6H_{14}O_4$	Triethylene glycol	150.176	1008.7	1282.2	481.0	0.243	1.2715	12.677	133.2[15]
125	C_7H_8	Toluene	92.141	790.8	1059.1	587.8	0.263	0.2415	8.914	106.8[25]
126	C_7H_8O	*o*-Cresol	108.140	835.5	1255.6	726.0	0.272	0.4299	11.139	105.2[40]
127	C_7H_{14}	Methylcyclohexane	98.189	673.4	1030.2	504.4	0.271	0.2362	7.825	128.3[25]
128	C_7H_{14}	Ethylcyclopentane	98.189	677.9	1025.0	492.8	0.268	0.2712	7.739	128.8[25]
129	C_7H_{14}	1-Heptene	98.189	660.3	963.9	412.2	0.262	0.3467	7.168	140.9[20]
130	C_7H_{16}	*n*-Heptane	100.205	668.9	972.3	396.9	0.261	0.3403	7.430	147.5[25]
131	C_8H_8	Styrene	104.152	752.9	1146.4	559.0	0.261	0.2885	9.211	115.0[20]
132	C_8H_{10}	Ethylbenzene	106.168	736.8	1115.5	540.0	0.265	0.2981	8.783	123.1[25]
133	C_8H_{10}	*m*-Xylene	106.168	742.1	1114.6	510.0	0.264	0.3086	8.818	123.5[25]
134	C_8H_{10}	*o*-Xylene	106.168	751.6	1138.0	530.0	0.266	0.2904	8.987	121.2[25]
135	C_8H_{10}	*p*-Xylene	106.168	740.7	1112.8	500.0	0.265	0.3304	8.769	124.0[25]
136	C_8H_{16}	Ethylcyclohexane	112.216	728.9	1084.7	453.9	0.265	0.3041	7.739	143.1[25]
137	C_8H_{16}	*n*-Propylcyclopentane	112.216	727.4	1062.5	406.5	0.253	0.3386	7.894	143.7[16]
138	C_8H_{18}	*n*-Octane	114.232	717.9	1024.9	362.1	0.258	0.3992	7.551	163.5[25]
139	$C_8H_{18}O_5$	Tetrnethylene glycol	194.229	1065.8	1432.4	304.4	0.205	0.8162	12.113	172.1[15]
140	C_9H_8	Indene	116.163	819.2	1245.5	553.6	0.250	0.3064	9.647	116.6[20]

141	C_9H_{10}	Indan	118.179	810.3	1225.9	526.6	0.251	0.2912	9.334	122.6[20]
142	C_9H_{10}	Methylstyrene	118.179	797.7	1192.6	500.0	0.255	0.3191	9.002	129.7[20]
143	C_9H_{12}	1-Ethyl-2-methylbenzene	120.195	788.7	1172.0	441.0	0.247	0.2970	8.839	136.4[20]
144	C_9H_{12}	*n*-Propylbenzene	120.195	778.3	1149.0	464.1	0.261	0.3446	8.661	139.4[20]
145	C_9H_{18}	*n*-Propylcyclohexane	126.243	773.8	1114.5	369.2	0.248	0.3617	7.886	159.2[20]
146	C_9H_{20}	*n*-Nonane	128.259	763.1	1071.0	331.0	0.254	0.4439	7.649	179.6[25]
147	$C_{10}H_8$	Naphthalene	128.174	884.0	1347.0	576.1	0.258	0.2954	9.738	132.0[99]
148	$C_{10}H_{10}$	1-Methylindene	130.190	851.7	1266.2	483.0	0.247	0.3291	9.323	
149	$C_{10}H_{10}$	2-Methylindene	130.190	866.1	1286.2	486.5	0.246	0.3367	9.485	144.1[20]
150	$C_{10}H_{12}$	Dicyclopentadiene	132.206	797.7	1188.7	773.9	0.254	0.2767	8.398	142.1[35]
151	$C_{10}H_{14}$	*n*-Butylbenzene	134.222	821.6	1188.8	418.7	0.258	0.3929	8.425	156.1[20]
152	$C_{10}H_{14}$	1,2-Dimethyl-3-ethylbenzene	134.222	840.8	1224.1	453.6	0.262	0.3968	8.916	
153	$C_{10}H_{20}$	*n*-Butylcyclohexane	140.27	817.4	1162.4	353.9	0.252	0.4035	7.90	175.5[20]
154	$C_{10}H_{22}$	*n*-Decane	142.286	805.1	1114.0	306.0	0.251	0.4869	7.722	196.0[25]
155	$C_{11}H_{10}$	1-Methylnaphthalene	142.201	932.0	1384.5	517.6	0.254	0.3607	9.770	139.4[20]
156	$C_{11}H_{10}$	2-Methylnaphthalene	142.201	925.6	1371.4	508.1	0.256	0.3647	9.660	
157	$C_{11}H_{24}$	*n*-Undecane	156.313	844.3	1152.0	282.0	0.248	0.521	7.790	212.2[25]
158	$C_{12}H_8$	Acenaphthalene	152.196	977.7	1434.5	467.2	0.237	0.3733	10.018	169.3[16]
159	$C_{12}H_{10}$	Diphenyl	154.212	951.1	1420.0	557.0	0.276	0.3638	9.891	155.8[74]
160	$C_{12}H_{12}$	2,7-Dimethylnaphthalene	156.228	965.1	1400.7	467.4	0.257	0.4232	9.760	
161	$C_{12}H_{14}$	1,2,3-Trimethylindene	158.244	909.3	1296.4	384.1	0.242	0.4271	8.955	
162	$C_{12}H_{26}$	*n*-Dodecane	170.328	881.0	1188.3	261.6	0.245	0.561	7.840	228.6[25]
163	$C_{13}H_{10}$	Fluorene	166.223	1027.9	1480.1	434.2	0.234	0.4512	10.136	
164	$C_{13}H_{14}$	1-Methylethylnaphthalene	170.255	986.7	1393.4	408.6	0.233	0.5044	10.03	
165	$C_{13}H_{14}$	2,3,5-Trimethylnaphthalene	170.255	1004.7	1418.9	408.6	0.232	0.5044	10.121	
166	$C_{13}H_{28}$	*n*-Tridecane	184.367	915.5	1219.0	250.0	0.242	0.6002	7.890	244.9[25]
167	$C_{14}H_{10}$	Phenanthrene	178.234	1103.0	1531.8	420.4	0.228	0.4396	10.524	
168	$C_{14}H_{30}$	*n*-Tetradecane	198.394	948.1	1251.0	230.0	0.240	0.640	7.920	261.3[25]
169	$C_{15}H_{12}$	1-Phenylindene	192.261	1071.3	1518.6	391.0	0.230	0.4644	9.933	
170	$C_{15}H_{14}$	2-Ethylfluorene	194.277	1047.9	1459.9	357.5	0.230	0.5175	9.636	
171	$C_{15}H_{32}$	*n*-Pentadecane	212.421	978.8	1278.0	220.0	0.237	0.6743	7.960	277.8[25]
172	$C_{16}H_{10}$	Fluoranthene	202.256	1199.1	1685.9	378.1	0.221	0.4930	10.426	
173	$C_{16}H_{10}$	Pyrene	202.256	1143.3	1605.7	378.1	0.224	0.4988	10.222	
174	$C_{16}H_{12}$	1-Phenylnaphthalene	204.272	1076.7	1512.2	381.8	0.228	0.5034	10.283	
175	$C_{16}H_{34}$	*n*-Hexadecane	226.448	1007.9	1305.0	206.0	0.236	0.7078	7.990	294.1[25]
176	$C_{18}H_{12}$	Chrysene	228.294	1298.1	1788.5	346.4	0.213	0.5676	10.691	

Part B

Number	Empirical Formula	Name	a_1	a_2	a_3	a_4	a_5	A_1	A_2	A_3
Inorganic Chemicals										
1	Ar	Argon	4.9647	0.0	0.0	0.0	0.0	5.42578	1499.0	463.9195
2	Br_2	Bromine	8.552	0.8334 E-3	−0.5053 E-06	0.1098 E-09	0.0	5.53786	5563.552	409.318
3	CCl_4	Carbon tetrachloride	18.36077	0.1932811 E-01	−0.2576049 E-04	0.173446 E-07	−0.4549234 E-11	6.199663	6110.034	441.2806
4	CO	Carbon monoxide	6.956012	0.591124 E-04	0.5075809 E-06	0.7641183 E-09	−0.6540363 E-12	5.712089	1385.883	462.6165
5	$COCl_2$	Phosgene	13.76767	0.1093685 E-01	−0.1226482 E-04	0.7900403 E-08	−0.2079814 E-11	5.870425	4545.777	412.5742
6	CO_2	Carbon dioxide	8.378605	−0.6475766 E-02	−0.3555025 E-05	0.1194595 E-08	−0.1851702 E-12	6.470232	3521.259	455.869
7	CS_2	Carbon disulfide	11.53044	0.123864 E-01	0.4778188 E-05	−0.8568489 E-08	0.2966357 E-11	6.263774	6389.82	486.9933
8	C_2OCl_4	Trichloroacetyl chloride	23.70705	0.2731643 E-01	−0.3266946 E-04	0.2107581 E-07	−0.5450088 E-11	5.752994	5751.971	363.6816
9	ClH	Hydrogen chloride	6.959	0.2236 E-03	0.7333 E-06	−0.1776 E-09	0.0	5.688540	3244.028	442.2680
10	Cl_2	Chlorine	7.973	0.18901 E-02	−0.12101 E-05	0.26526 E-09	0.0	5.186832	3699.272	417.709
11	HI	Hydrogen iodide	6.948176	0.1457827 E-05	0.1104365 E-05	−0.5203962 E-09	0.7254255 E-13	5.362089	3840.331	424.3549
12	H_2	Hydrogen	6.647816	0.2472647 E-02	−0.4557635 E-05	0.3117701 E-08	−0.6643678 E-12	5.692657	418.1773	474.214
13	H_2O	Water	7.985742	0.4633191 E-03	0.1402841 E-05	−0.6578387 E-09	0.9795288 E-13	6.53247	7173.79	389.4747
14	H_2S	Hydrogen sulfide	8.031194	0.9868632 E-03	0.2388543 E-05	−0.159311 E-08	0.320329 E-12	5.445487	3535.867	432.235
15	H_3N	Ammonia	5.2765	0.39006 E-02	0.35245 E-06	−0.27402 E-09	0.0	6.152480	4253.826	415.9528
16	Ne	Neon	4.9647	0.0	0.0	0.0	0.0	5.560555	476.5174	464.7596
17	NO	Nitric oxide	7.255110	0.4551648 E-03	0.2640019 E-06	−0.1225439 E-09	0.133261 E-13	8.142411	2374.39	434.2132
18	NO_2	Nitrogen dioxide	8.495494	0.4921745 E-02	−0.1239651 E-05	−0.2704296 E-09	0.1240708 E-12	12.76017	11907.65	616.0504
19	N_2	Nitrogen	6.947138	0.6609477 E-04	0.5693395 E-06	0.3226862 E-10	−0.9683259 E-13	5.316656	1184.797	454.5328
20	N_2O	Nitrous oxide	8.767171	0.6369103 E-02	−0.3621806 E-05	0.1572094 E-08	−0.2566121 E-12	5.353828	2785.606	416.6335
21	O_2	Oxygen	6.996501	0.5581101 E-03	0.1399925 E-05	−0.1093827 E-08	0.2299662 E-12	5.15038	1404.466	452.1536
22	O_2S	Sulfur dioxide	9.134	0.532 E-02	−0.2323 E-05	0.3527 E-09	0.0	5.966623	4293.005	401.685
23	O_3S	Sulfur trioxide	10.964	0.1251 E-01	−0.6523 E-05	0.1328 E-08	0.0	4.828507	3199.785	234.315
Organic Chemicals										
24	$CHCl_3$	Chloroform	14.84	0.1245 E-01	−0.6495 E-05	0.1259 E-08	0.0	5.894057	5289.385	393.075
25	CHN	Hydrogen cyanide	8.194594	0.526853 E-02	−0.3123949 E-05	0.1256972 E-08	−0.2109817 E-12	6.97745	5672.753	443.761
26	CH_2O	Formaldehyde	8.209533	0.1838523 E-02	0.1697531 E-05	−0.1107293 E-08	0.2015218 E-12	5.525307	3890.399	402.114
27	CH_3Cl	Methyl chloride	5.964398	0.1006818 E-01	−0.8251344 E-07	−0.2858358 E-08	0.1064404 E-11	5.504941	3906.036	414.1819
28	CH_3I	Methyl iodide	9.71643	0.1105462 E-01	−0.3302857 E-05	−0.173936 E-09	0.3161217 E-12	5.235173	4840.0	399.9509
29	CH_4	Methane	8.245223	0.3806333 E-02	0.8864745 E-05	−0.7461153 E-08	0.1822959 E-11	5.14135	1742.638	452.974
30	CH_4O	Methanol	9.291084	0.8430542 E-02	0.6669185 E-05	−0.8208981 E-08	0.2500638 E-11	7.513334	6468.101	396.2652
31	CH_5N	Methylamine	11.192	0.1571 E-01	−0.43782 E-05	0.50592 E-09	0.0	5.973935	4216.777	389.9355
32	C_2HCl_3	Trichloroethylene	17.8198	0.1891162 E-01	−0.1588157 E-04	0.7817208 E-08	−0.1645299 E-11	5.814331	5636.178	391.6901
33	C_2HCl_3O	Dichloroacetyl chloride	21.08973	0.2396316 E-01	−0.2415185 E-04	0.1440388 E-07	−0.3583915 E-11	6.437229	6108.109	369.1736
34	C_2H_2	Acetylene	9.89	0.8273 E-02	−0.3783 E-05	0.7457 E-09	0.0	6.109766	3305.991	444.4562
35	$C_2H_2Cl_2O$	Chloroacetyl chloride	18.47242	0.2060988 E-02	−0.1563425 E-04	0.7711953 E-08	−0.1717712 E-11	5.875686	5522.555	341.0137
36	C_2H_3Cl	Vinyl chloride	11.52336	0.1776248 E-01	−0.9084331 E-05	0.2459001 E-08	−0.1792789 E-12	5.033325	3650.037	391.3080
37	C_2H_3ClO	Acetyl chloride	15.8551	0.1725661 E-01	−0.7116618 E-05	0.1060025 E-08	0.1484101 E-12	[illegible]	[illegible]	[illegible]

38	$C_2H_3Cl_3$	1,1,2-Trichloroethane	19.37069	0.2598217 E-01	−0.1790523 E-04	0.7161791 E-08	−0.1193551 E-11	6.877873	6958.502	411.7562
39	C_2H_3N	Acetonitrile	11.5361	0.1232096 E-01	−0.1200452 E-05	−0.2031388 E-08	0.7743102 E-12	6.393303	6059.675	411.6977
40	C_2H_4	Ethylene	9.326018	0.1393929 E-01	0.1010831 E-05	−0.7516552 E-08	0.3615367 E-11	5.27791	2568.994	433.9156
41	$C_2H_4Cl_2$	1,1-Dichloroethane	16.548	0.22237 E-01	−0.92549 E-05	0.15584 E-08	0.0	5.34928	4694.036	371.5705
42	$C_2H_4Cl_2$	1,2-Dichloroethane	17.38636	0.1985922 E-01	−0.8175161 E-05	0.1505784 E-08	0.9333614 E-13	5.768529	5524.353	383.4458
43	C_2H_4	Acetaldehyde	11.90924	0.1481123 E-01	0.9439146 E-06	−0.501431 E-08	0.172932 E-11	6.49856	5121.453	419.9494
44	C_2H_4O	Ethylene oxide	10.14899	0.1762188 E-01	0.4347253 E-05	−0.1164214 E-07	0.4326094 E-11	5.630604	4460.616	399.9853
45	$C_2H_4O_2$	Acetic acid	14.63924	0.229877 E-01	−0.1021997 E-04	0.2589452 E-08	−0.2804407 E-12	7.203594	7376.157	410.1814
46	$C_2H_4O_2$	Methyl formate	14.31964	0.2105721 E-01	−0.3231842 E-05	−0.5463847 E-08	0.2608819 E-11	6.023216	4906.897	396.03
47	C_2H_5Cl	Ethyl chloride	13.436	0.21267 E-01	−0.64893 E-05	0.6832 E-09	0.0	5.696013	4424.781	404.411
48	C_2H_6	Ethane	11.51606	0.140309 E-01	0.854034 E-05	−0.1106078 E-07	0.3162199 E-11	5.383894	2847.921	434.898
49	C_2H_6O	Dimethyl ether	15.91995	0.1599677 E-01	0.7899362 E-05	−0.1293053 E-07	0.4398304 E-11	5.77524	3918.305	415.2581
50	C_2H_6O	Ethanol	14.04853	0.2153149 E-01	−0.2153442 E-05	−0.4602256 E-08	0.1893692 E-11	7.43437	6162.36	359.3826
51	$C_2H_6O_2$	Ethylene glycol	18.11978	0.2404298 E-01	0.1265575 E-05	−0.1072173 E-07	0.4248091 E-11	7.258288	8088.817	311.8854
52	C_2H_6S	Dimethyl sulfide	16.23989	0.1919445 E-01	−0.3534516 E-06	−0.5604401 E-08	0.2328362 E-11	5.610757	4769.088	396.909
53	C_2H_6S	Ethyl mercaptan	15.73943	0.2175969 E-01	−0.4178643 E-05	−0.2550827 E-08	0.1279568 E-11	5.631324	4709.722	394.2954
54	C_2H_7N	Ethylamine	14.61684	0.2301337 E-01	0.5042536 E-05	−0.1298503 E-07	0.470142 E-11	5.841118	4333.688	377.3129
55	C_3H_3N	Acrylonitrile	13.77061	0.1984967 E-01	−0.8937427 E-05	0.193298 E-08	−0.2797383 E-13	6.038654	5459.573	396.7914
56	C_3H_4	Methylacetylene	13.17061	0.1775777 E-01	−0.7296423 E-05	0.1921976 E-08	−0.242782 E-12	5.179851	3470.383	387.1061
57	C_3H_4	Propadiene	12.6505	0.1928835 E-01	−0.6452827 E-05	−0.1674653 E-08	0.1813724 E-11	2.443058	1832.002	317.5695
58	C_3H_6	Propylene	13.63267	0.2106998 E-01	0.249545 E-05	−0.1146863 E-07	0.5247386 E-11	5.44467	3375.447	418.4319
59	C_3H_6O	Acetone	16.13621	0.2340064 E-01	−0.1479392 E-05	−0.4143552 E-08	0.1323724 E-11	6.244412	5356.715	397.5293
60	$C_3H_6O_2$	Ethyl formate	20.94868	0.273312 E-01	−0.146055 E-05	−0.8986131 E-08	0.3692011 E-11	5.94826	4965.502	377.2637
61	$C_3H_6O_2$	Methyl acetate	21.04651	0.2395065 E-01	0.154732 E-05	−0.9770737 E-08	0.3676818 E-11	6.253272	5251.863	385.1996
62	$C_3H_6O_2$	Propionic acid	20.17881	0.2781613 E-01	−0.2700043 E-05	−0.7554358 E-08	0.323127 E-11	6.838962	6770.055	340.8683
63	C_3H_7NO	Dimethylformamide	20.8472	0.3068996 E-01	−0.4238415 E-05	−0.6471348 E-08	0.287579 E-11	5.298043	5665.834	313.254
64	C_3H_8	Propane	15.58683	0.2504953 E-01	0.1404258 E-04	−0.3526261 E-07	0.1864467 E-10	5.353418	3371.084	414.488
65	C_3H_8O	Isopropanol	18.703	0.3374798 E-01	−0.8097677 E-05	−0.4524869 E-08	0.2586334 E-11	7.180215	5596.813	327.2833
66	C_3H_8O	n-Propanol	18.71145	0.2788756 E-01	0.858526 E-06	−0.9785116 E-08	0.3679178 E-11	6.683944	5414.961	303.9864
67	C_3H_9N	Trimethylamine	19.09535	0.3856445 E-01	−0.136958 E-04	0.2035707 E-08	−0.1282133 E-13	5.552747	4030.388	398.7676
68	C_4H_4	Vinylacetylene	5.297392	0.171349 E-01	−0.11425 E-05	−0.3775036 E-08	0.1440128 E-11	5.297392	3879.835	381.4085
69	C_4H_4S	Thiophene	5.520119	0.3754804 E-01	−0.2222312 E-04	0.6967862 E-08	−0.709689 E-12	5.520119	5164.732	366.4536
70	C_4H_5N	Methacrylonitrile	19.23704	0.2314625 E-01	−0.2793527 E-05	−0.45453 E-08	0.1908719 E-11	5.824528	5313.429	366.5642
71	C_4H_6	Dimethylacetylene	16.76823	0.2517102 E-01	−0.8454522 E-05	0.2326427 E-08	−0.4824367 E-12	5.637212	4482.741	388.6972
72	C_4H_6	Ethylacetylene	17.38834	0.2778978 E-01	−0.116434 E-04	0.3040897 E-08	−0.3742009 E-12	5.606554	4103.138	387.8234
73	C_4H_6	1,2-Butadiene	17.15982	0.26213 E-01	−0.5937819 E-05	−0.2361299 E-08	0.1011447 E-11	6.184923	4644.865	419.7079
74	C_4H_6	1,3-Butadiene	16.47292	0.3392027 E-01	−0.1392511 E-04	−0.4786315 E-08	0.5611304 E-11	5.69864	4105.731	409.9939
75	C_4H_8	1-Butene	17.96141	0.3297022 E-01	−0.605339 E-05	−0.569609 E-08	0.2826942 E-11	5.58272	3941.014	404.741
76	C_4H_8	cis-2-Butene	16.54537	0.2966393 E-01	0.5471621 E-05	−0.1883127 E-07	0.8437562 E-11	5.456285	3977.563	394.4956
77	C_4H_8	Isobutene	18.93086	0.3101008 E-01	−0.4930015 E-05	−0.6036954 E-08	0.3200886 E-11	5.616762	3953.678	405.9166
78	C_4H_8	trans-2-Butene	18.84267	0.2761259 E-01	0.3097447 E-05	−0.1337556 E-07	0.5631517 E-11	5.487073	3984.406	400.0703
79	C_4H_8O	Isobutyraldehyde	20.75125	0.3284207 E-01	−0.3152369 E-06	−0.1104319 E-07	0.4330567 E-11	6.508418	5396.492	379.294
80	C_4H_8O	Methyl ethyl ketone	22.30645	0.2959044 E-01	−0.3506391 E-06	−0.8248579 E-08	0.3038054 E-11	5.885353	5097.27	356.3834
81	$C_4H_8O_2$	n-Butyric acid	23.98619	0.3727046 E-01	−0.3625636 E-05	−0.1019473 E-07	0.4365542 E-11	7.444973	7372.927	330.4845
82	$C_4H_8O_2$	Ethyl acetate	24.90819	0.3329732 E-01	0.7316711 E-06	−0.1247032 E-07	0.4824152 E-11	6.3307	5440.049	373.48

Part B (cont'd)

Number	Empirical Formula	Name	a_1	a_2	a_3	a_4	a_5	A_1	A_2	A_3
Organic Chemicals										
83	$C_4H_8O_2$	Methyl propionate	24.90819	0.3329732 E-01	0.7816711 E-06	-0.1247032 E-07	0.4824152 E-11	6.280916	5462.483	372.7137
84	$C_4H_8O_2$	Propyl formate	24.90819	0.3329732 E-01	0.7316711 E-06	-0.1247032 E-07	0.4824152 E-11	5.956599	5225.881	363.1314
85	C_4H_9NO	Dimethyl acetamide	24.63017	0.4015238 E-01	-0.5139106 E-05	-0.913829 E-08	0.4017948 E-11	4.812879	5134.59	279.0569
86	C_4H_{10}	Isobutane	20.41853	0.3462286 E-01	0.1415619 E-04	-0.4246126 E-07	0.2296993 E-10	5.611805	3870.419	409.949
87	C_4H_{10}	*n*-Butane	20.79783	0.3143287 E-01	0.1928511 E-04	-0.4588652 E-07	0.2380972 E-10	5.741624	4126.385	409.5179
88	$C_4H_{10}O$	Isobutanol	17.908	0.3086043 E-01	0.2615677 E-04	-0.3727992 E-07	0.1247926 E-10	7.134107	5843.713	310.811
89	$C_4H_{10}O$	*n*-Butanol	22.86768	0.4421951 E-01	-0.1487031 E-04	-0.4450266 E-09	0.139999 E-11	6.303186	5225.124	274.4291
90	$C_4H_{10}O$	*t*-Butyl alcohol	23.80689	0.4378233 E-01	-0.1467142 E-04	0.8051186 E-09	0.1541653 E-11	6.180797	4882.792	274.7841
91	$C_4H_{10}O$	Diethyl ether	23.43495	0.3456899 E-01	0.6985382 E-05	-0.1902477 E-07	0.6906888 E-11	5.976844	4614.723	288.3025
92	$C_4H_{10}O_3$	Diethylene glycol	26.63047	0.4356575 E-01	0.6483778 E-05	-0.2359434 E-07	0.8904581 E-11	9.238843	10861.34	363.948
93	$C_5H_4O_2$	Furfural	20.38649	0.3085299 E-01	-0.4999507 E-05	-0.7442546 E-08	0.3466989 E-11	8.278279	9658.592	4.9.7815
94	C_5H_{10}	2-Methyl-1-butene	23.51432	0.416842 E-01	-0.6797959 E-05	-0.1216479 E-07	0.7590583 E-11	5.655016	4383.237	287.8013
95	C_5H_{10}	2-Methyl-2-butene	22.08508	0.3932158 E-01	-0.3039504 E-05	-0.1105363 E-07	0.511218 E-11	5.701977	4531.679	296.7817
96	C_5H_{10}	3-Methyl-1-butene	24.98621	0.4544002 E-01	-0.2709002 E-04	0.1719799 E-07	0.6539064 E-11	5.554918	4210.159	304.7817
97	C_5H_{10}	Cyclopentane	16.21714	0.4643893 E-01	0.5947453 E-05	-0.2901838 E-07	0.1338546 E-10	5.429031	4462.042	306.4612
98	C_5H_{10}	1-Pentene	23.09041	0.4065747 E-01	-0.7117898 E-05	-0.5289083 E-08	0.1708107 E-11	5.452355	4326.393	288.5993
99	C_5H_{10}	*cis*-2-Pentene	21.12406	0.4169782 E-01	-0.3053253 E-05	-0.1195115 E-07	0.4474386 E-11	5.625241	4412.304	282.3593
100	C_5H_{10}	*trans*-2-Pentene	22.95406	0.3853433 E-01	-0.1306019 E-05	-0.1368152 E-07	0.6325655 E-11	5.722727	4491.719	287.2958
101	$C_5H_{10}O$	Diethyl ketone	24.50795	0.4231144 E-01	-0.117334 E-05	-0.1375883 E-07	0.5488549 E-11	6.159896	5631.04	361.7281
102	$C_5H_{10}O_2$	*n*-Propyl acetate	28.73052	0.4269 E-01	-0.9959801 E-07	-0.1517593 E-07	0.5975479 E-11	6.302585	5536.313	355.9455
103	C_5H_{12}	Isopentane	24.94637	0.4446726 E-01	0.7054883 E-05	-0.3344167 E-07	0.1774503 E-10	5.49978	4221.154	287.287
104	C_5H_{12}	*n*-Pentane	25.64627	0.397176 E-01	0.2397294 E-04	-0.5842615 E-07	0.3079918 E-10	5.853654	4598.287	304.4148
105	C_5H_{12}	Neopentane	25.46761	0.461177 E-01	0.1147232 E-04	-0.4605143 E-04	0.2506343 E-10	5.692011	4148.025	404.42
106	$C_6H_3Cl_3$	1,2,4-Trichlorobenzene	25.75694	0.4831912 E-01	-0.3089766 E-04	0.1057239 E-07	-0.1390436 E-11	6.592514	8014.486	364.6567
107	$C_6H_4Cl_2$	*m*-Dichlorobenzene	22.87009	0.4456102 E-01	-0.2128264 E-04	0.2990787 E-08	0.7361333 E-12	11.37776	15451.49	682.6184
108	$C_6H_4Cl_2$	*o*-Dichlorobenzene	22.87009	0.4456102 E-01	-0.2128264 E-04	0.2990787 E-08	0.7361333 E-12	5.981208	6798.548	345.1776
109	$C_6H_4Cl_2$	*p*-Dichlorobenzene	22.87009	0.4456102 E-01	-0.2128264 E-04	0.2990787 E-08	0.7361333 E-12	6.813621	7773.248	396.0557
110	C_6H_5Br	Bromobenzene	20.36329	0.4011145 E-01	-0.1108768 E-04	-0.4813553 E-08	0.2980795 E-11	5.881747	6571.377	365.2812
111	C_6H_5Cl	Chlorobenzene	19.98323	0.4080291 E-01	-0.1166762 E-04	-0.4590812 E-08	0.2862703 E-11	5.85808	6222.695	372.2756
112	C_6H_5I	Iodobenzene	20.57765	0.3968462 E-01	-0.1067708 E-04	-0.50094 E-08	0.2927215 E-11	5.72827	6854.36	348.1382
113	C_6H_6	Benzene	16.39282	0.4020369 E-01	0.6925399 E-05	-0.4114202 E-07	0.2398098 E-10	5.658375	5307.813	379.456
114	C_6H_6O	Phenol	19.91816	0.4992518 E-01	-0.2451622 E-04	0.460471 E-08	0.4113815 E-12	6.535719	7250.359	321.6074
115	C_6H_7N	Aniline	20.11747	0.4538924 E-01	-0.5743054 E-05	-0.1216273 E-07	0.5366204 E-11	6.44519	7386.331	344.6331
116	C_6H_{12}	Cyclohexane	21.00016	0.5627391 E-01	0.1129438 E-04	-0.3606168 E-07	0.1482606 E-10	5.473055	5030.253	371.2755

117	C_6H_{12}	Methylcyclopentane	22.02735	0.5465972 E-01	0.5935187 E-05	−0.3442291 E-07	0.164543 E-10	5.567563	4936.44	375.9433
118	C_6H_{12}	1-Hexene	27.87277	0.4926029 E-01	−0.7512748 E-05	−0.9298869 E-08	0.3952236 E-11	5.711574	4783.217	374.7552
119	C_6H_{14}	2,2-Dimethylbutane	29.64918	0.550671 E-01	0.1806208 E-05	−0.2478314 E-07	0.9570332 E-11	5.50245	4486.167	381.1012
120	C_6H_{14}	2,3-Dimethylbutane	29.27018	0.5595826 E-01	−0.2028283 E-05	−0.2494276 E-07	0.1323425 E-10	5.61351	4672.79	380.1172
121	C_6H_{14}	*n*-Hexane	30.17847	0.5199263 E-01	0.3048799 E-05	−0.2763996 E-07	0.1346731 E-10	6.039243	5085.758	382.794
122	C_6H_{14}	2-Methylpentane	30.30218	0.5351181 E-01	0.5716877 E-05	−0.3870868 E-07	0.2132741 E-10	5.7088	4700.639	375.5984
123	C_6H_{14}	3-Methylpentane	30.17174	0.5189874 E-01	0.366338 E-05	−0.2860809 E-07	0.1391842 E-10	5.7023	4700.526	376.1611
124	$C_6H_{14}O_4$	Triethylene glycol	38.88318	0.6252653 E-01	0.5449502 E-05	−0.2983416 E-07	0.1149462 E-10	9.707385	11860.26	356.528
125	C_7H_8	Toluene	21.17722	0.4639546 E-01	0.9961368 E-05	−0.4628264 E-07	0.2585787 E-10	5.944251	5836.287	374.745
126	C_7H_8O	*o*-Cresol	24.15791	0.5181666 E-01	−0.7496517 E-05	−0.1323952 E-07	0.5990957 E-11	5.749559	6394.925	286.9147
127	C_7H_{14}	Methylcyclohexane	27.06932	0.6729289 E-01	0.5750553 E-05	−0.3885885 E-07	0.1837708 E-10	5.608872	5338.374	370.0705
128	C_7H_{14}	Ethylcyclopentane	24.63008	0.9883192 E-01	−0.1351091 E-03	0.1674966 E-06	−0.8292246 E-10	5.698096	5369.766	364.7743
129	C_7H_{14}	1-Heptene	32.68419	0.5769426 E-01	−0.724699 E-05	−0.1448889 E-07	0.6897952 E-11	5.922457	5212.626	362.3801
130	C_7H_{16}	*n*-Heptane	34.96845	0.608752 E-01	0.1213345 E-05	−0.293693 E-07	0.1454746 E-10	5.98627	5278.902	359.5259
131	C_8H_8	Styrene	24.82866	0.5843 E-01	−0.25693 E-04	0.3432486 E-08	0.8297016 E-12	6.071326	6329.575	358.5947
132	C_8H_{10}	Ethylbenzene	26.37827	0.5526271 E-01	0.1239678 E-04	−0.5839197 E-07	0.3331962 E-10	5.747492	5862.905	349.8527
133	C_8H_{10}	*m*-Xylene	26.42788	0.5188146 E-01	0.122123 E-04	−0.4900955 E-07	0.2628339 E-10	5.949452	6049.457	354.6467
134	C_8H_{10}	*o*-Xylene	27.89247	0.5103585 E-01	0.5908631 E-05	−0.3659655 E-07	0.1949676 E-10	5.922098	6141.641	354.0417
135	C_8H_{10}	*p*-Xylene	26.39662	0.4982215 E-01	0.1658367 E-04	−0.5289838 E-07	0.276508 E-10	5.94371	6033.046	355.99
136	C_8H_{16}	Ethylcyclohexane	32.07366	0.7610546 E-01	−0.7343807 E-05	−0.4881198 E-07	0.2469959 E-10	5.769319	5751.059	355.93
137	C_8H_{16}	*n*-Propylcyclopentane	30.7991	0.8393195 E-01	0.7343807 E-05	0.9086445 E-08	−0.10736 E-11	5.957854	5754.086	352.481
138	C_8H_{18}	*n*-Octane	39.77987	0.6930903 E-01	−0.3576344 E-04	−0.3456095 E-07	0.1749419 E-10	6.4141	5947.491	360.26
139	$C_8H_{18}O_5$	Tetraethylene glycol	50.93845	0.8159435 E-01	0.1479927 E-05	−0.3636893 E-07	0.141849 E-10	10.89268	14787.51	439.2803
140	C_9H_8	Indene	26.11577	0.6007207 E-01	−0.1628819 E-04	−0.7372481 E-08	0.4361004 E-11	6.176081	7190.945	371.053
141	C_9H_{10}	Indan	27.27218	0.6712433 E-01	−0.1535148 E-04	−0.1126863 E-07	0.5886033 E-11	6.049353	6821.739	357.362
142	C_9H_{10}	Methylstyrene	40.40845	0.5092828 E-01	0.1423367 E-04	−0.204508 E-07	0.9784106 E-11	6.087191	6638.097	352.369
143	C_9H_{12}	1-Ethyl-2-methylbenzene	32.7457	0.6787234 E-01	−0.2692206 E-04	0.5325566 E-08	−0.3666534 E-12	6.202647	6541.084	351.7732
144	C_9H_{12}	*n*-Propylbenzene	30.85809	0.7397426 E-01	−0.333376 E-04	0.8236172 E-08	−0.8488248 E-12	5.919976	6180.323	340.82
145	C_9H_{18}	*n*-Propylcyclohexane	36.93022	0.9596314 E-01	−0.3752096 E-04	0.6920047 E-08	−0.3686077 E-11	6.022487	6079.604	343.4018
146	C_9H_{20}	*n*-Nonane	44.6198	0.7738344 E-01	0.2963375 E-05	−0.4134716 E-07	0.2114216 E-10	6.22189	6662.655	330.96
147	$C_{10}H_8$	Naphthalene	26.38315	0.7107626 E-01	−0.303242 E-04	0.2599732 E-08	0.1536979 E-11	5.464939	7090.598	305.1725
148	$C_{10}H_{10}$	1-Methylindene	29.92083	0.696464 E-01	−0.1746532 E-04	−0.9807097 E-08	0.5436545 E-11	6.139705	7223.491	343.832
149	$C_{10}H_{10}$	2-Methylindene	29.5297	0.7131178 E-01	−0.181527 E-04	−0.990292 E-08	0.5540522 E-11	6.165742	6479.445	340.573
150	$C_{10}H_{12}$	Dicyclopentadiene	35.24185	0.8077631 E-01	−0.3064237 E-04	−0.1037675 E-08	0.3171173 E-11	5.97896	6534.868	353.37
151	$C_{10}H_{14}$	*n*-Butylbenzene	35.57803	0.8354658 E-01	−0.3733832 E-04	0.919402 E-08	−0.951656 E-12	6.089988	6534.868	330.3357
152	$C_{10}H_{14}$	1,2-Dimethyl-3-Ethylbenzene	32.18688	0.7623887 E-01	−0.7317236 E-05	−0.2192313 E-07	0.9362406 E-11	6.180938	6838.277	330.4982
153	$C_{10}H_{20}$	*n*-Butylcyclohexane	41.74714	0.1046007 E-01	−0.3964926 E-04	0.6648178 E-08	−0.214681 E-12	6.094088	6369.972	329.0528
154	$C_{10}H_{22}$	*n*-Decane	49.42138	0.8602711 E-01	0.2049705 E-05	−0.4415409 E-07	0.2256651 E-10	6.33557	6213.998	317.6512
155	$C_{11}H_{10}$	1-Methylnaphthalene	29.3571	0.7475587 E-01	−0.1560299 E-04	−0.1428024 E-07	0.7089941 E-11	6.080512	7676.997	323.8246

Part B (cont'd)

Number	Empirical Formula	Name	a_1	a_2	a_3	a_4	a_5	A_1	A_2	A_3
Organic Chemicals										
156	$C_{11}H_{10}$	2-Methylnaphthalene	29.3571	0.7475587 E-01	−0.1360299 E-04	−0.1428024 E-07	0.7059941 E-11	6.101162	7630.143	325.2701
157	$C_{11}H_{24}$	*n*-Undecane	54.25211	0.9427374 E-01	0.2727295 E-05	−0.4957262 E-07	0.2544979 E-10	7.21247	7475.258	350.7821
158	$C_{12}H_8$	Acenaphthlene	30.48077	0.7755508 E-01	−0.2664829 E-04	−0.5063562 E-08	0.4429521 E-11	6.216864	8047.648	313.565
159	$C_{12}H_{10}$	Diphenyl	32.02568	0.9116691 E-01	−0.4408667 E-04	0.7505404 E-08	0.9059193 E-12	6.194778	7947.647	317.1246
160	$C_{12}H_{12}$	2,7-Dimethylnaphthalene	33.16177	0.8467461 E-01	−0.1714886 E-04	−0.1655051 E-07	0.8135765 E-11	6.707037	8521.498	331.2805
161	$C_{12}H_{14}$	1,2,3-Trimethylindene	37.49874	0.8872509 E-01	−0.1961391 E-04	−0.1486368 E-07	0.7642585 E-11	6.452743	7497.763	321.886
162	$C_{12}H_{26}$	*n*-Dodecane	59.0528	0.1029143	0.2243202 E-05	−0.5378563 E-07	0.279613 E-10	6.561135	6739.22	292.574
163	$C_{13}H_{10}$	Fluorene	34.75668	0.8111078 E-01	−0.2232686 E-04	−0.1036036 E-07	0.6152866 E-11	8.197664	11632.66	435.9648
164	$C_{13}H_{14}$	1-Methylethylnaphthalene	38.92984	0.9421013 E-01	−0.1816491 E-04	−0.1913785 E-07	0.9260544 E-11	6.678618	8234.079	295.939
165	$C_{13}H_{14}$	2,3,5-Trimethylnaphthalene	36.96391	0.9458171 E-01	−0.1866141 E-04	−0.188505 E-07	0.9196502 E-11	6.667748	8366.407	292.104
166	$C_{13}H_{28}$	*n*-Tridecane	63.85792	0.111595	0.1116408 E-05	−0.5633991 E-07	0.2630431 E-10	6.65466	6995.694	281.4988
167	$C_{14}H_{10}$	Phenanthrene	34.43893	0.9086123 E-01	−0.2523545 E-04	−0.1184692 E-07	0.7013306 E-11	5.543959	7914.989	244.9414
168	$C_{14}H_{30}$	*n*-Tetradecane	68.69802	0.1195599	0.269646 E-05	−0.6341006 E-07	0.3319885 E-10	6.75784	7203.471	269.269
169	$C_{15}H_{12}$	1-Phenylindene	39.22844	0.101567	−0.2937448 E-04	−0.1146747 E-07	0.7190597 E-11	6.502465	8771.184	284.573
170	$C_{15}H_{14}$	2-Ethylfluorene	40.82861	0.1076498	−0.286231 E-04	−0.1479421 E-07	0.8512086 E-11	6.695303	8621.0	283.702
171	$C_{15}H_{32}$	*n*-Pentadecane	73.51018	0.1251686	0.2315556 E-05	−0.6703845 E-07	0.3505542 E-10	6.82225	7400.305	257.5114
172	$C_{16}H_{10}$	Fluoranthene	40.95336	0.1036185	−0.4006217 E-04	−0.2144235 E-08	0.4437308 E-11	6.571647	9789.787	257.[illegible]
173	$C_{16}H_{10}$	Pyrene	38.96862	0.1053988	−0.3875499 E-04	−0.4808038 E-08	0.5453756 E-11	6.603641	9365.547	267.[illegible]
174	$C_{16}H_{12}$	1-Phenylnaphthalene	37.71548	0.1059567	−0.2424246 E-04	−0.189117 E-07	0.9723825 E-11	7.078733	9631.87	312.9423
175	$C_{16}H_{34}$	*n*-Hexadecane	78.32123	0.1367191	0.1674373 E-05	−0.7030701 E-07	0.3676587 E-10	6.92955	7569.57	248.[illegible]
176	$C_{18}H_{12}$	Chrysene	42.55082	0.1204639	−0.3831014 E-04	−0.1145987 E-07	0.8077914 E-11	6.810698	10647.46	229.[illegible]

VITA

Mr. Warin Iamteerapaiboon graduated high school from Debsirin school in 1984 and received a Bachelor Degree in Chemical Engineering from the Department of Chemical Engineering, Faculty of Engineering, King Mongkut Institute's of Technology Thonburi in 1989. After then he subsequently studied for a requirement of the Master's Degree in Chemical Engineering at the Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University from 1992 till 1994.

He also has an experience in working as process engineer at National Petrochemical Corporation in 1989 till 1990 and then working as process engineer for The Shell Company of Thailand Limited and Rayong Refinery Company Limited uptill the present.