

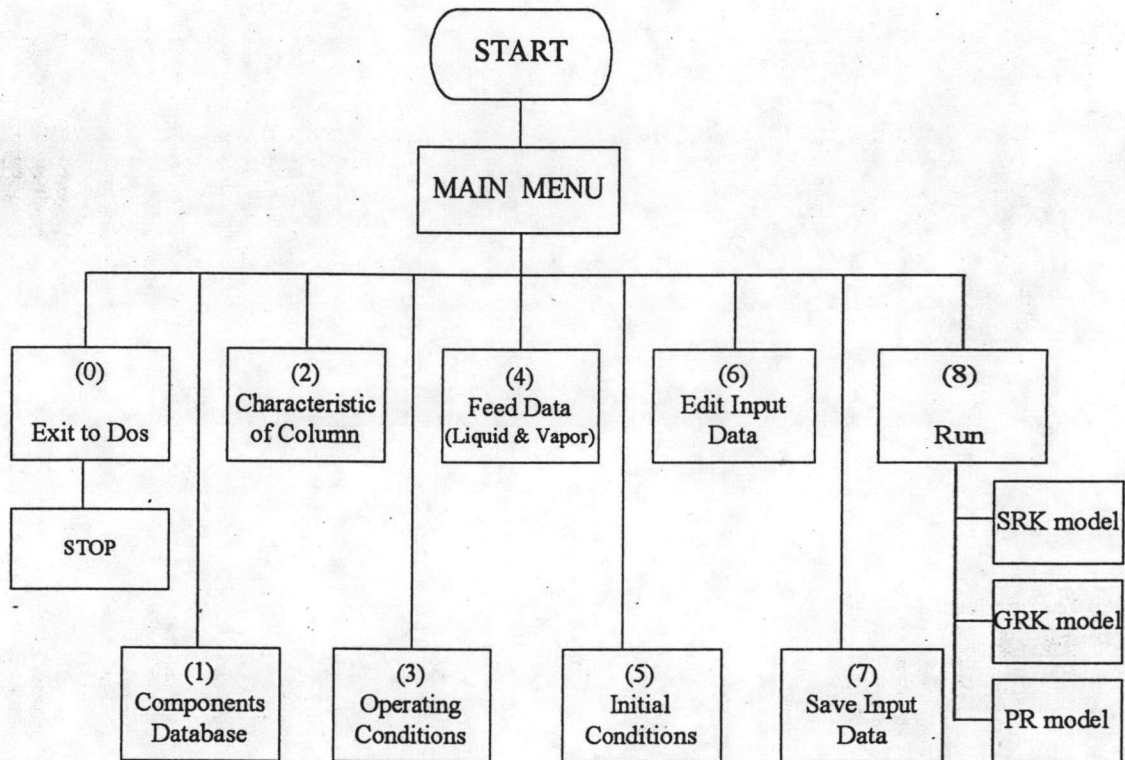
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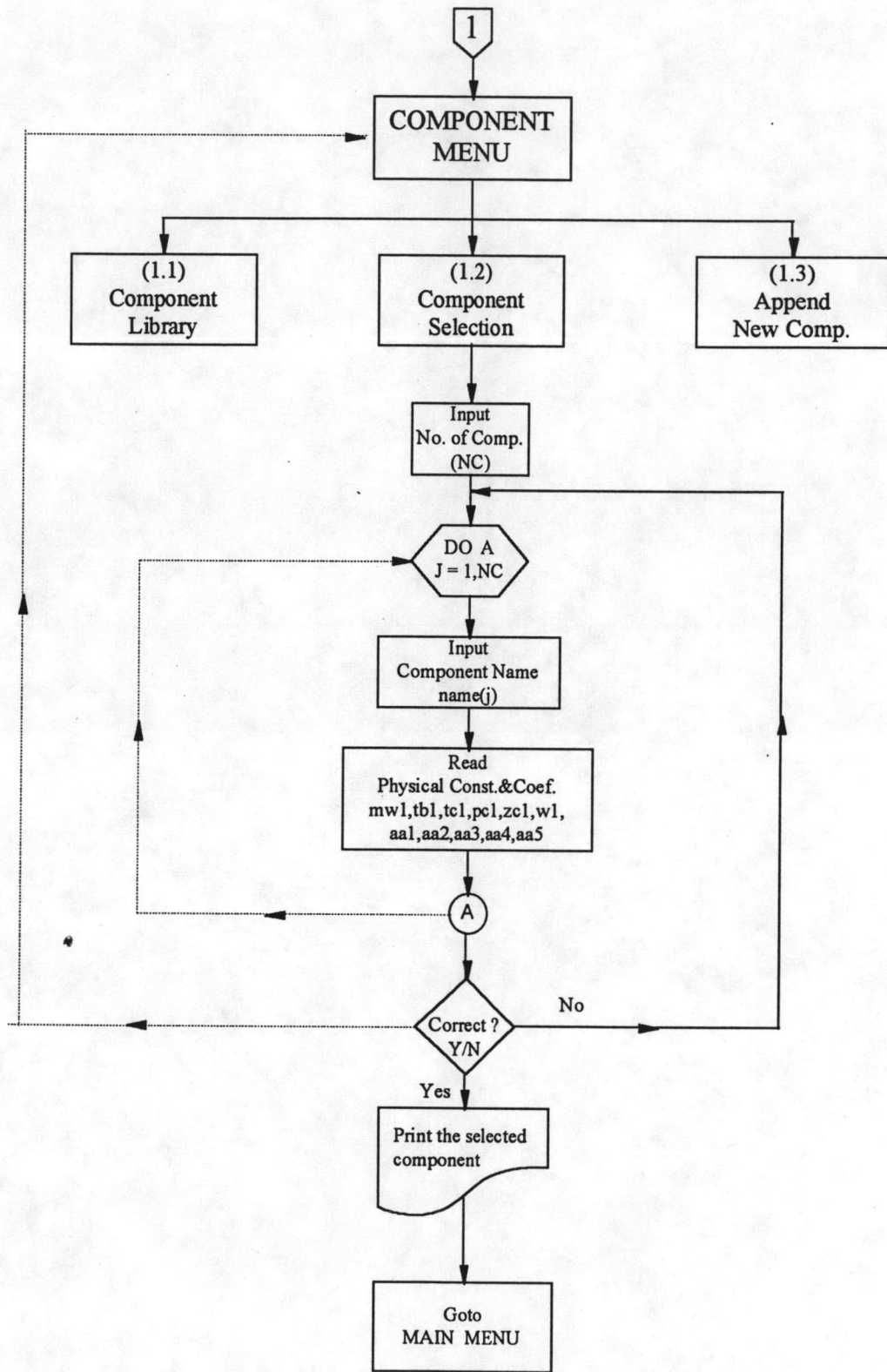
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Appendix A

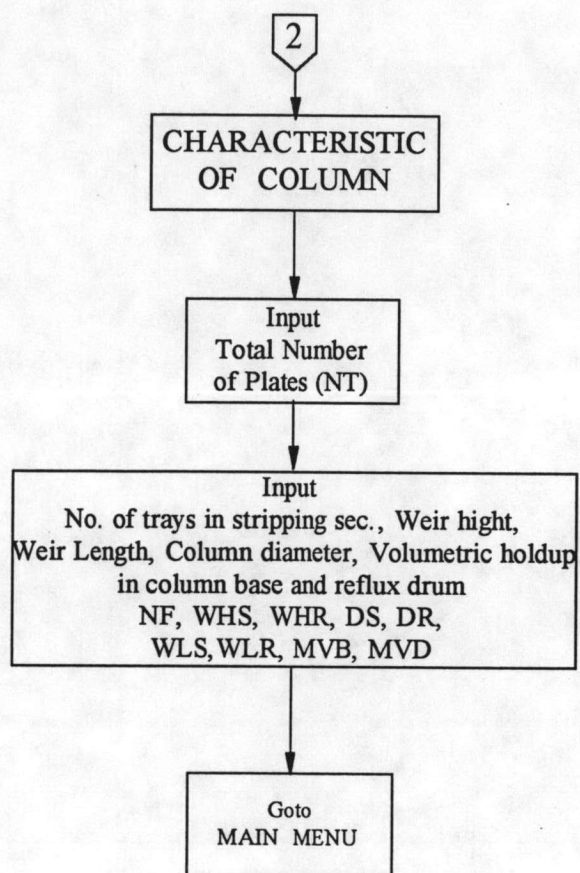
Computer Program Flow Chart



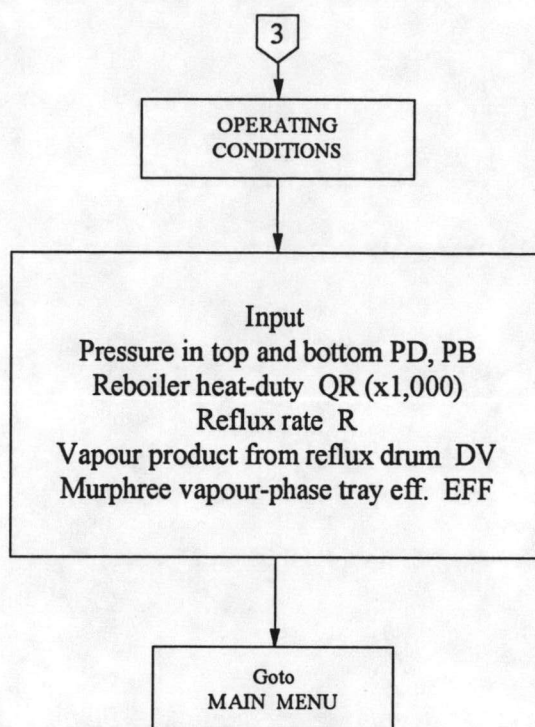
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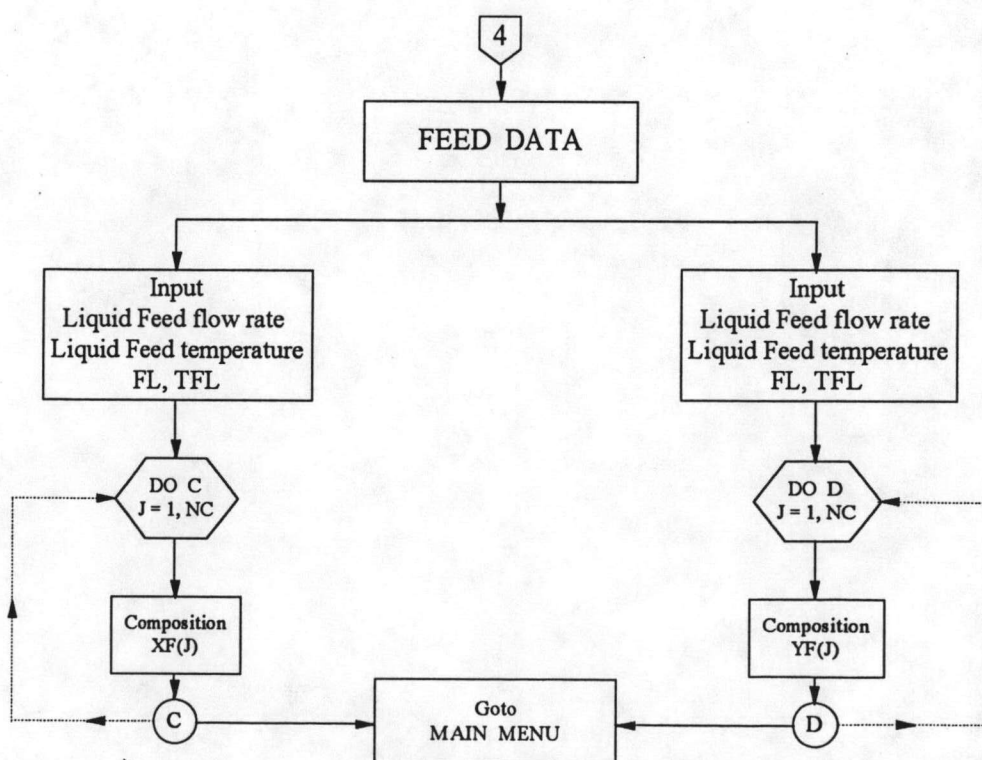
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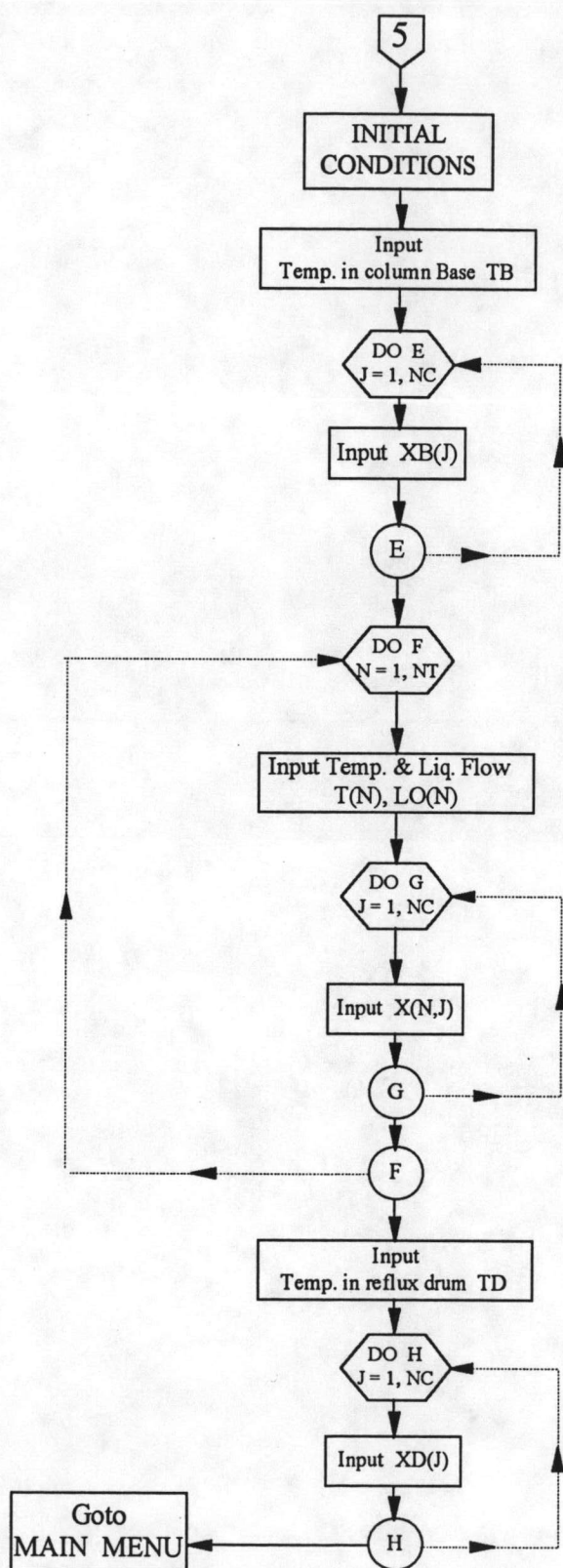
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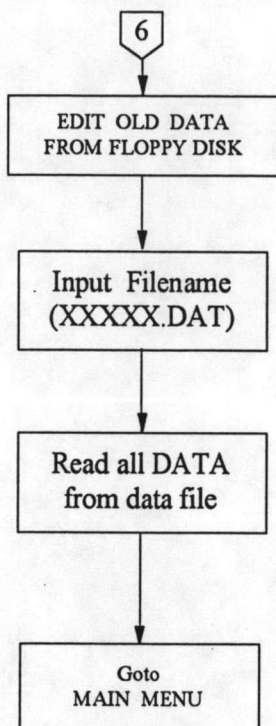
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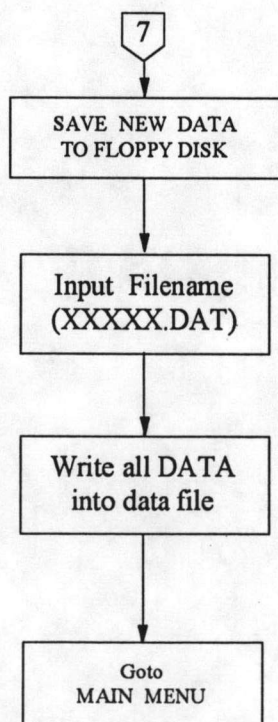
4) Feed Data



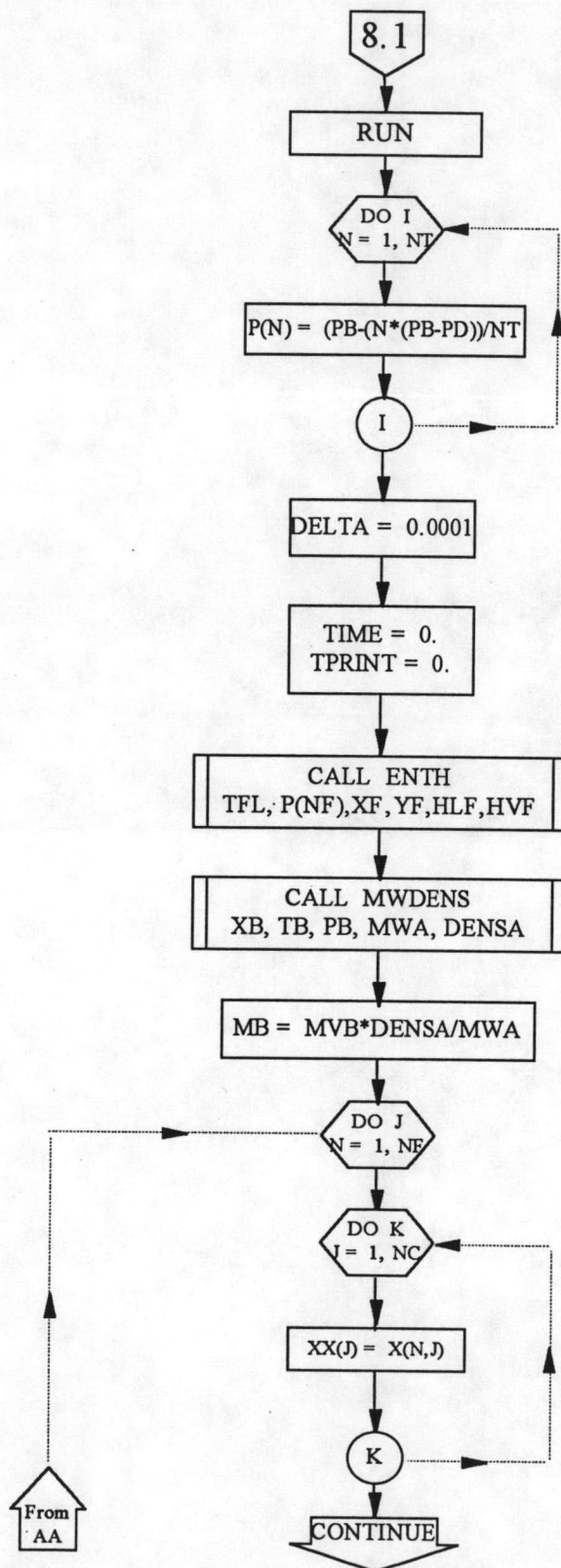
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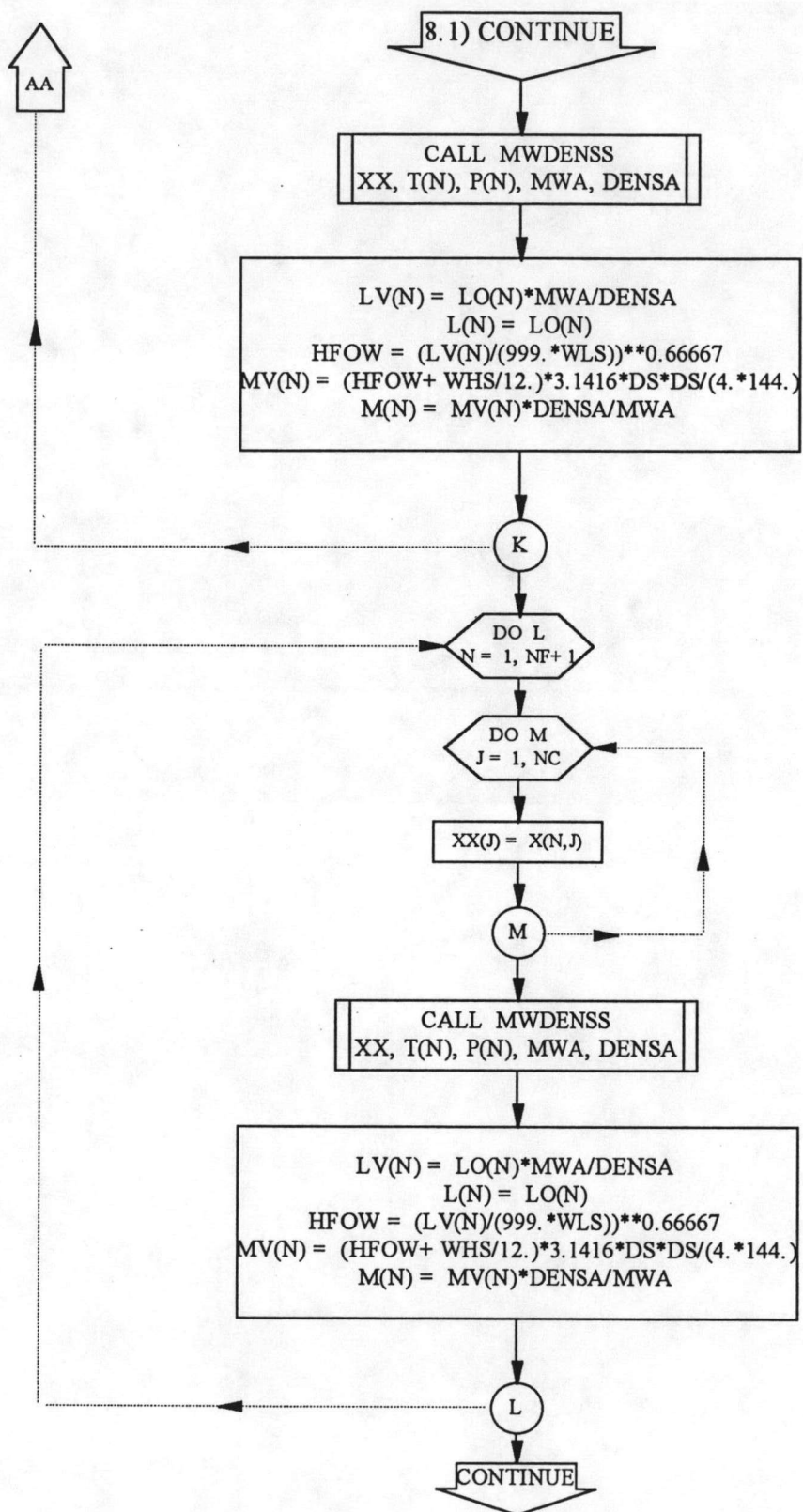
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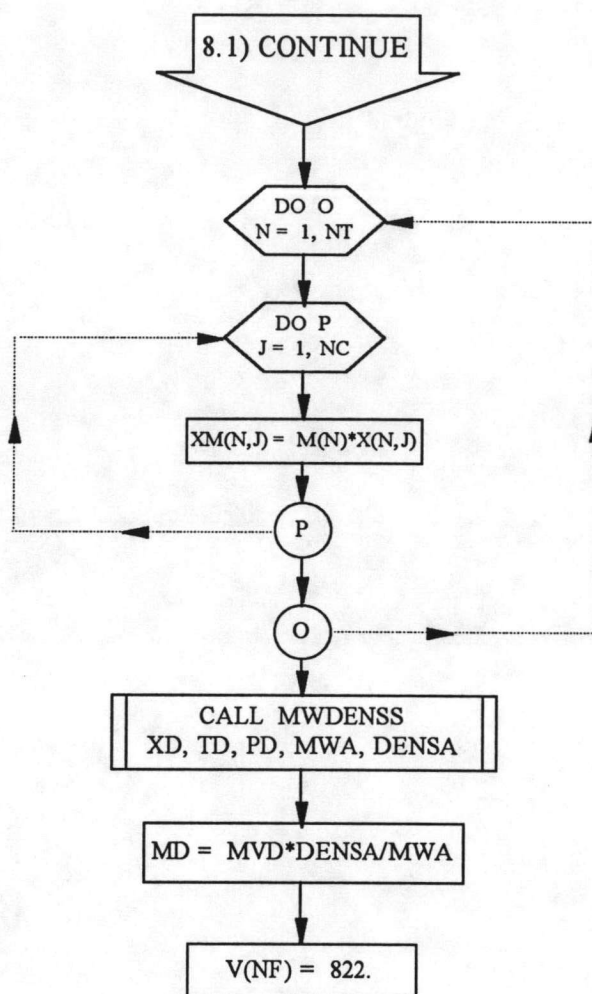
7) Save Input Data



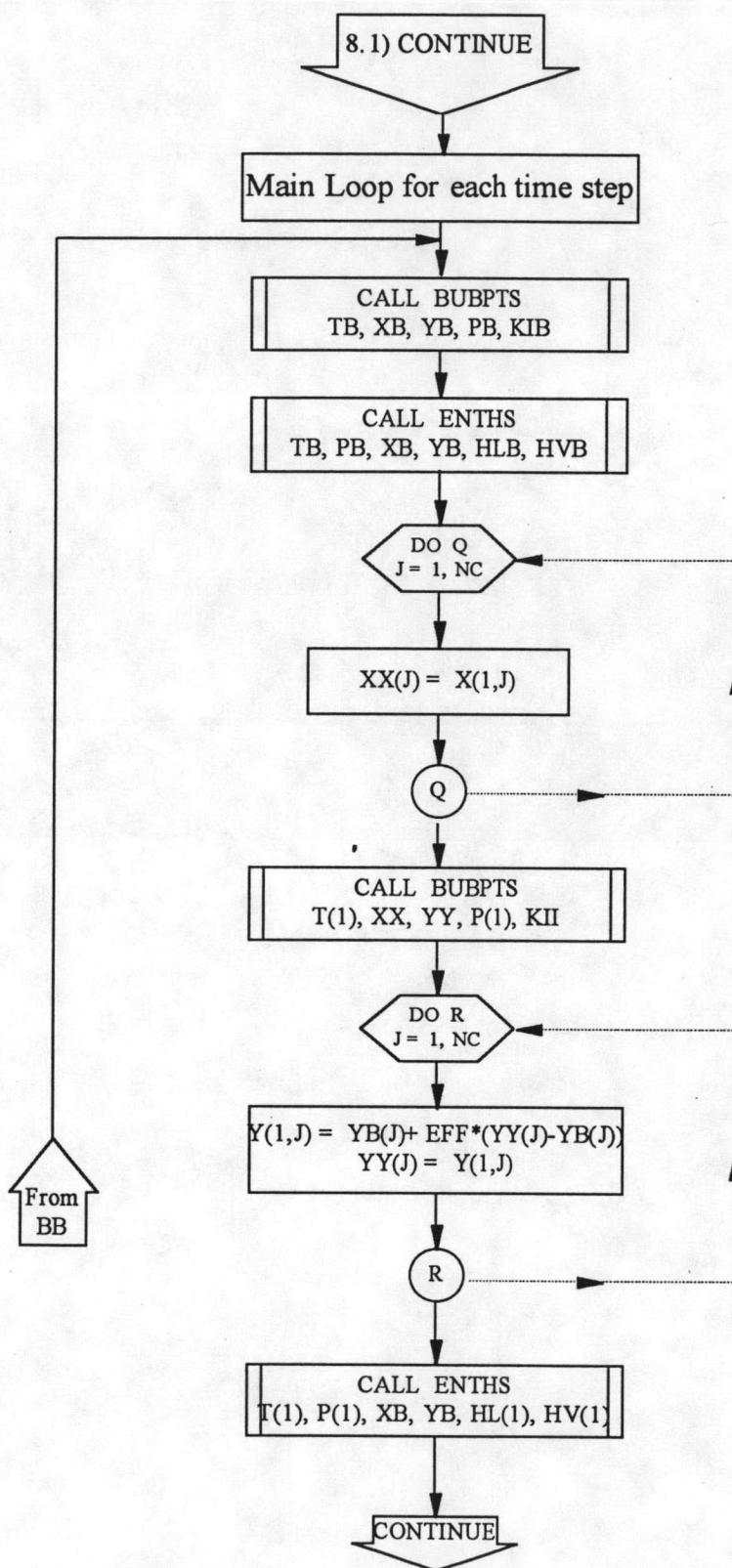
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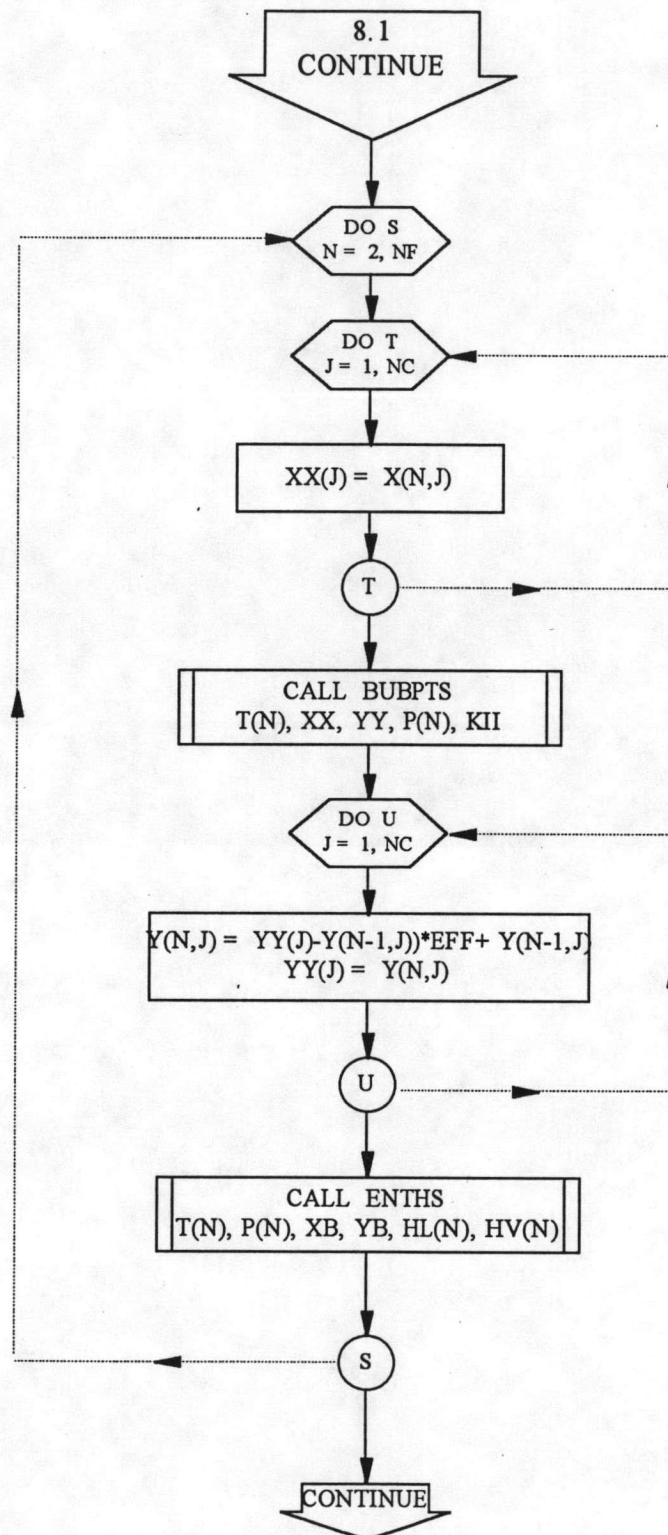
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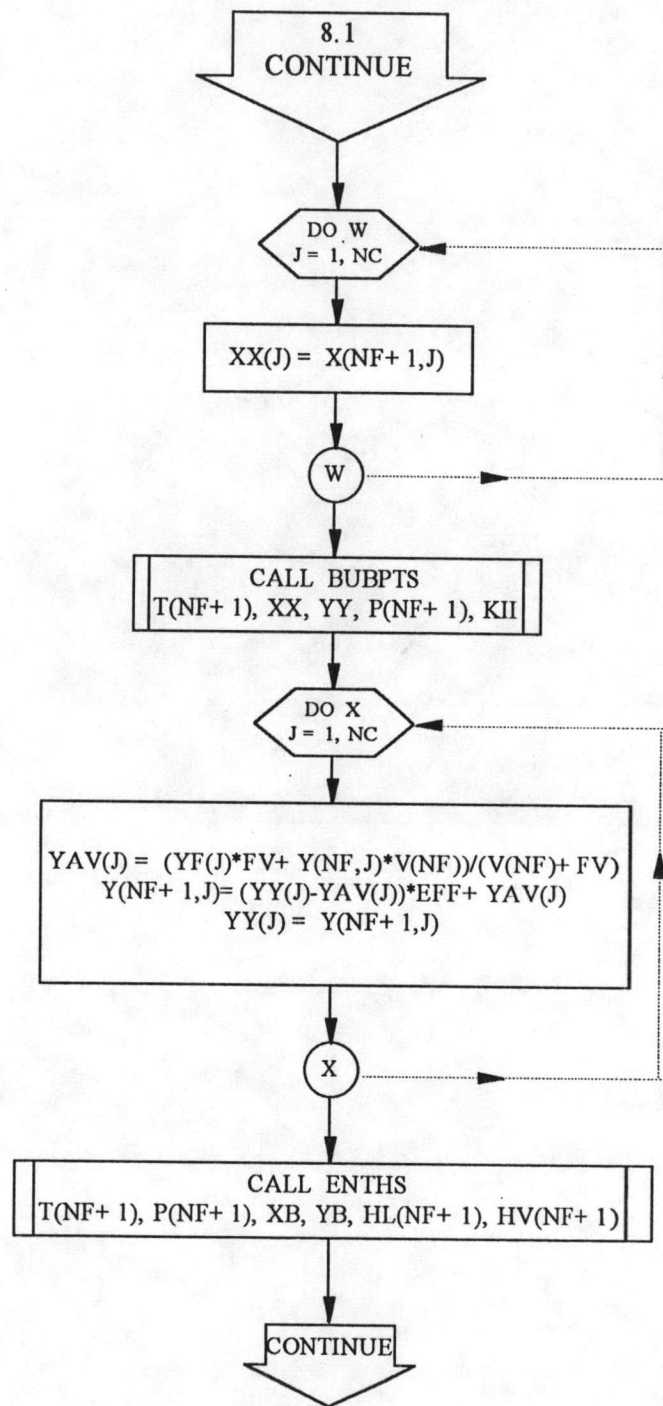
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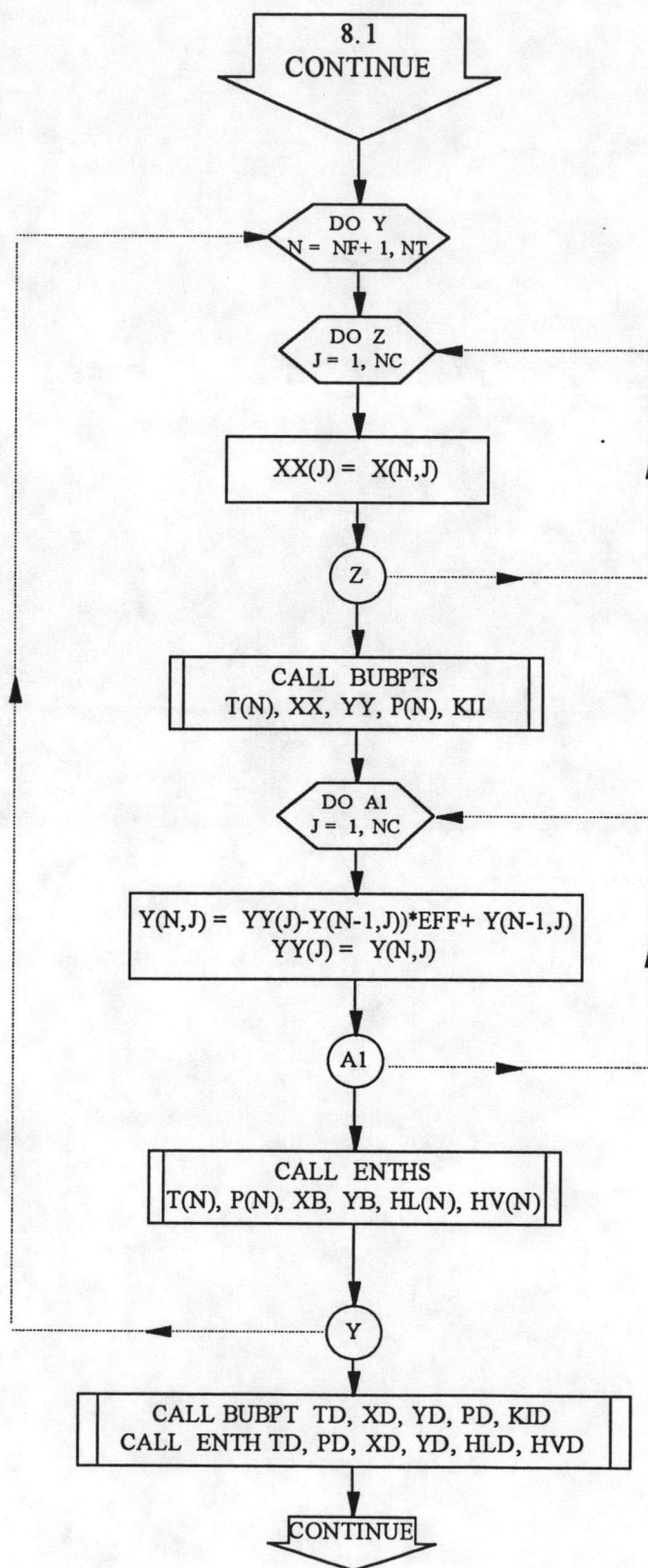
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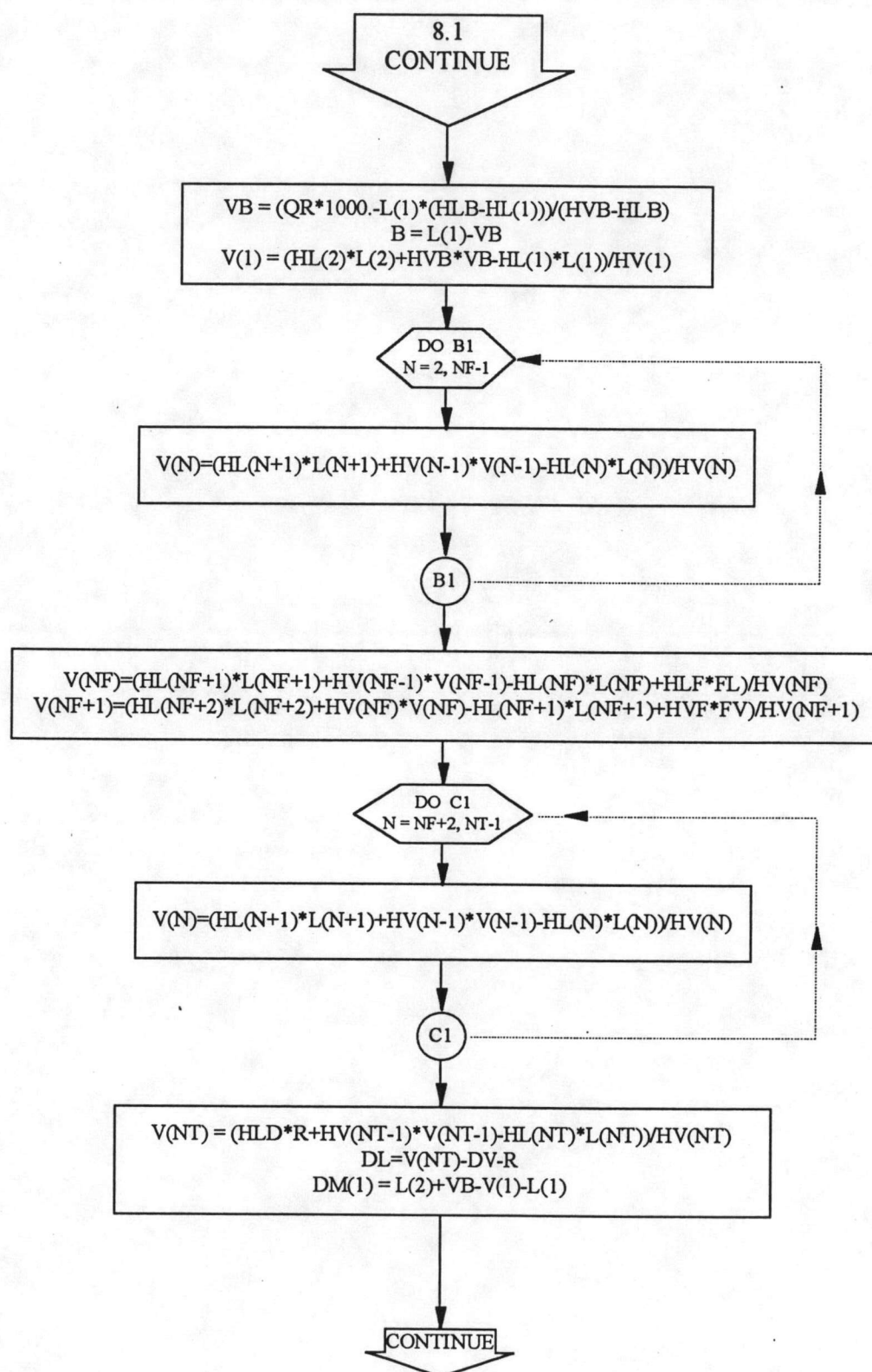
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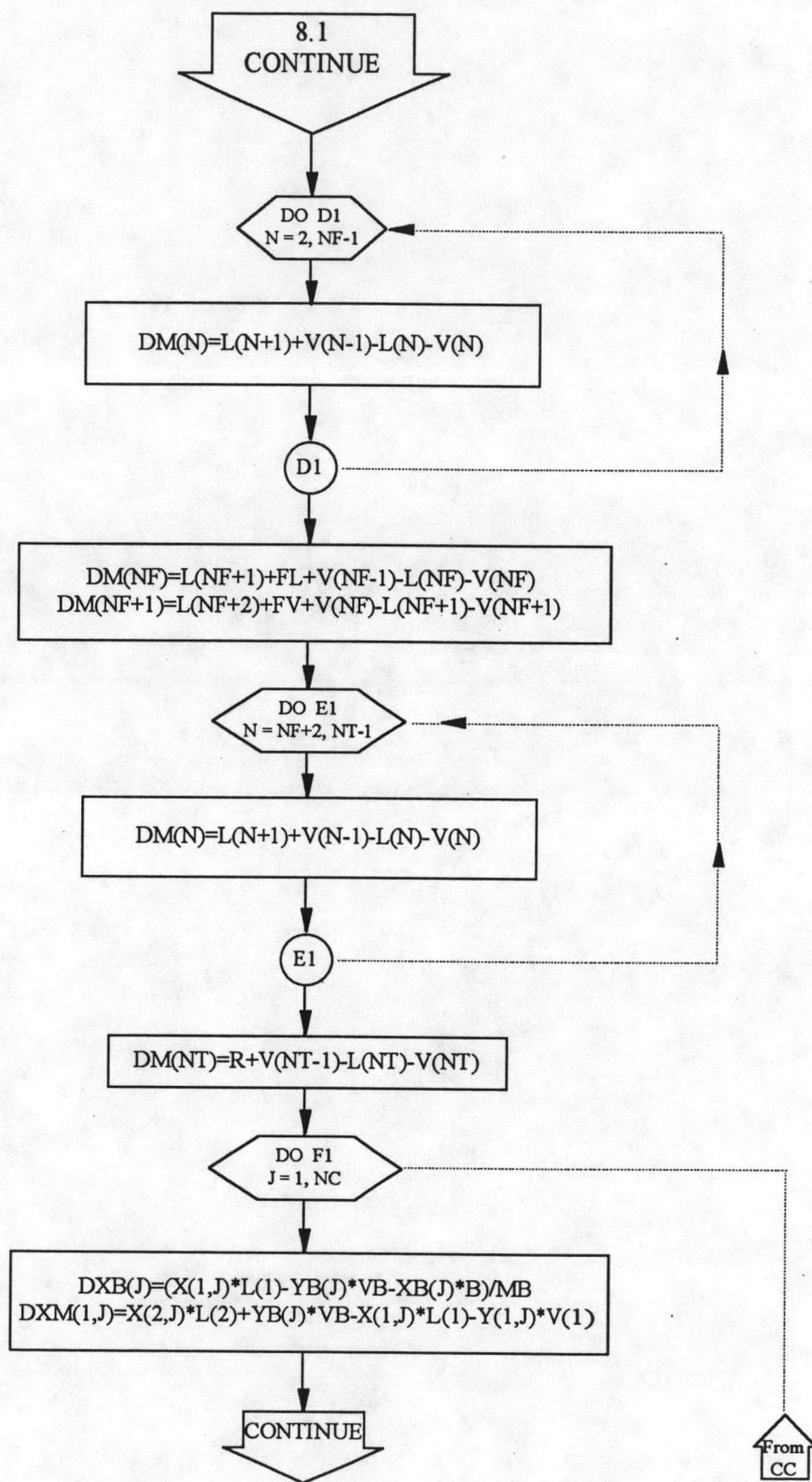
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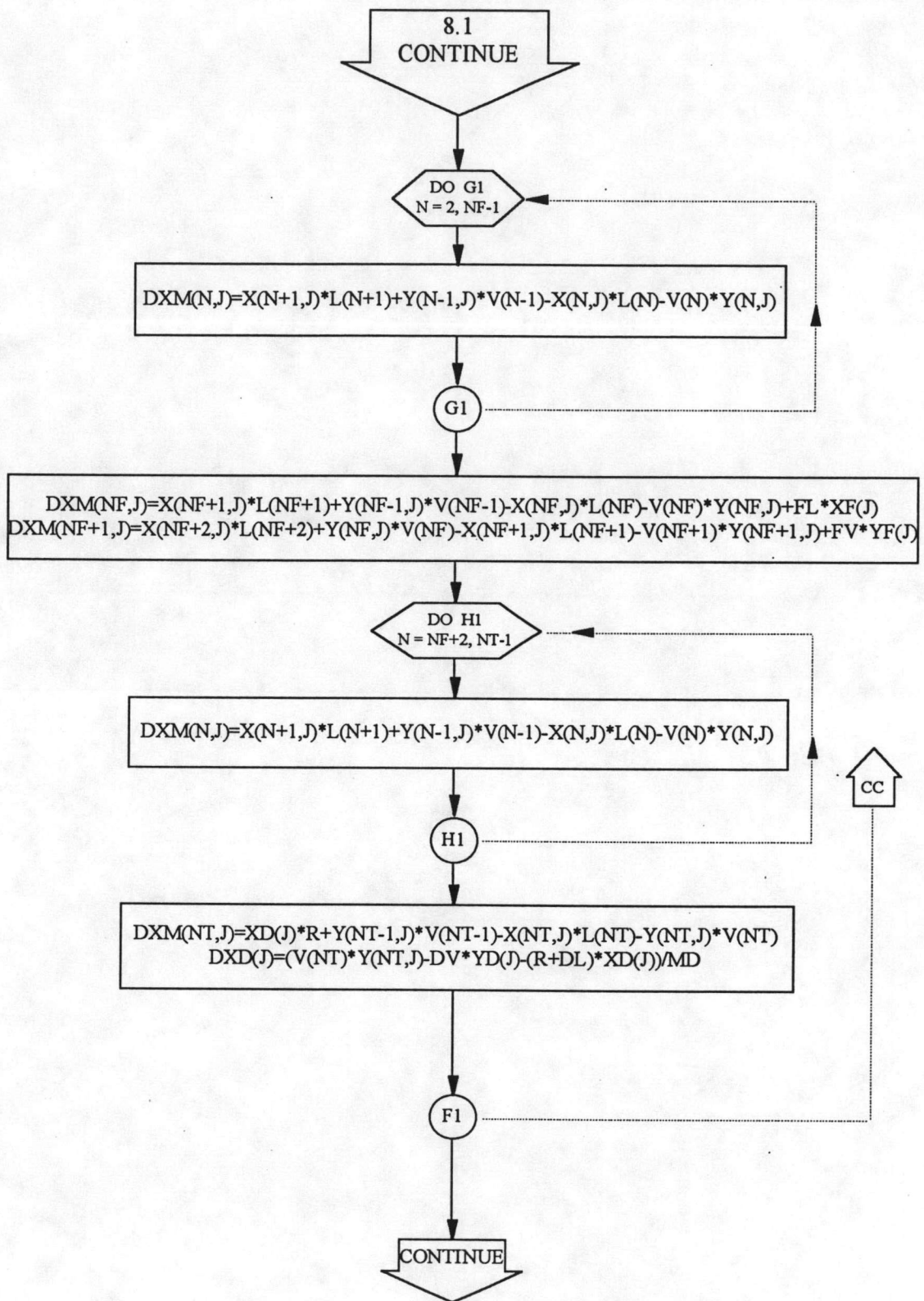
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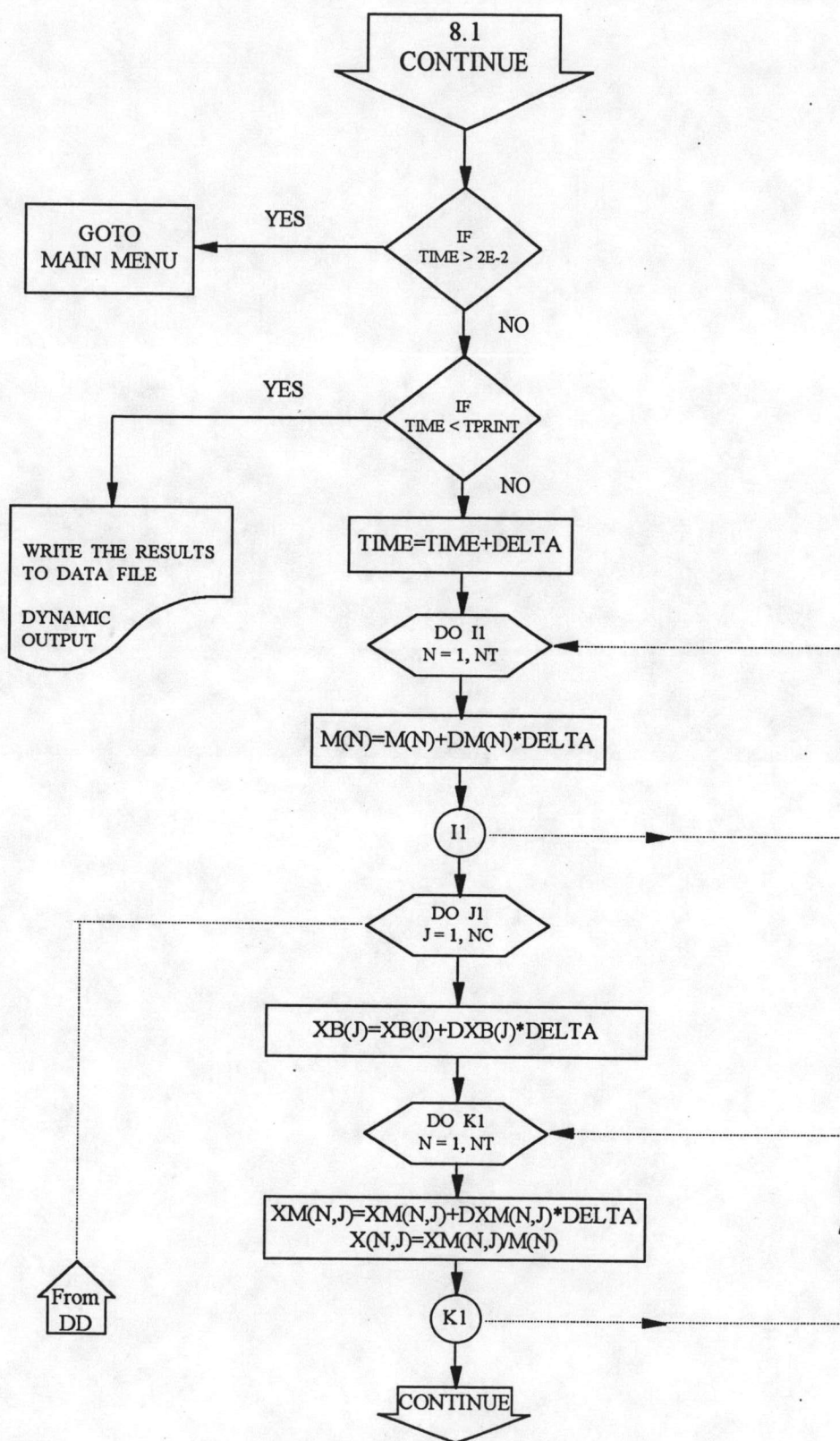
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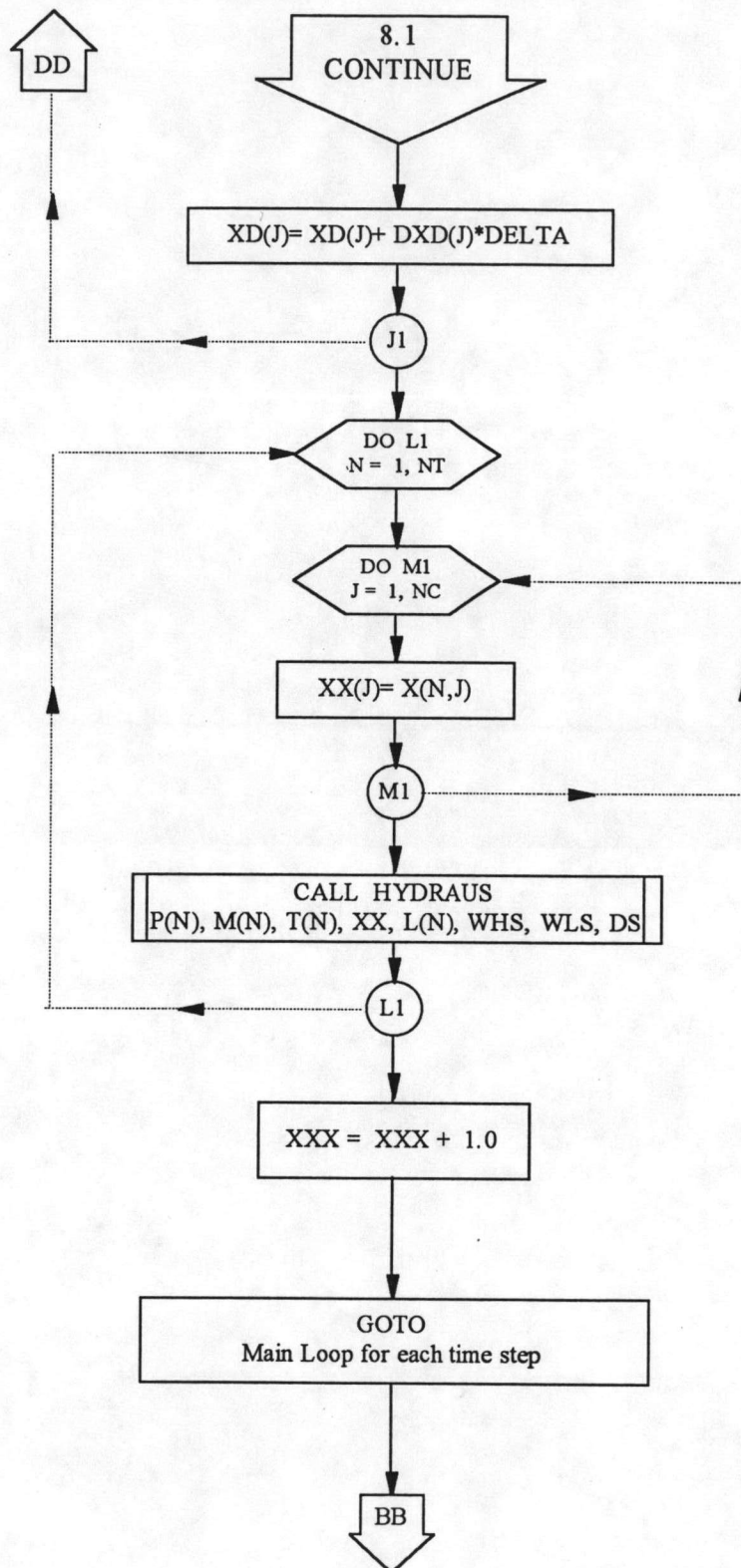
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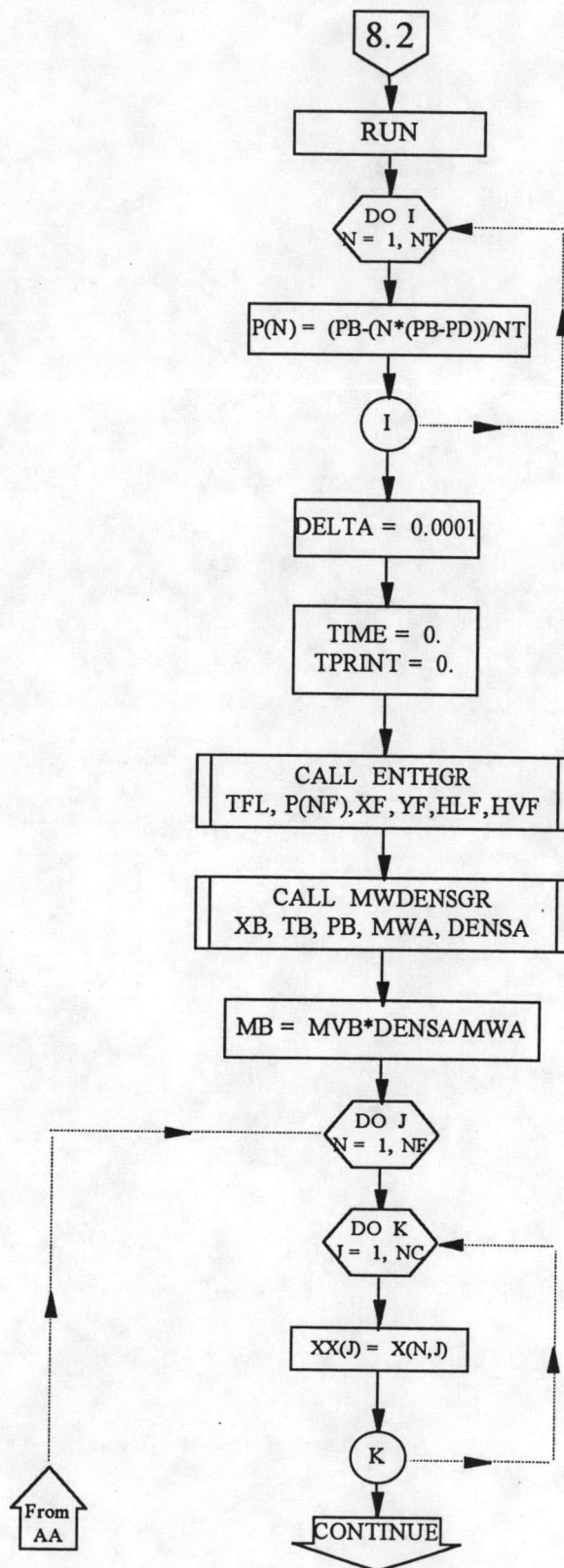
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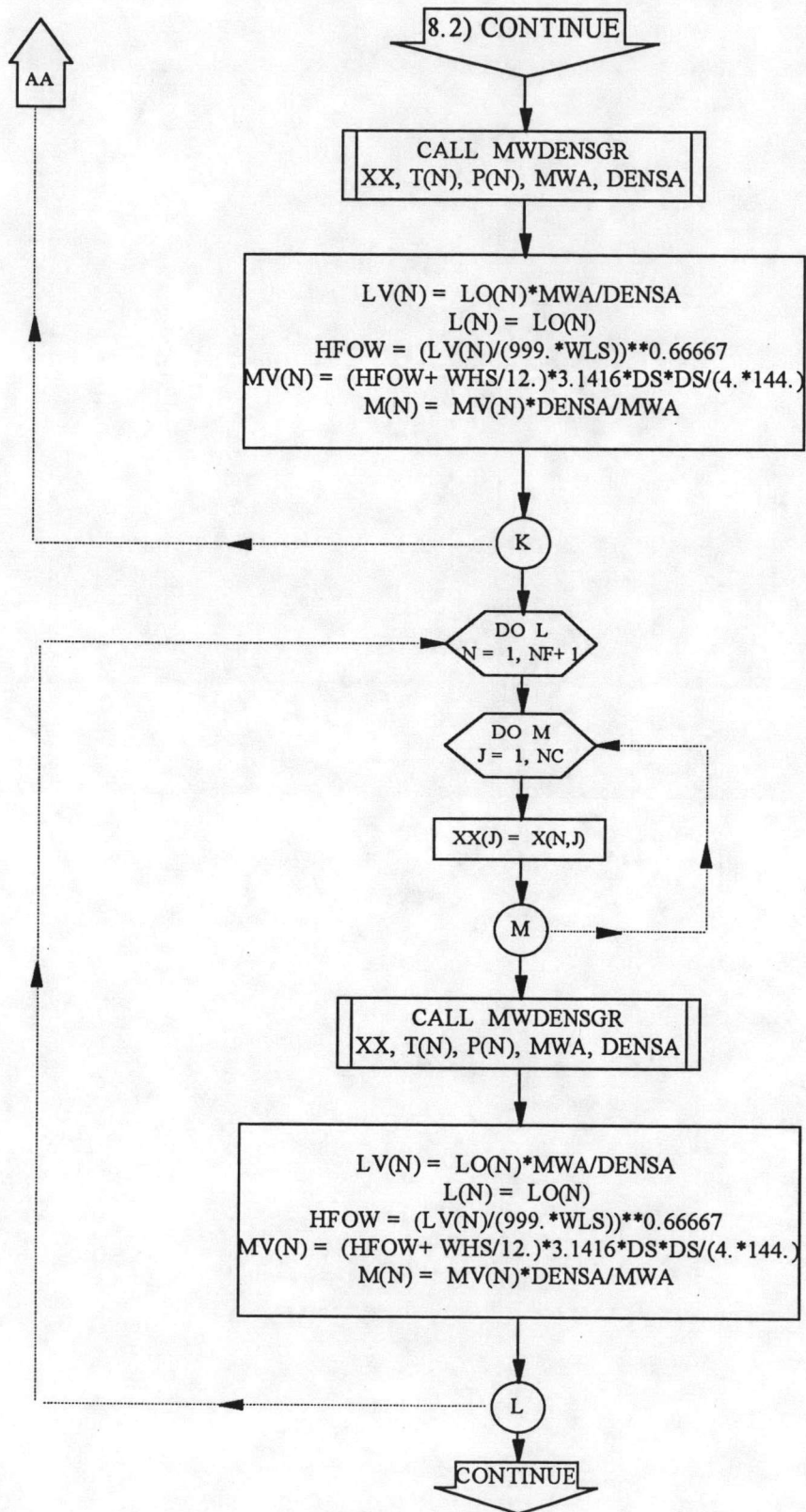
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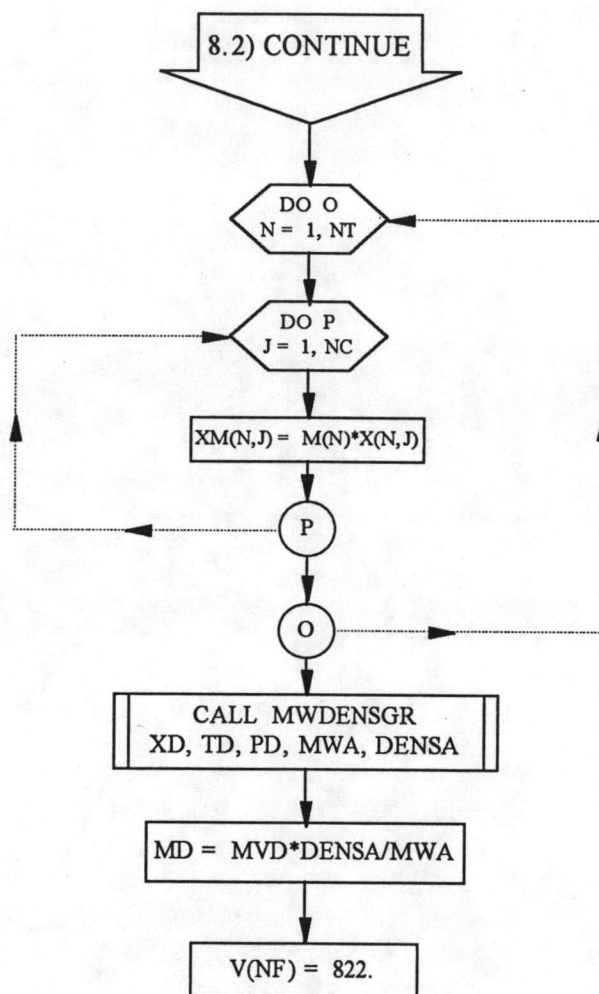
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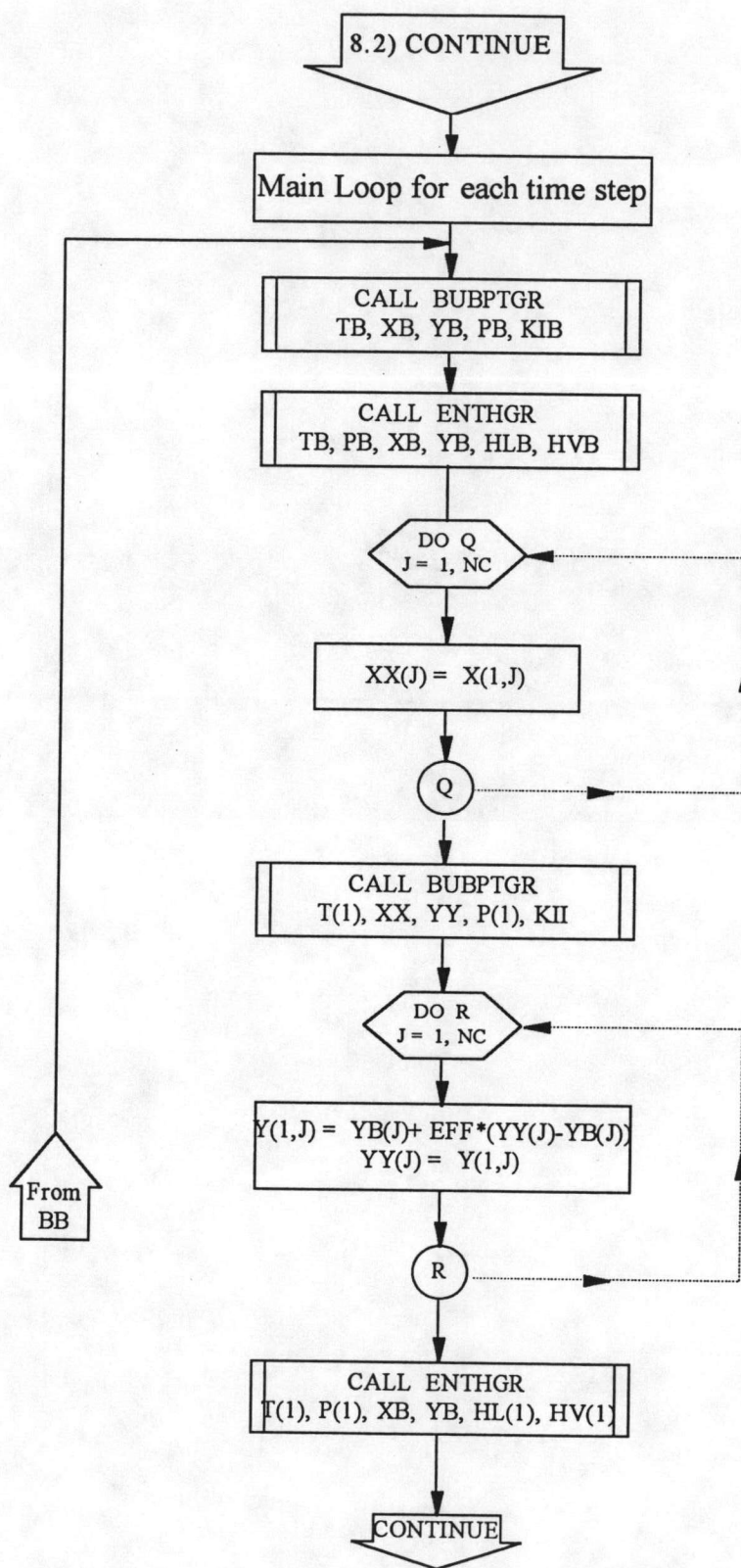
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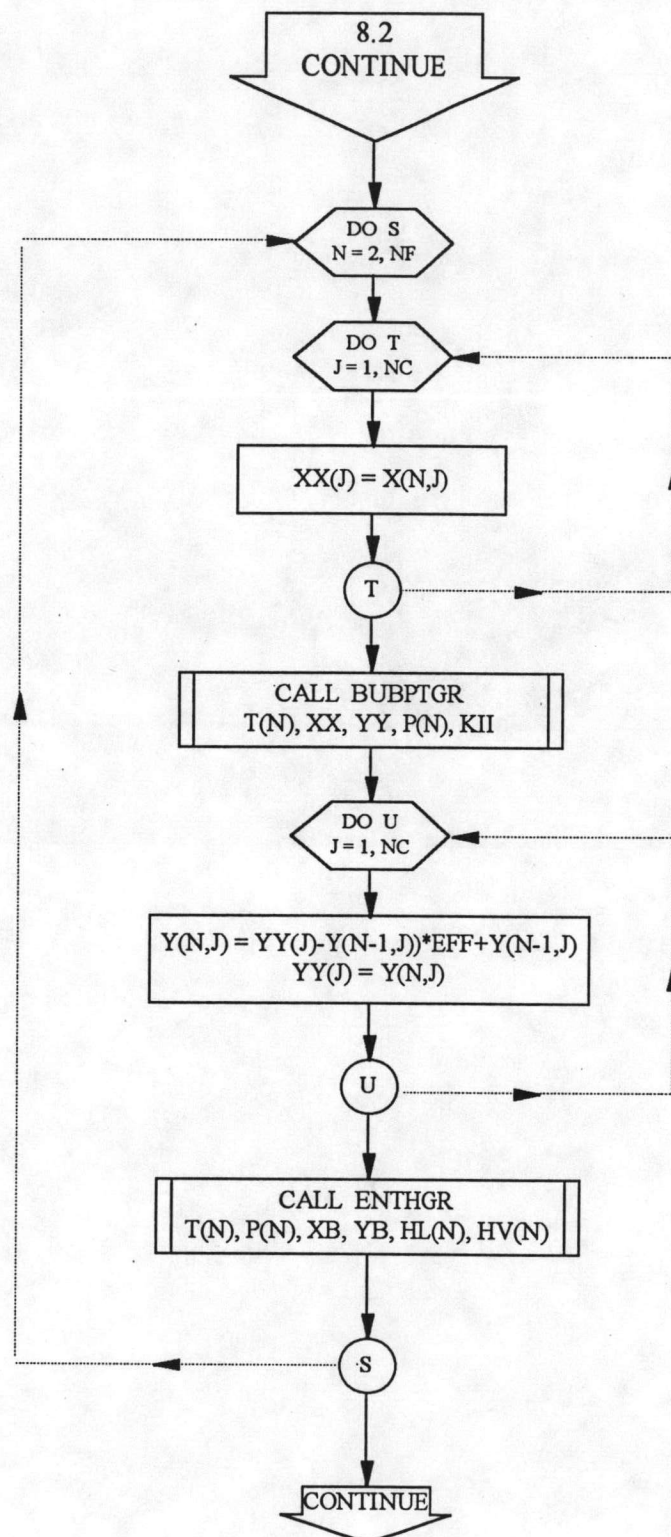
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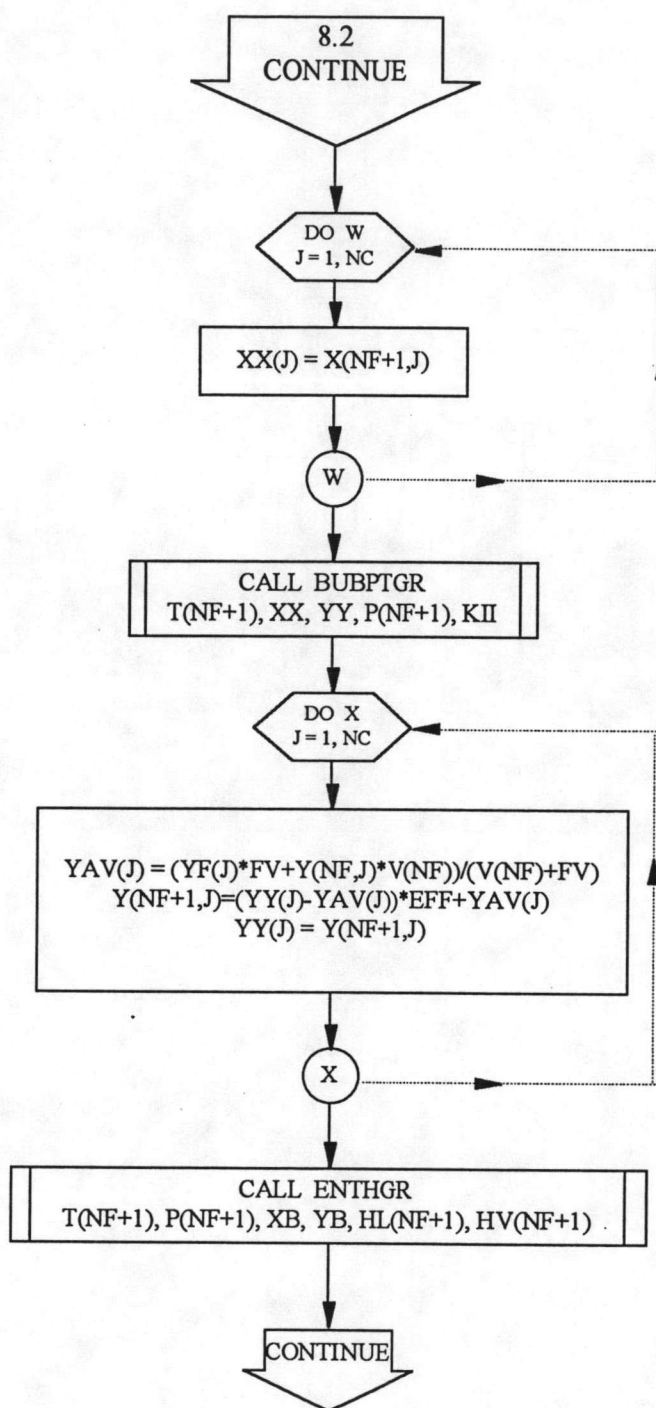
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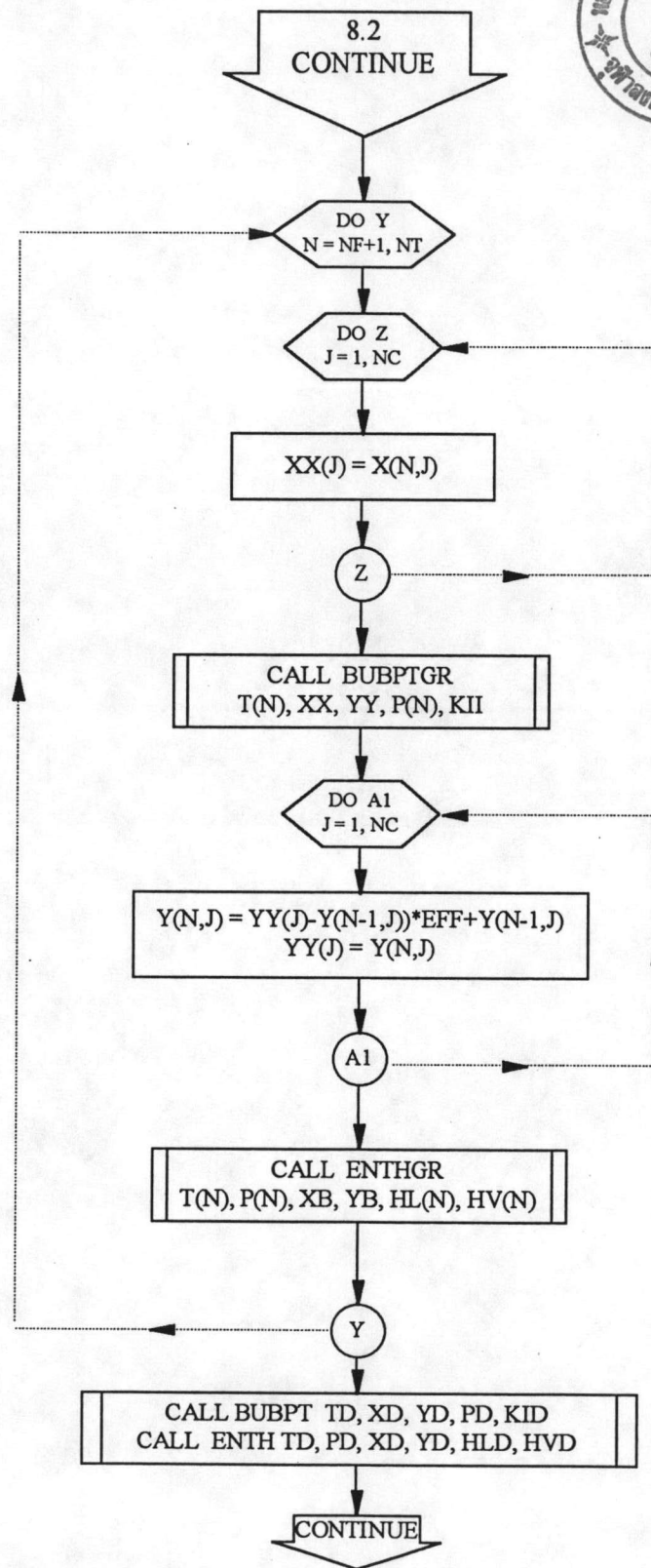
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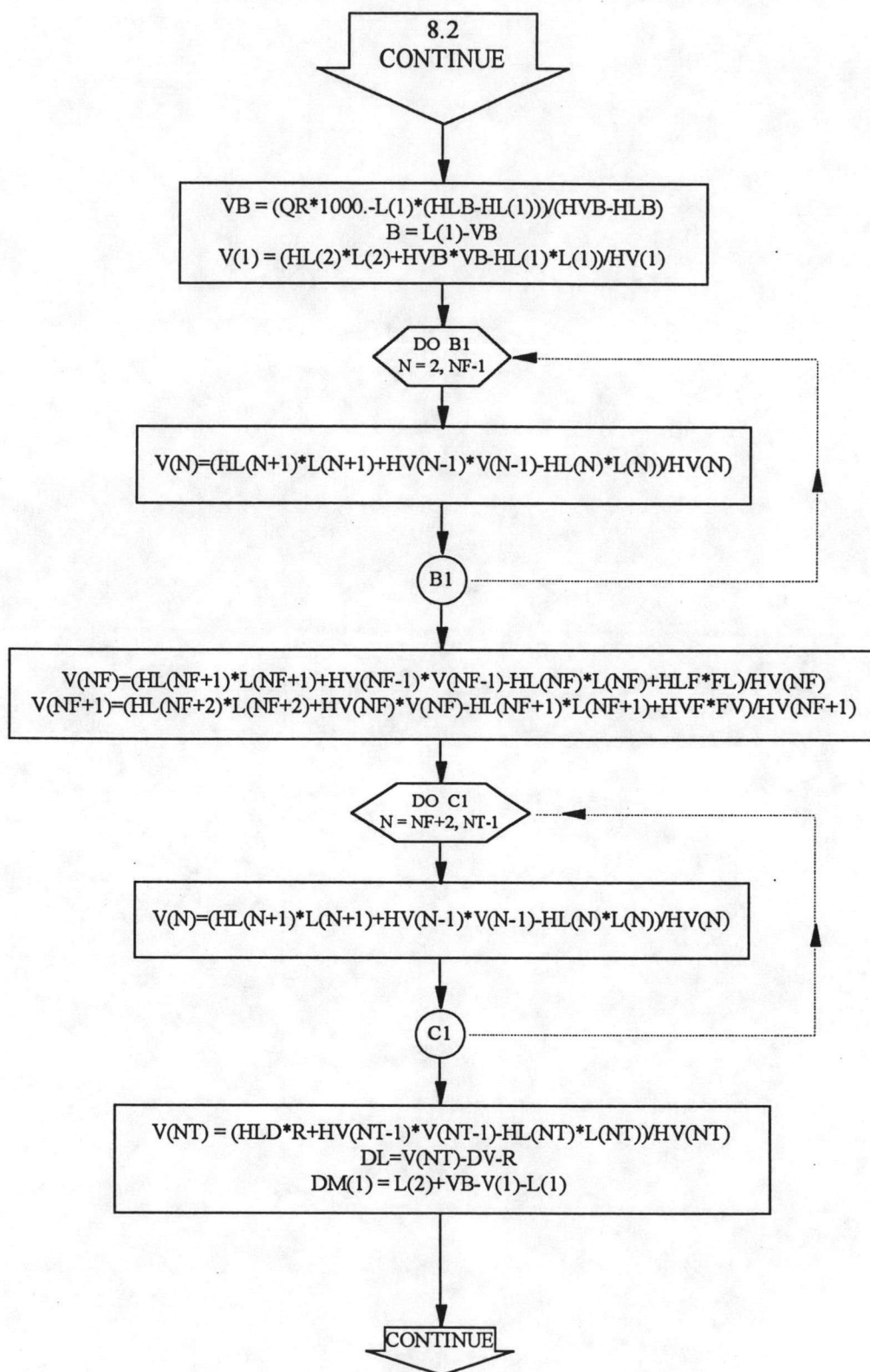
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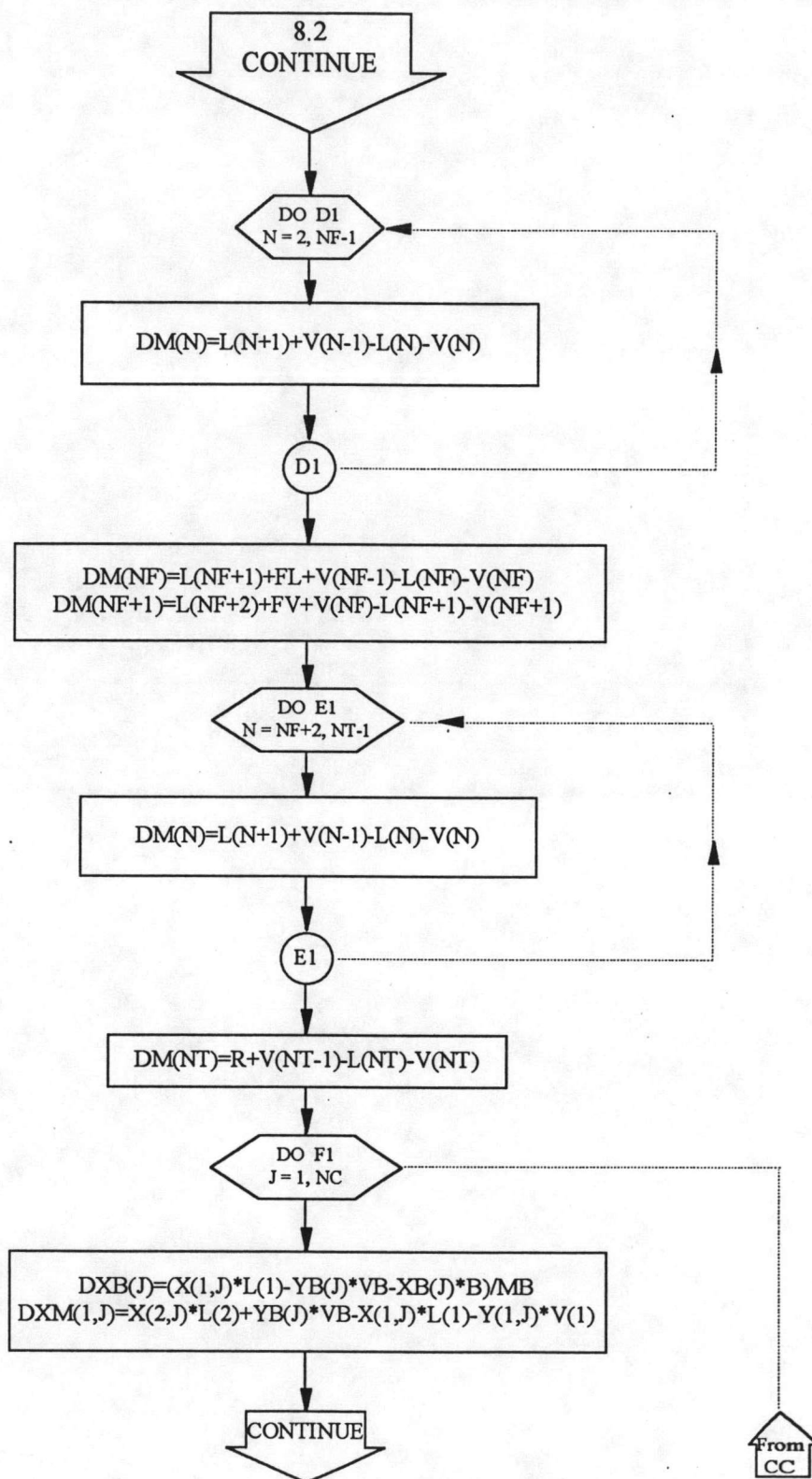
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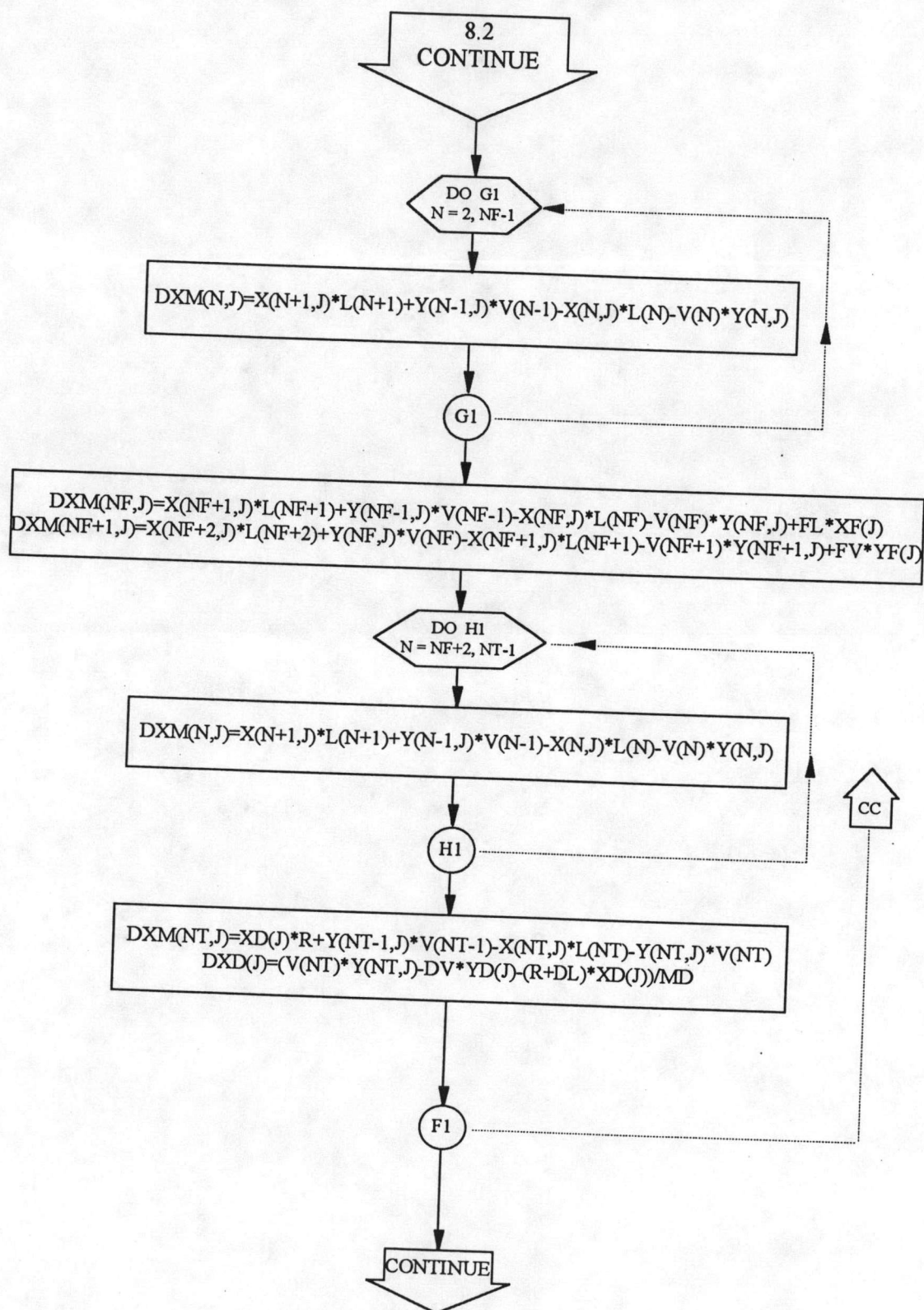
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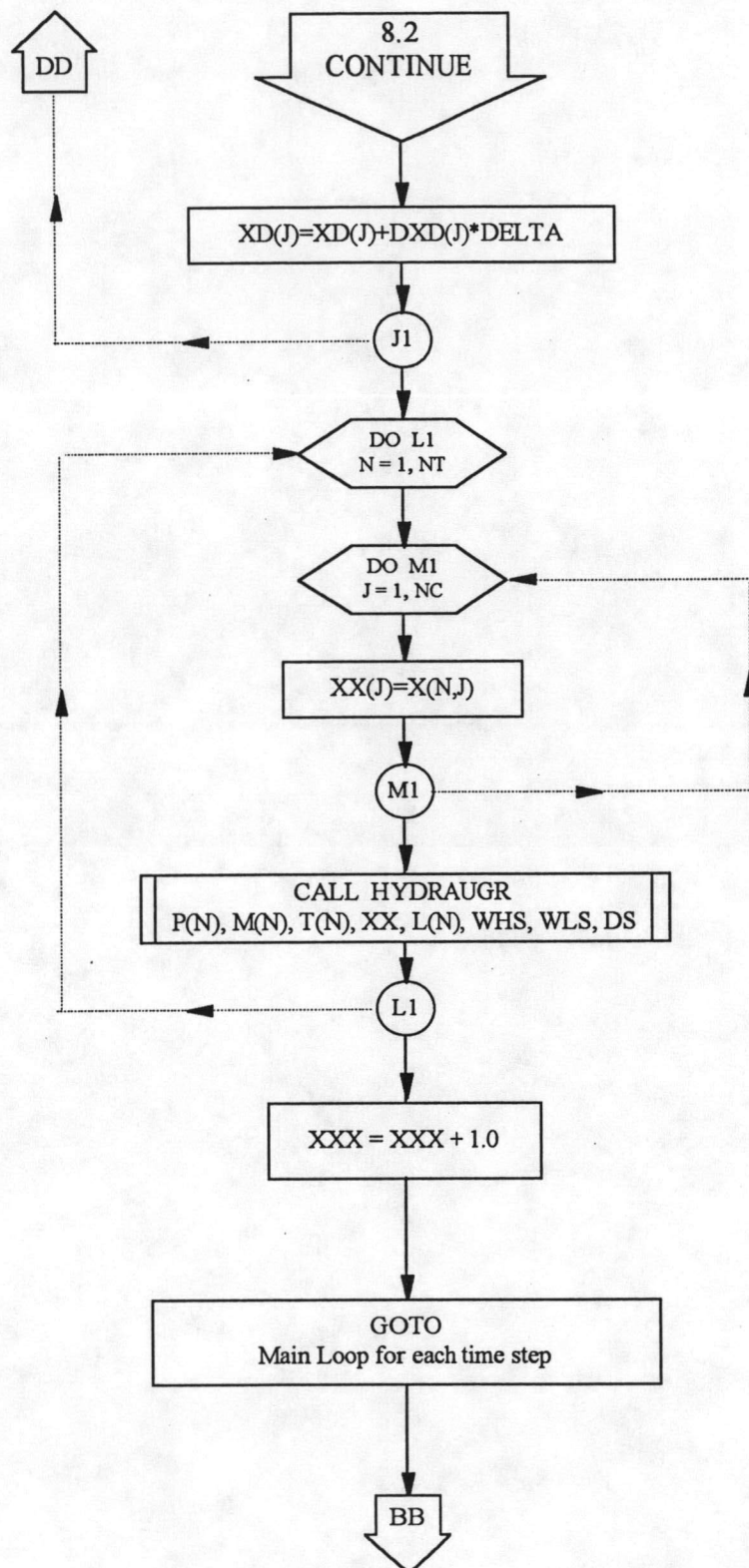
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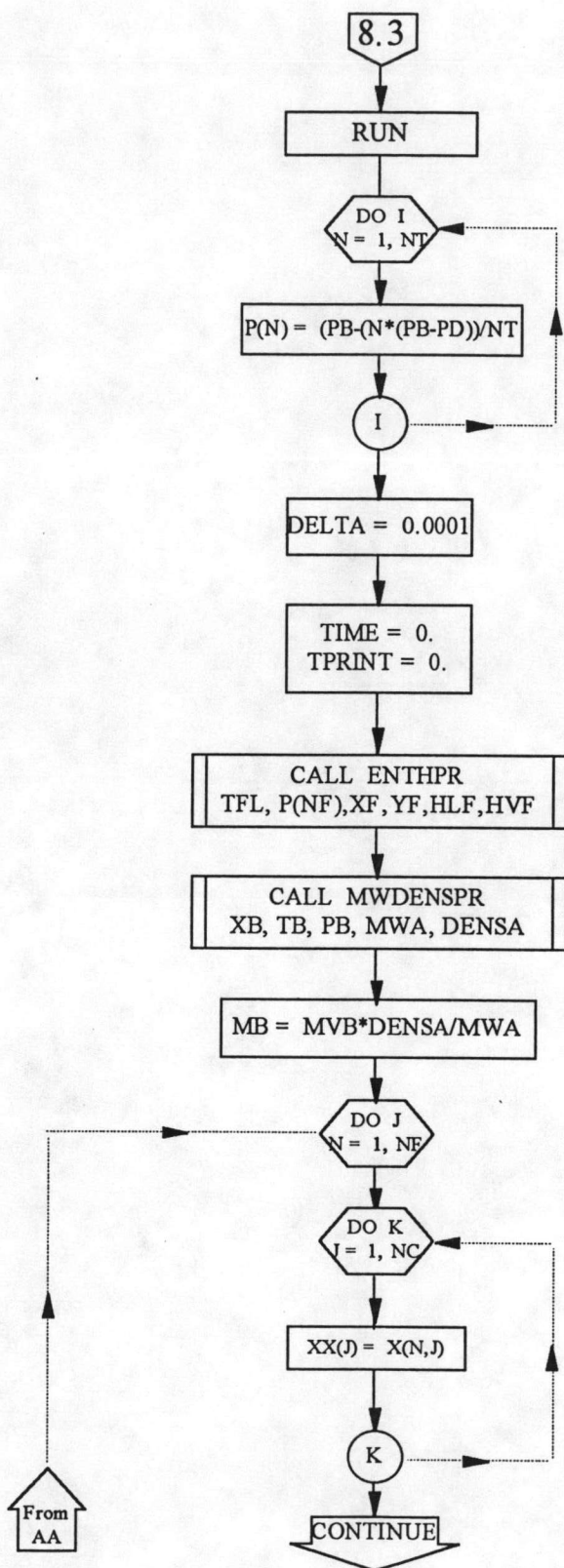
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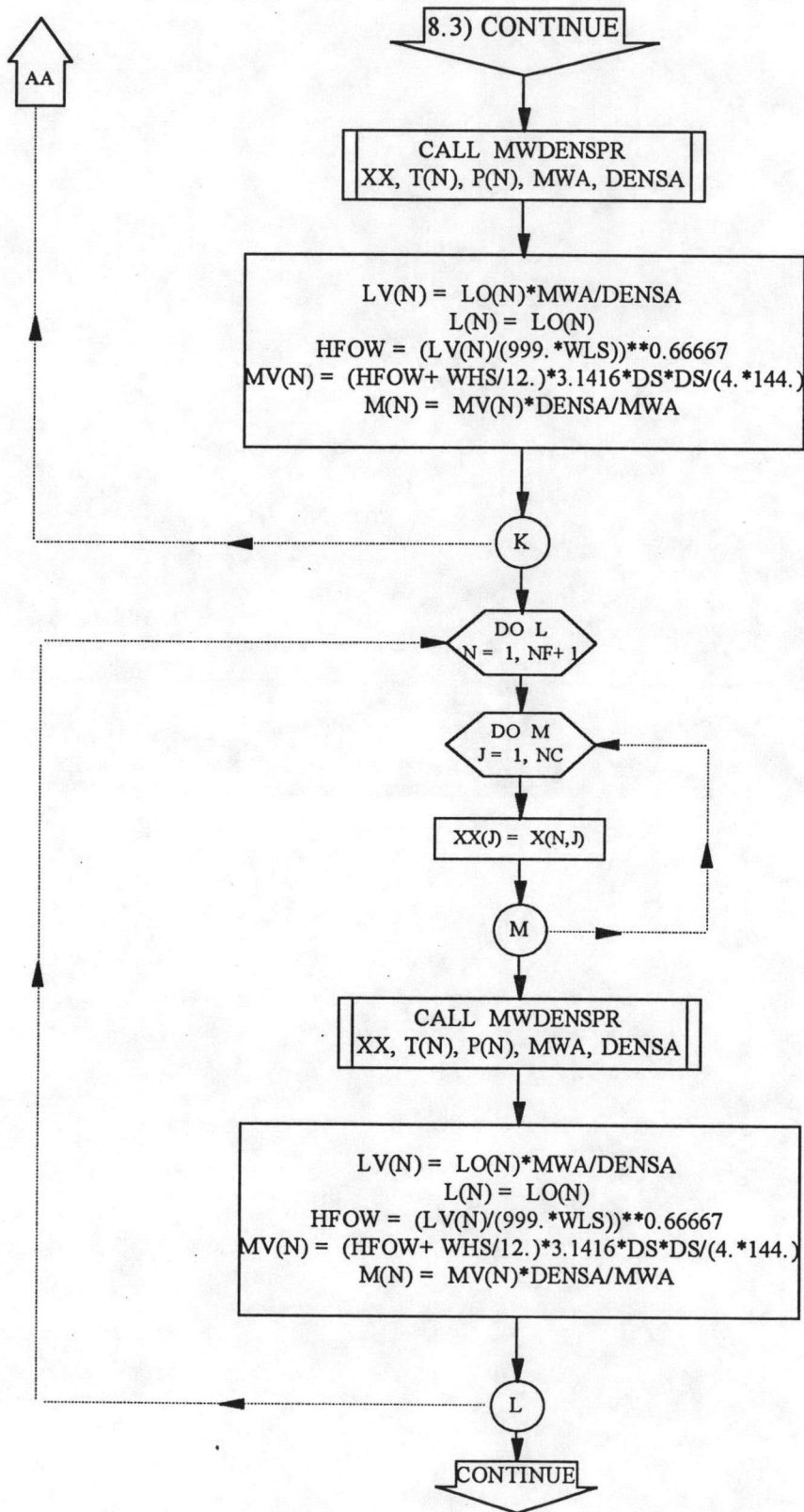
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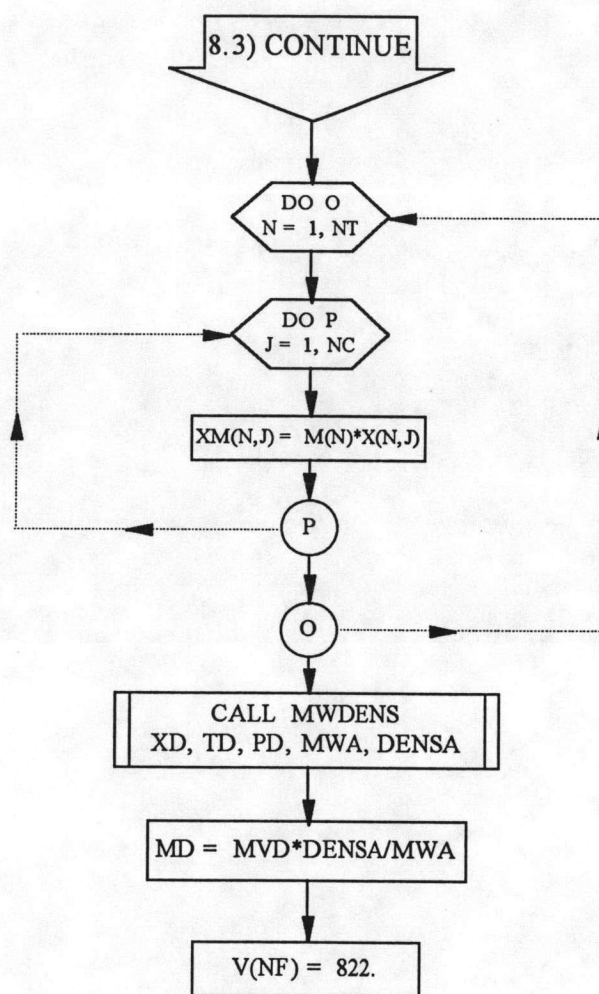
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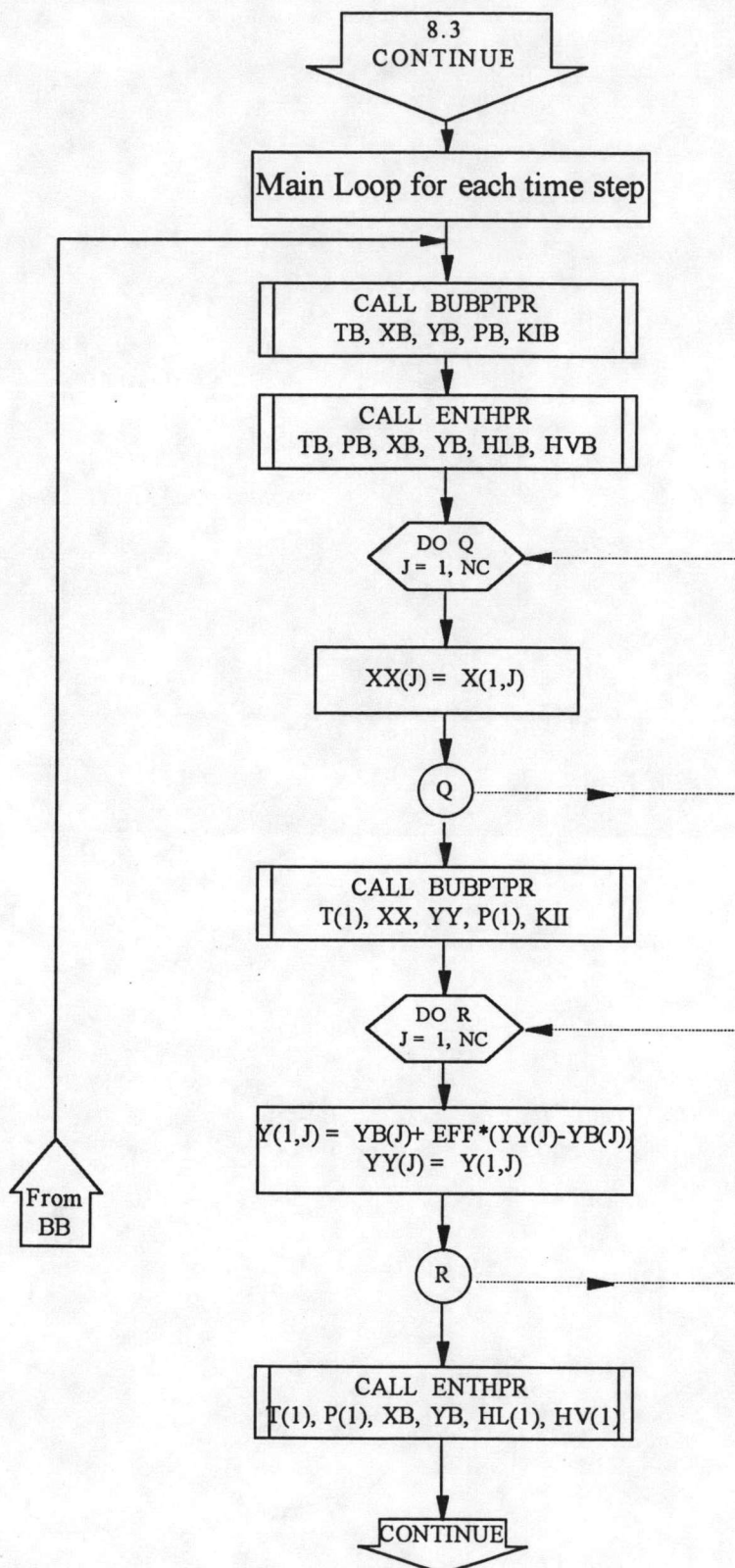
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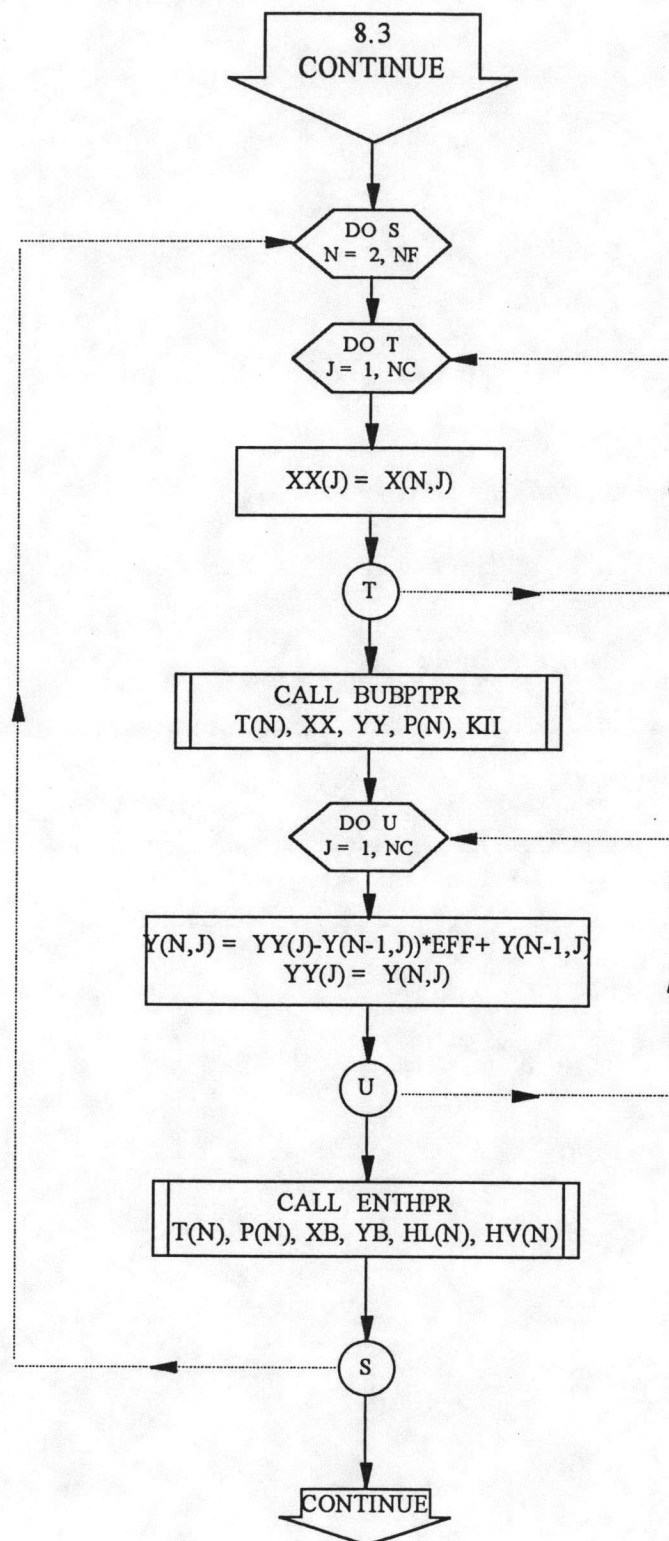
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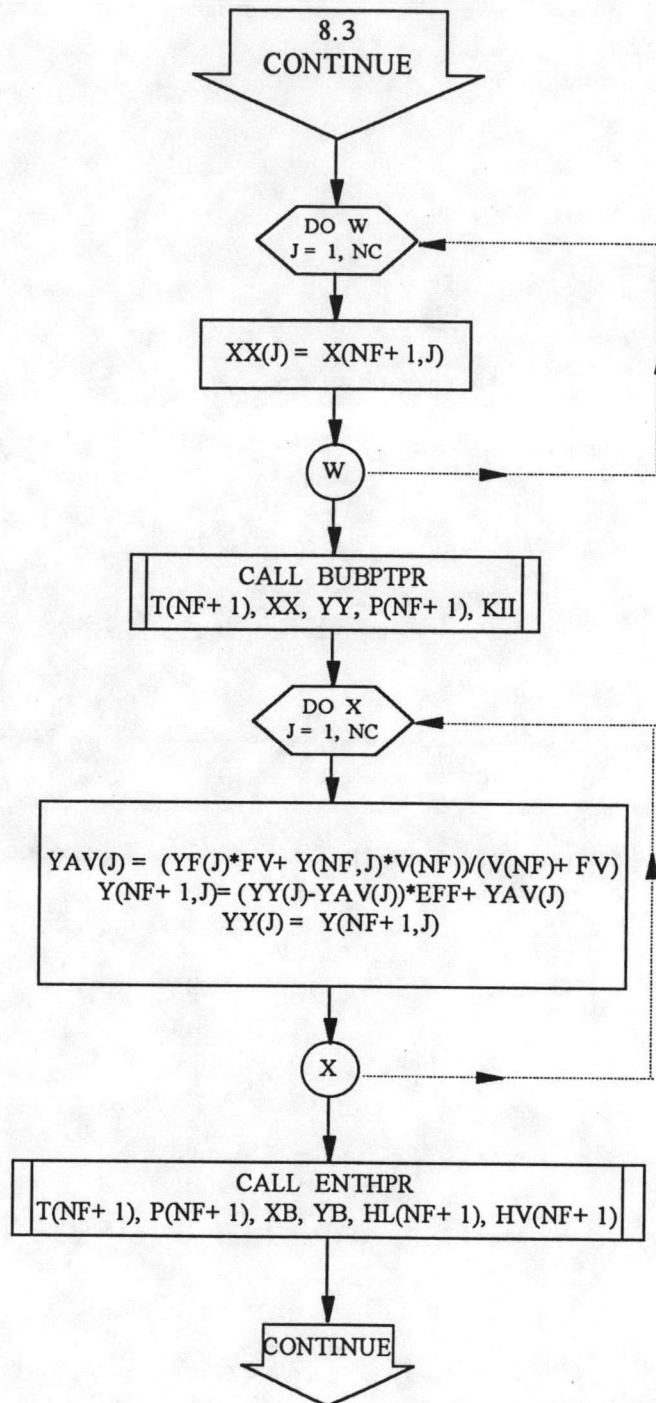
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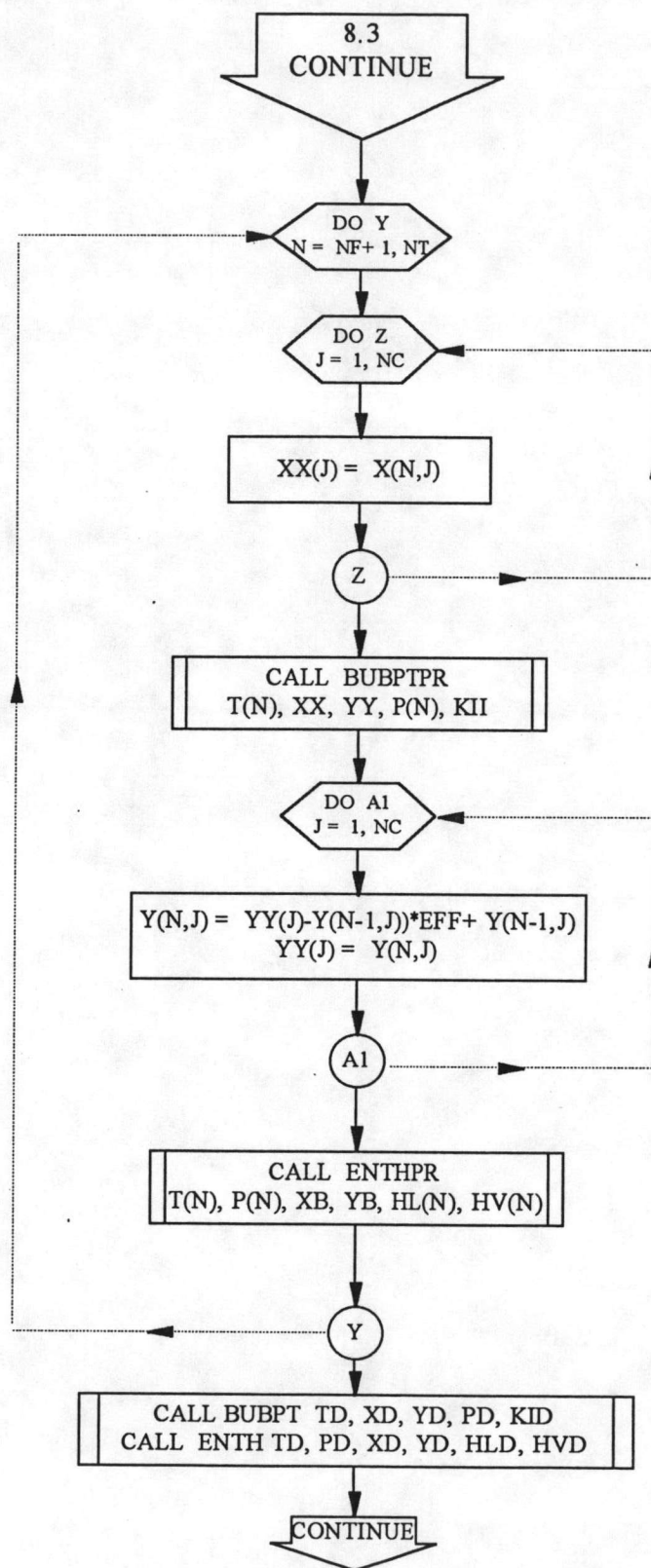
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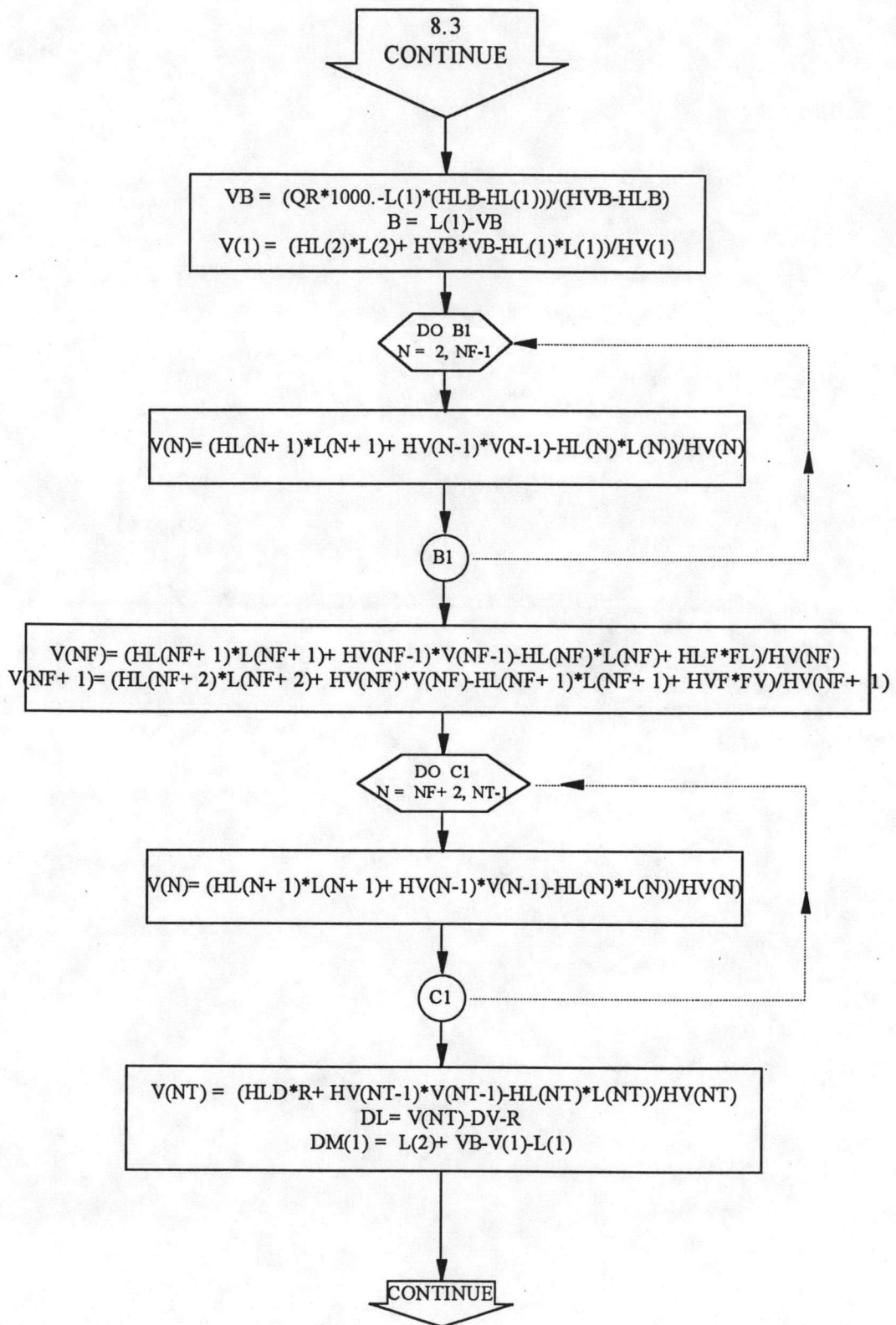
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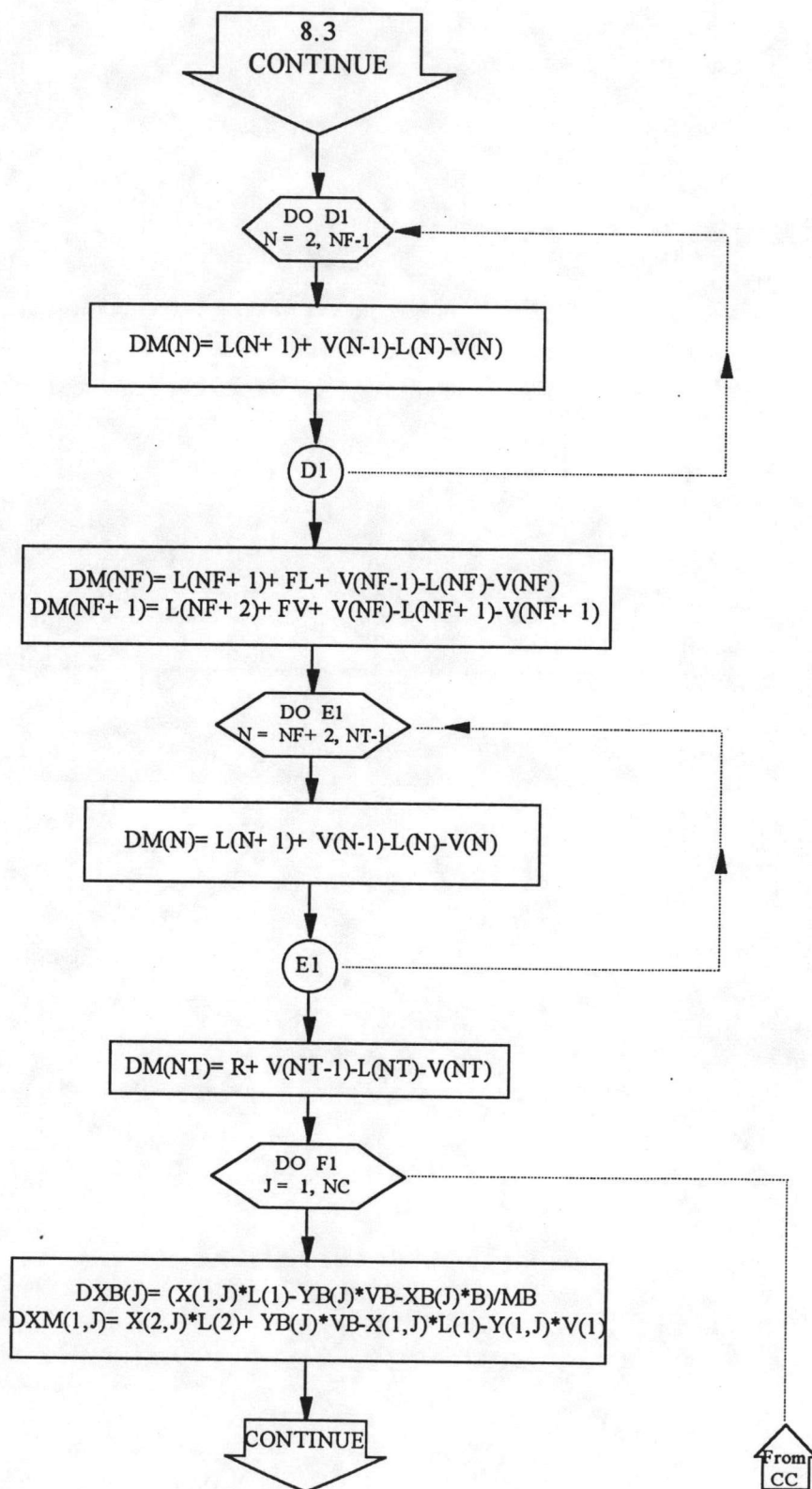
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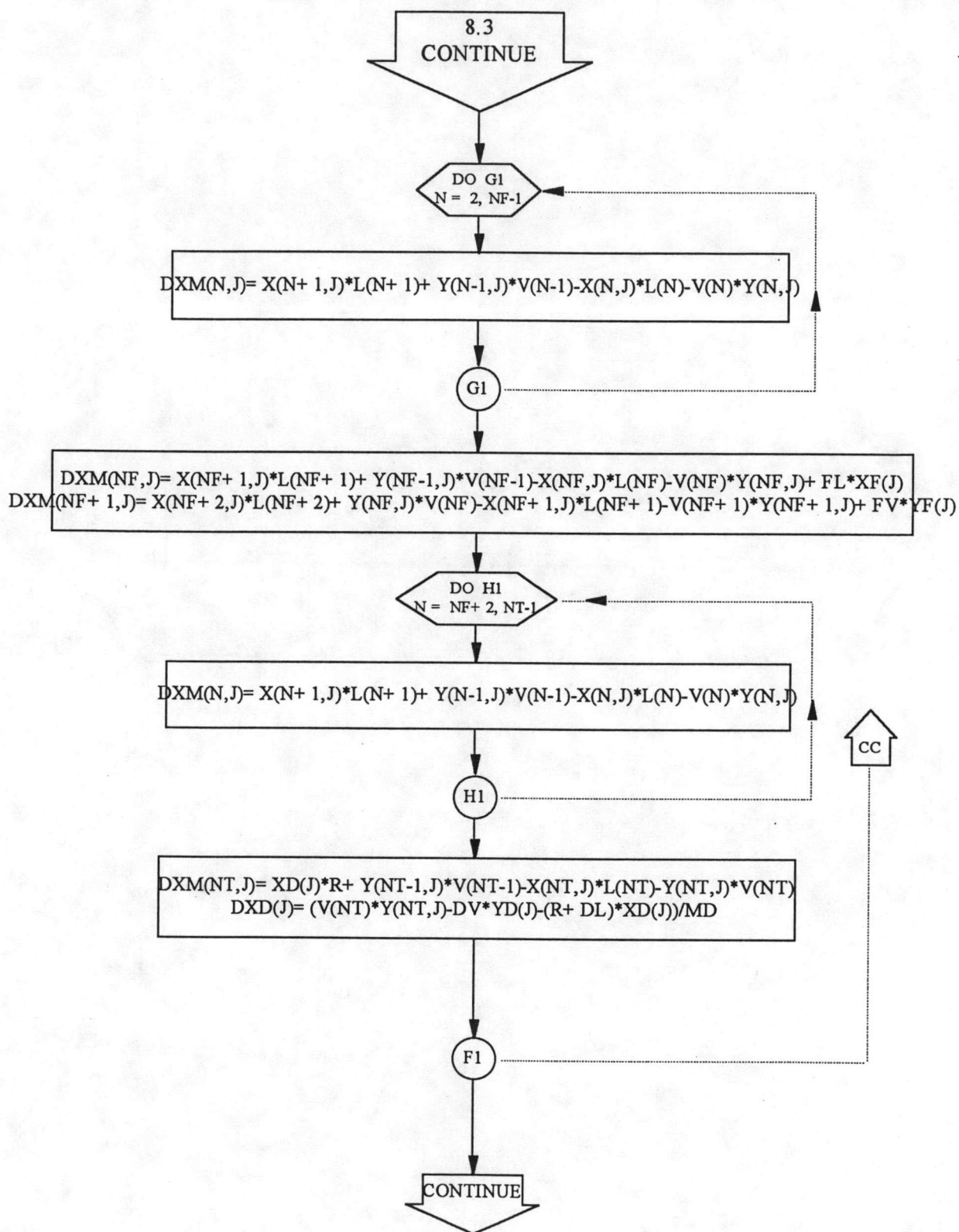
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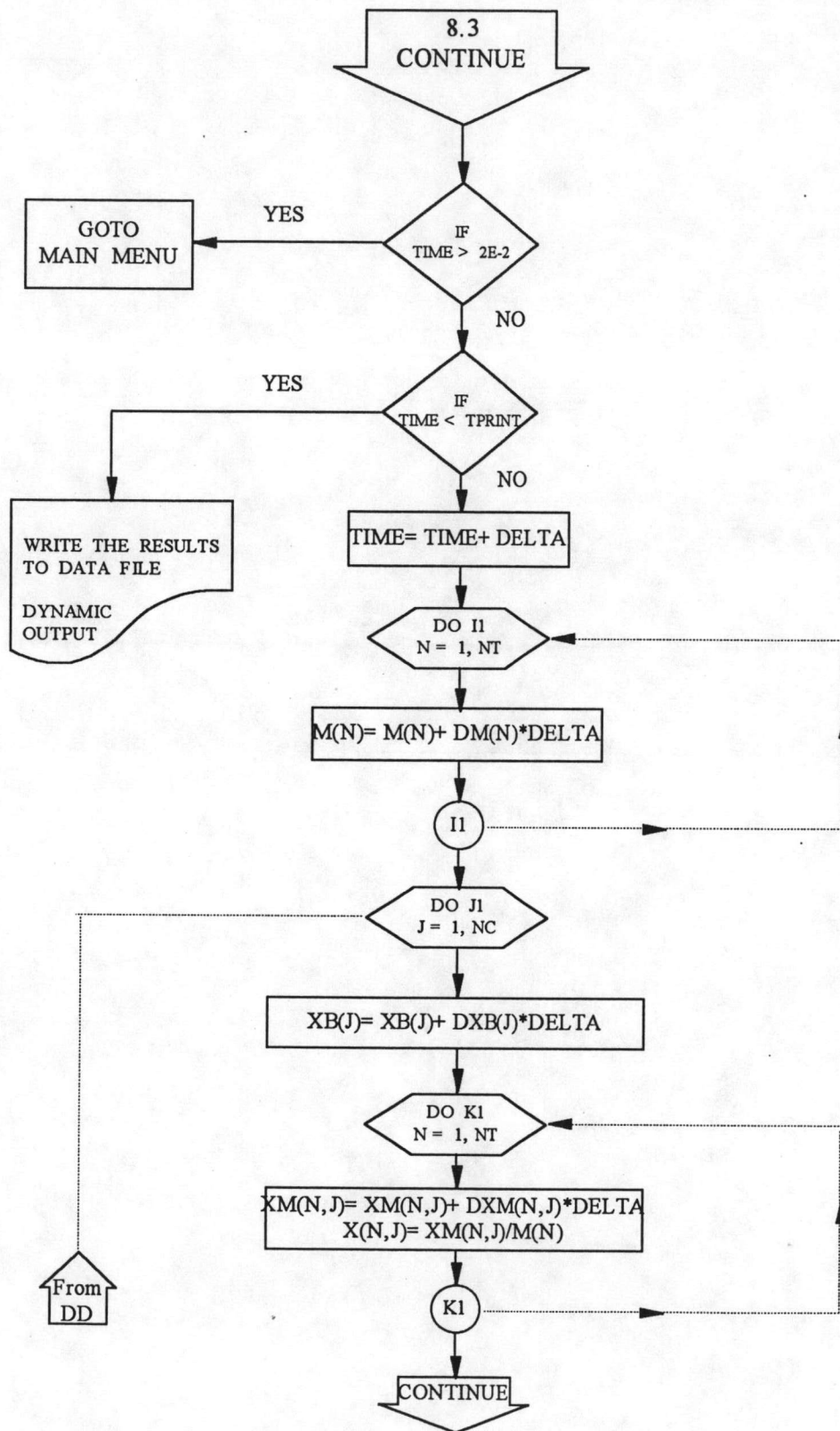
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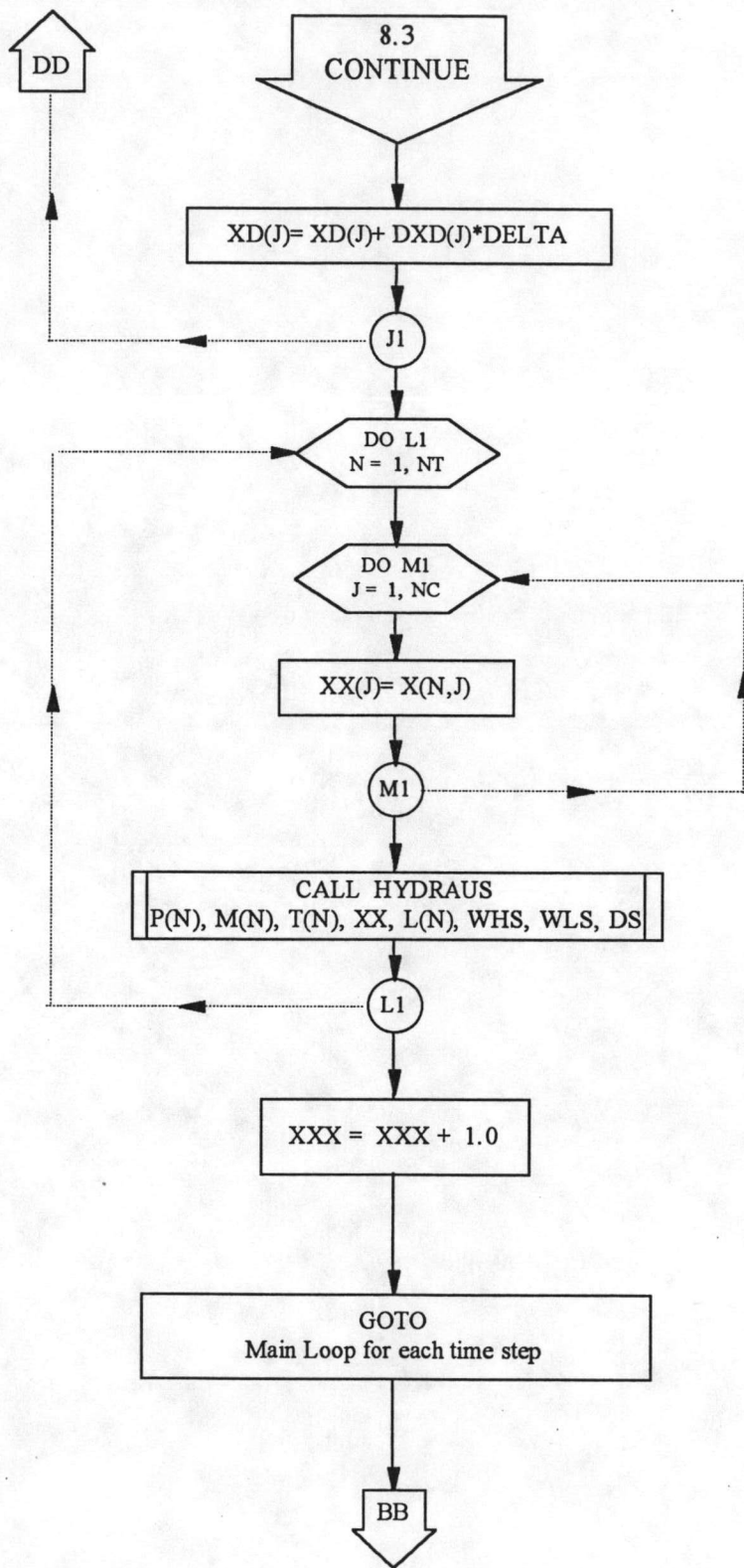
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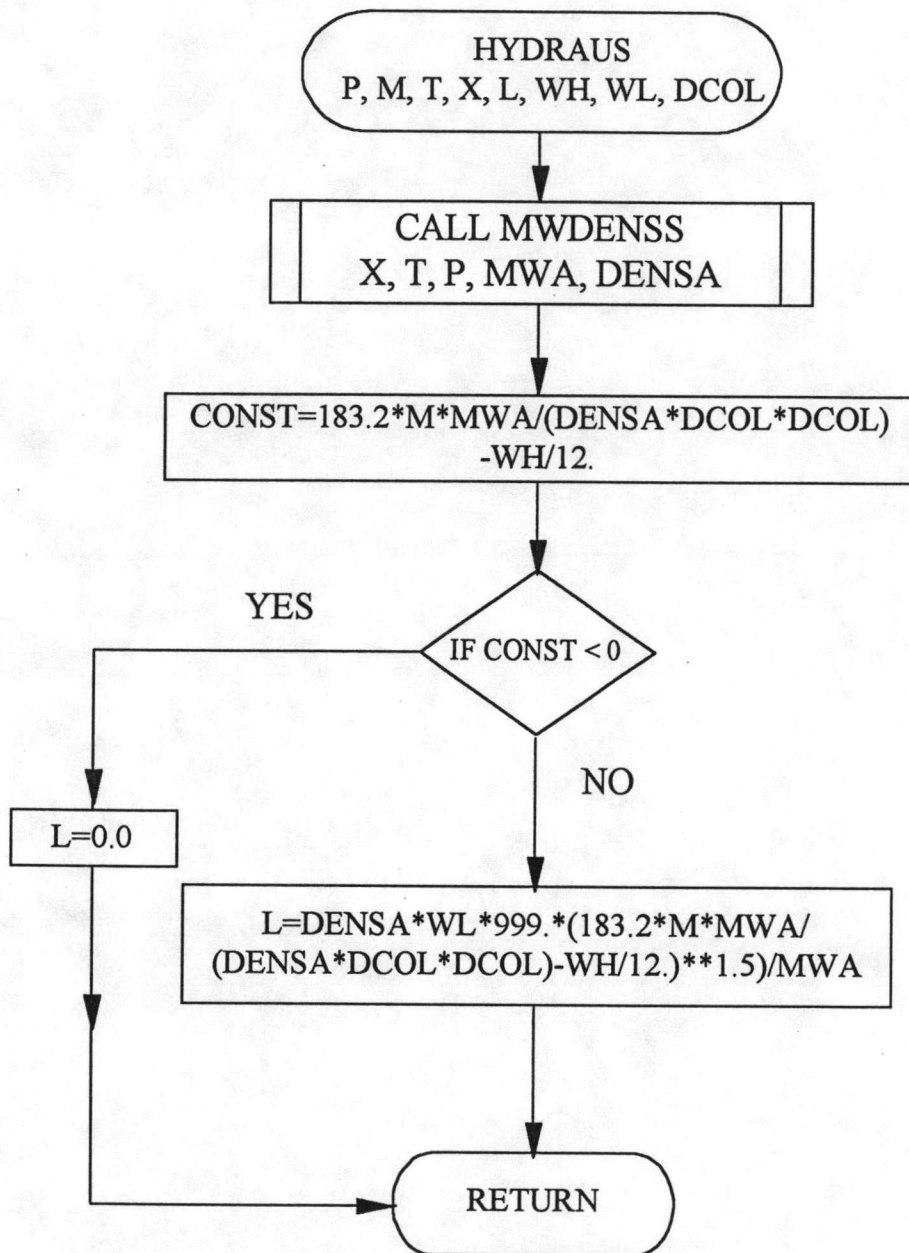
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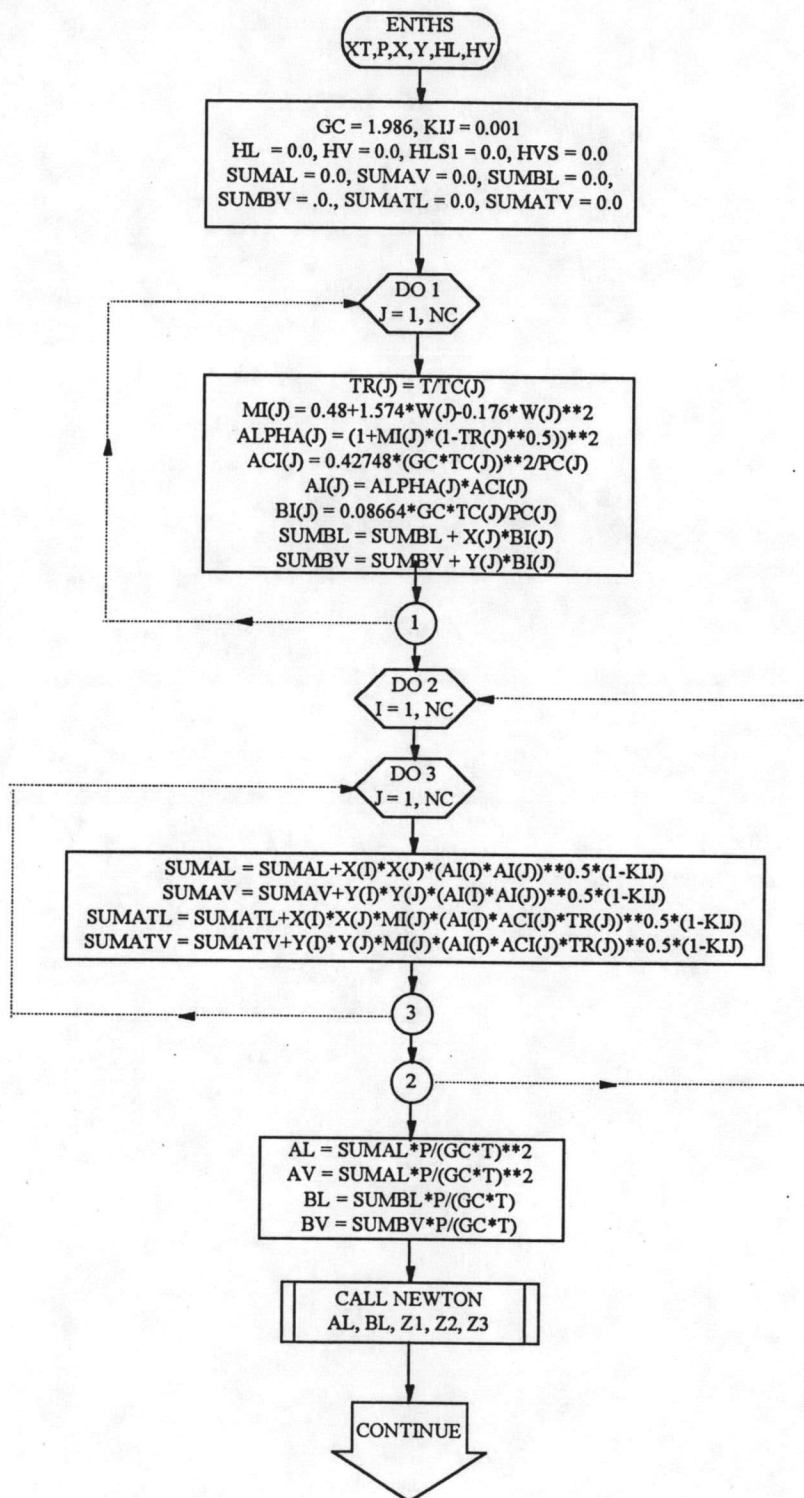
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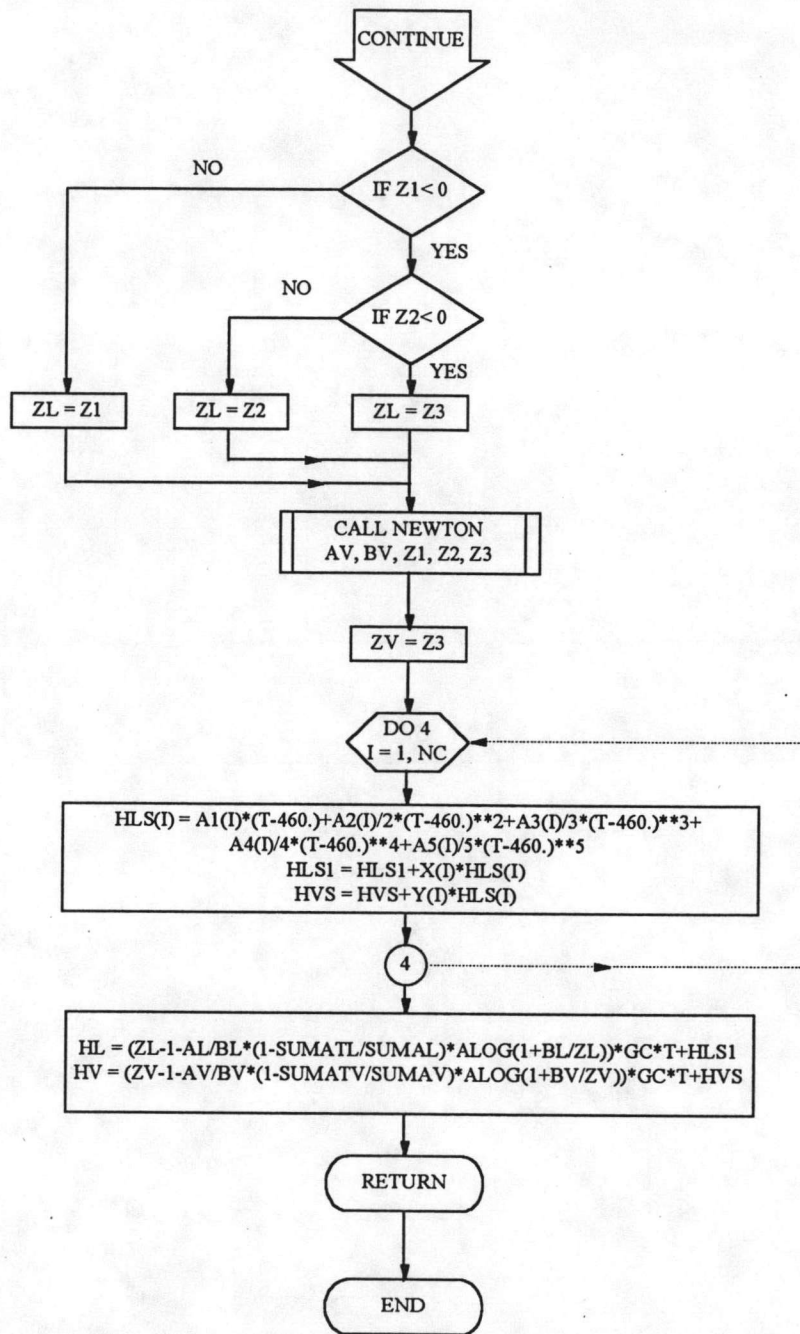
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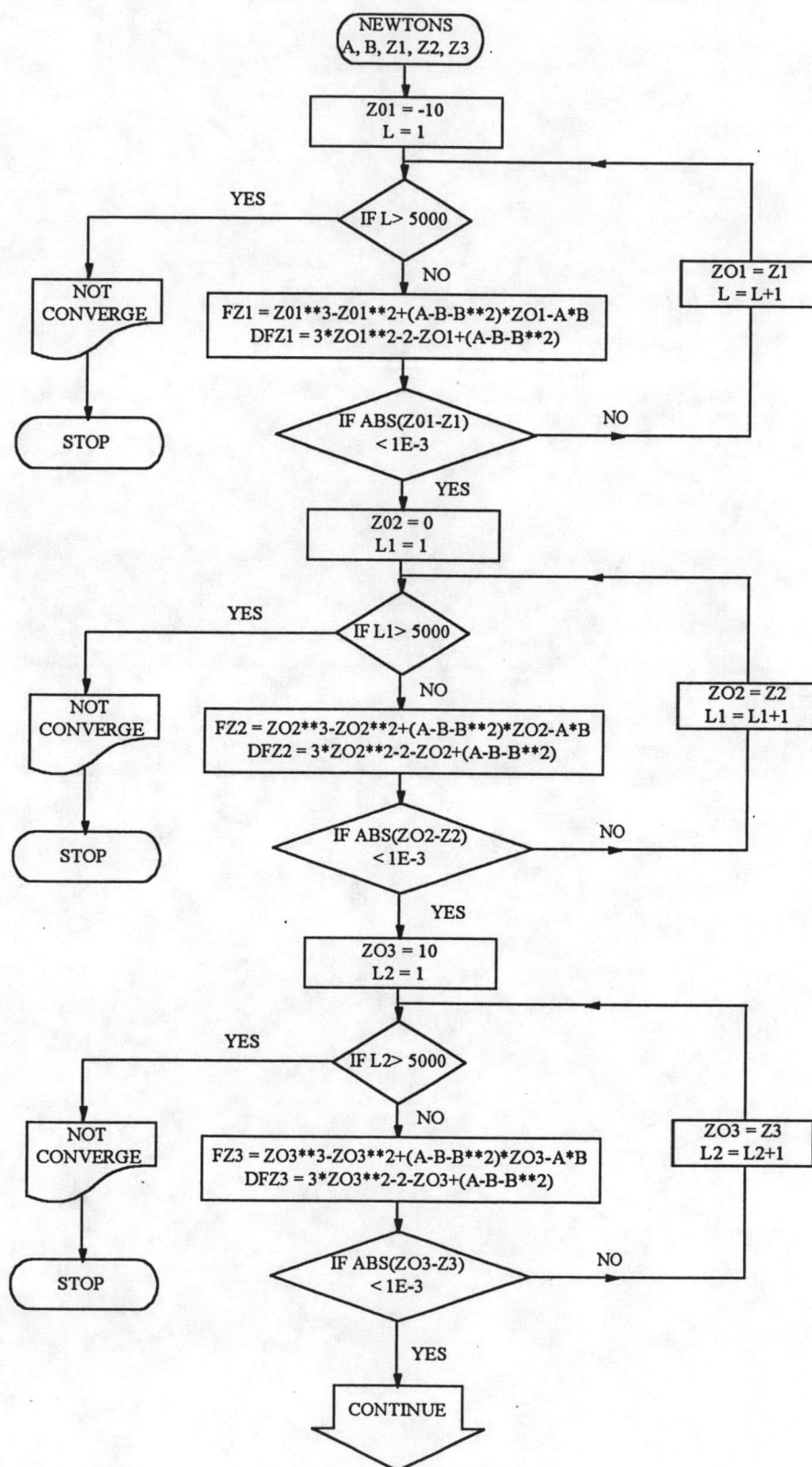
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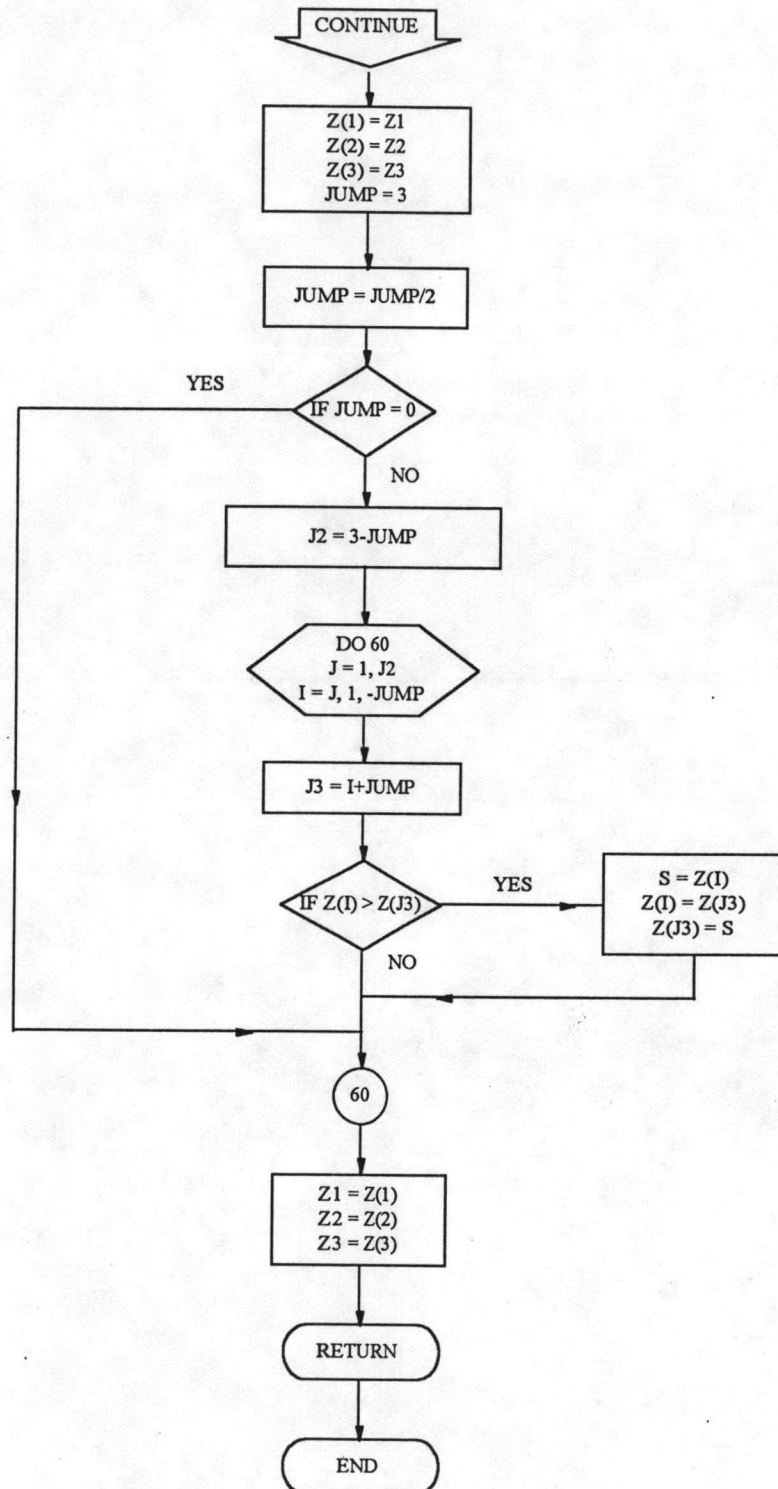
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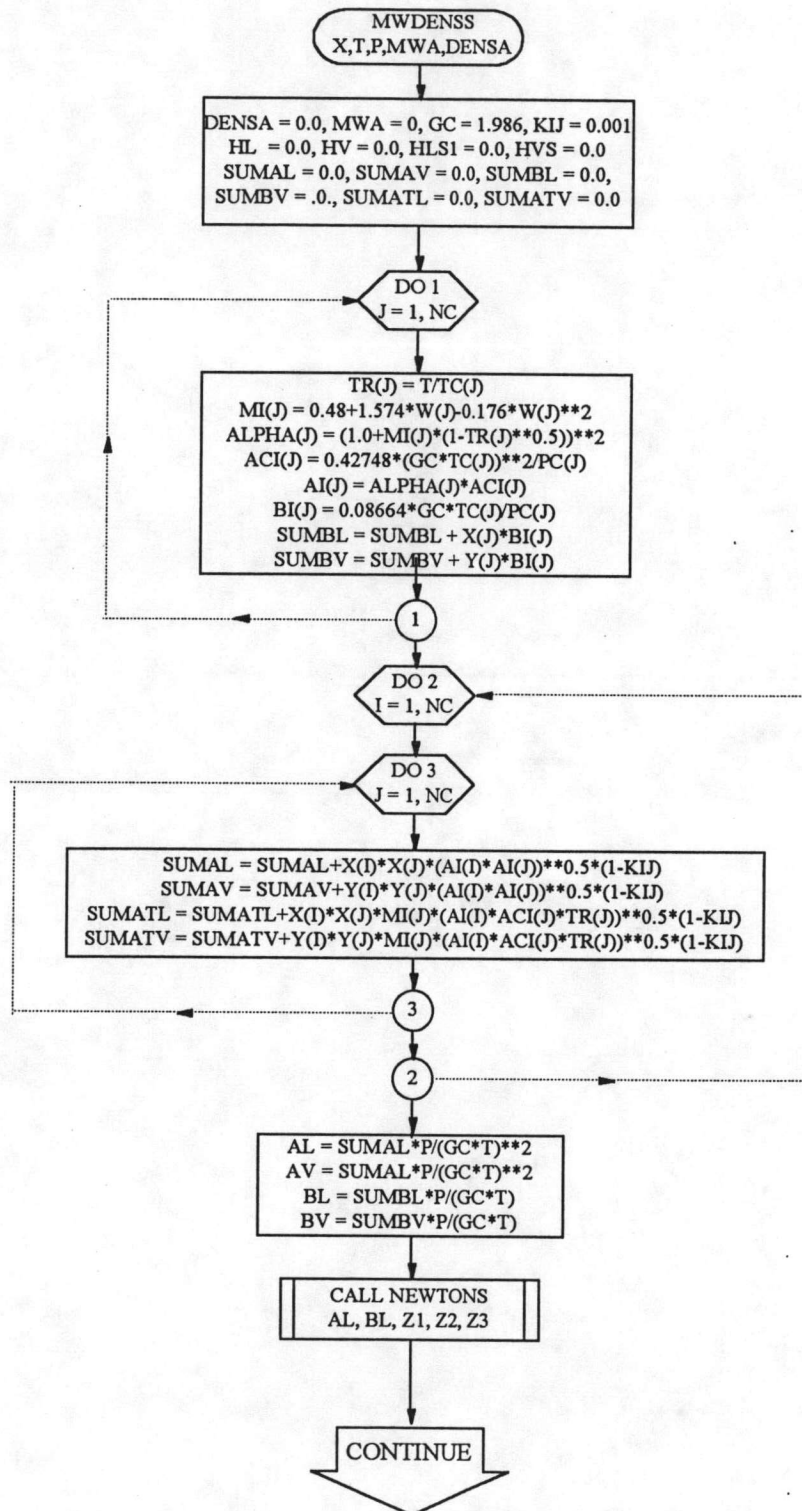
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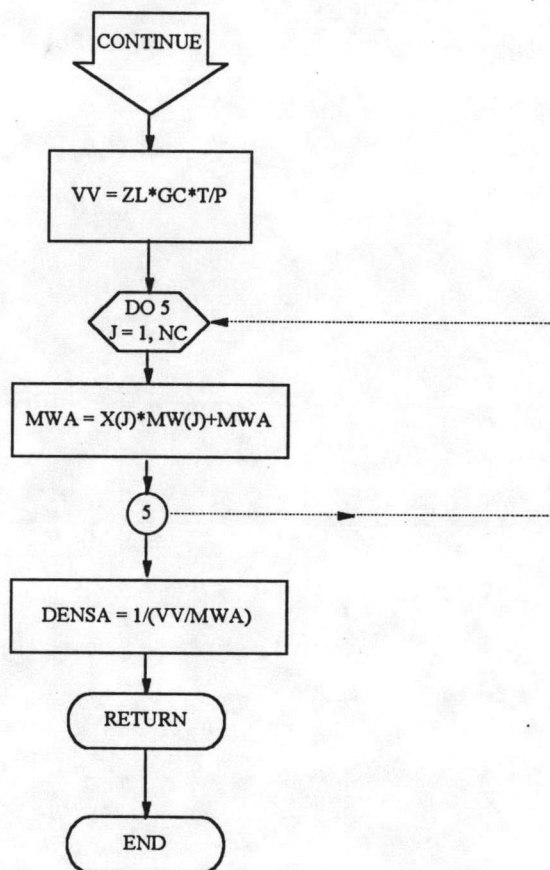
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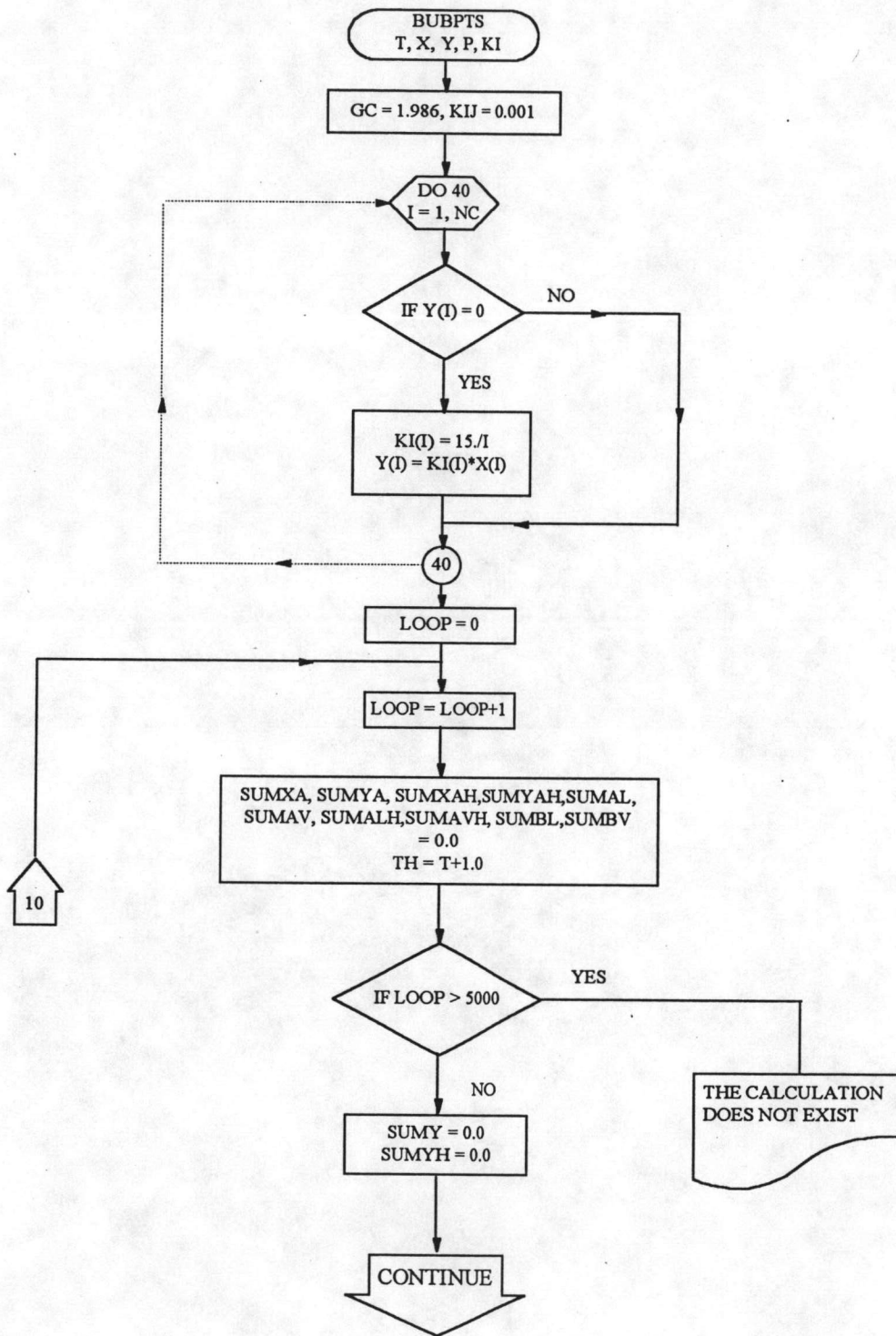
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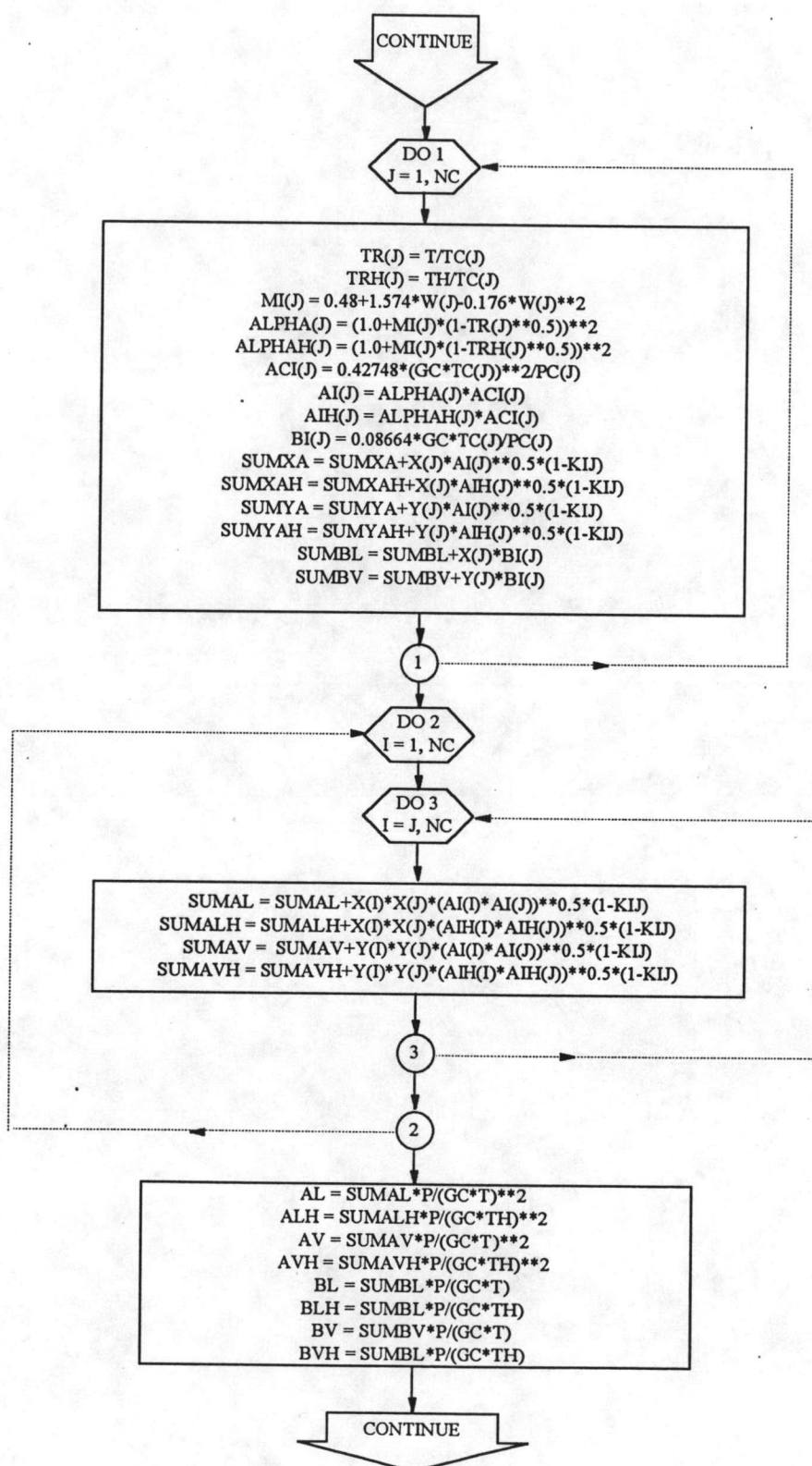
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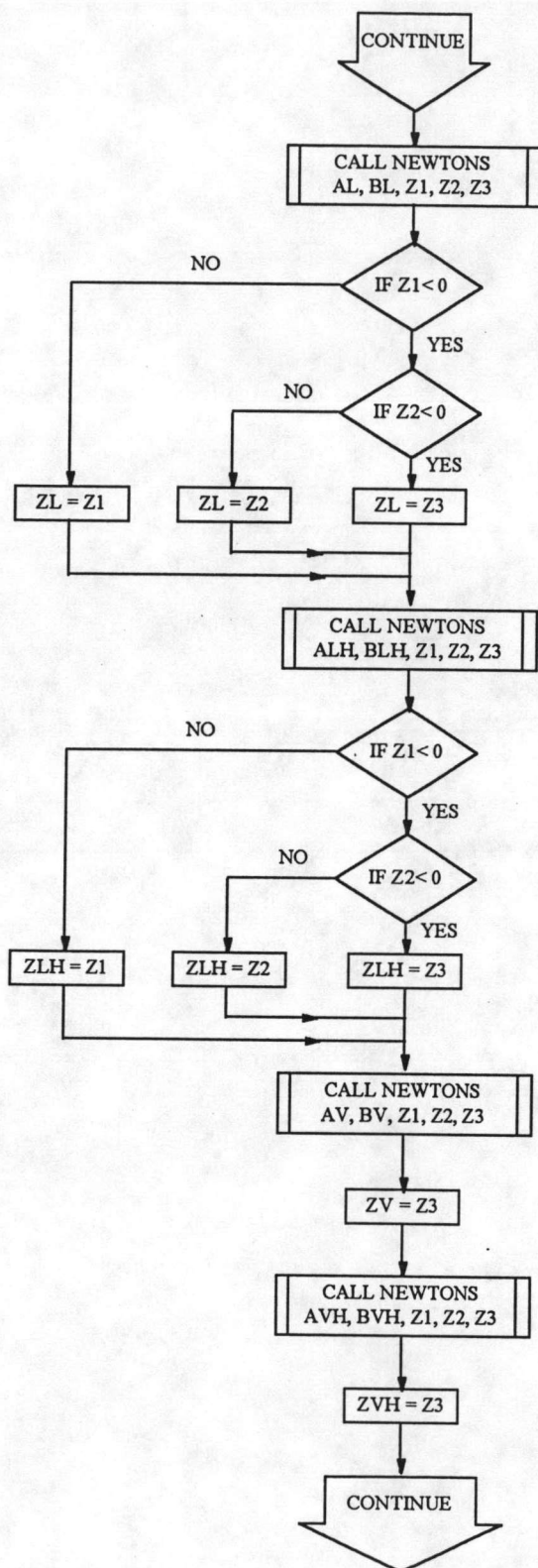
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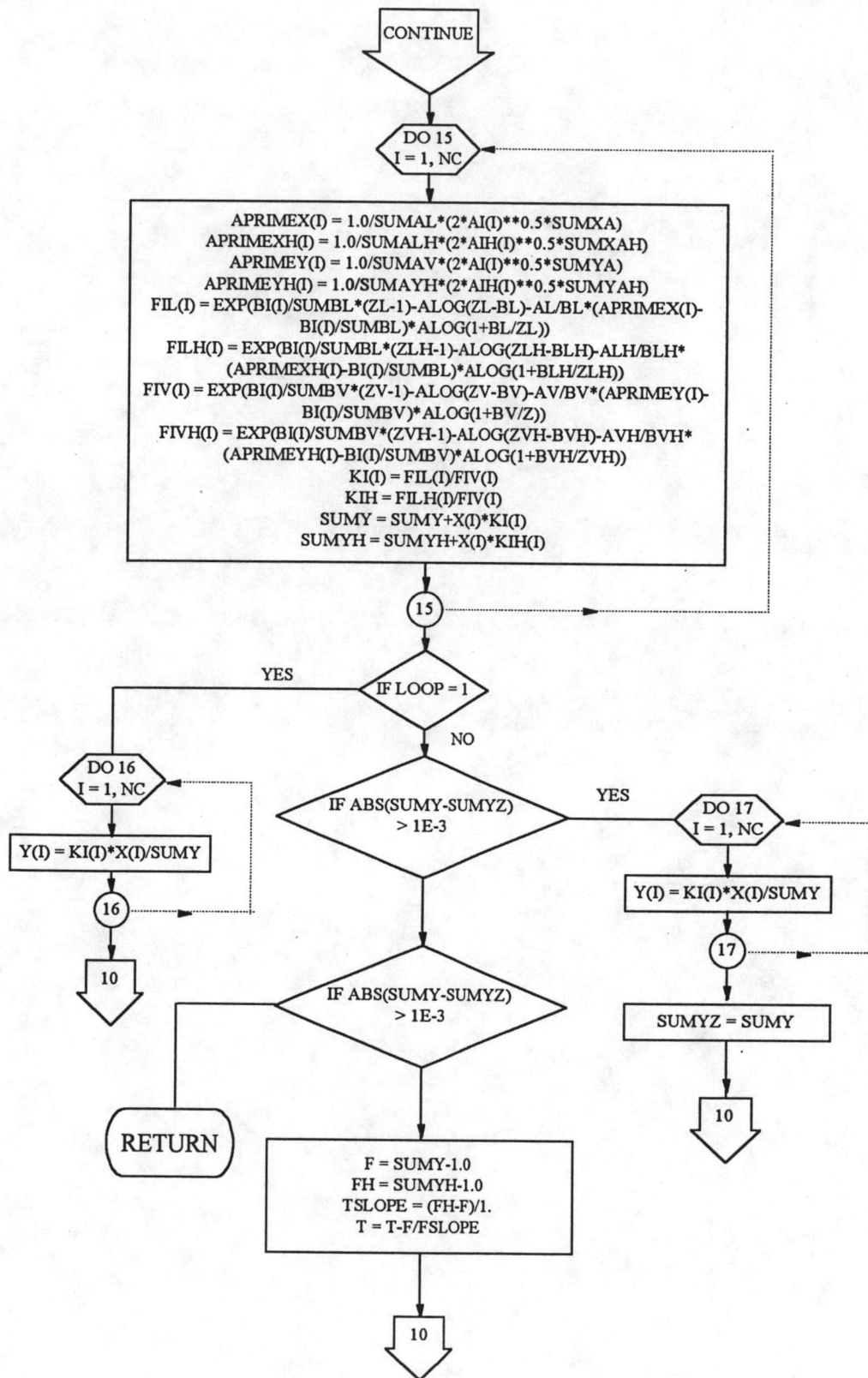
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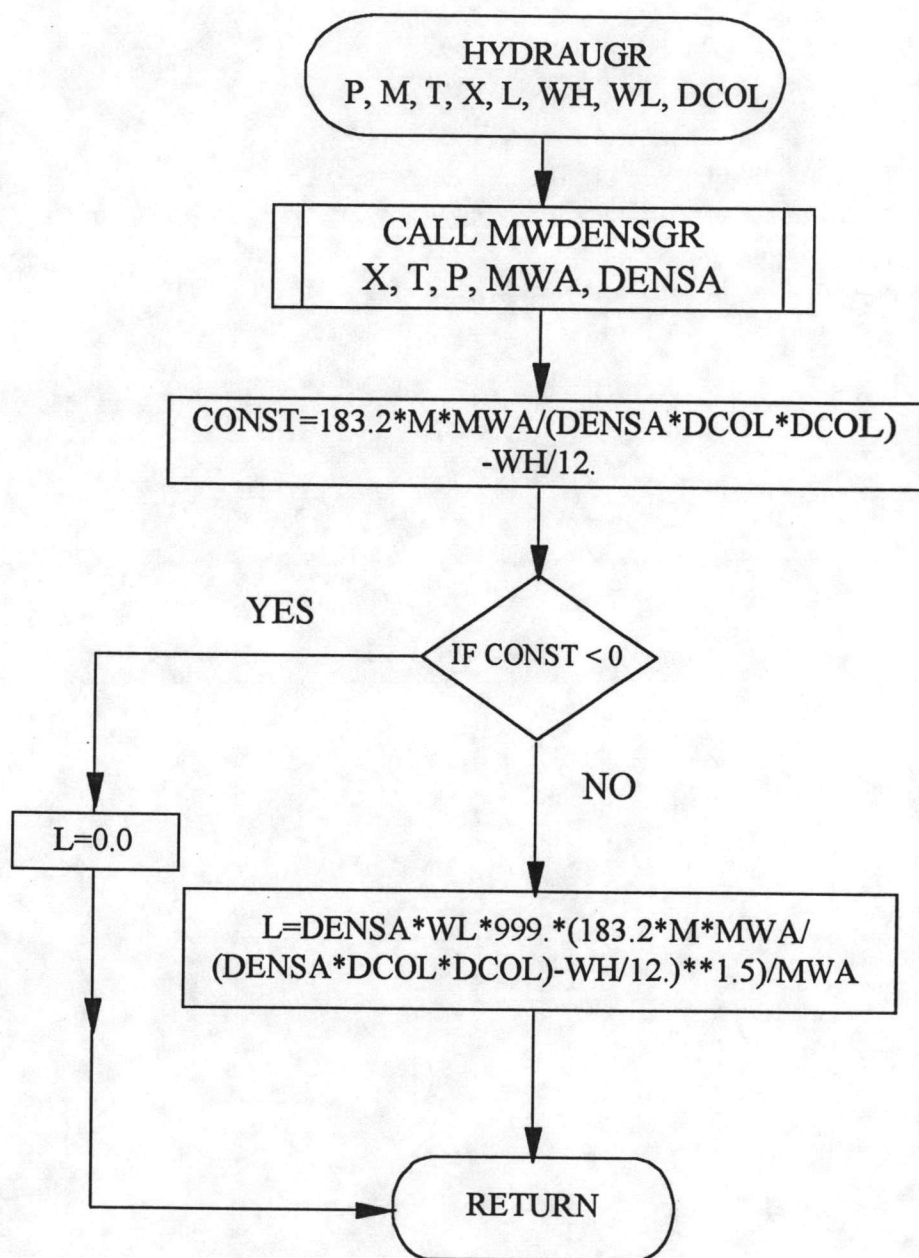
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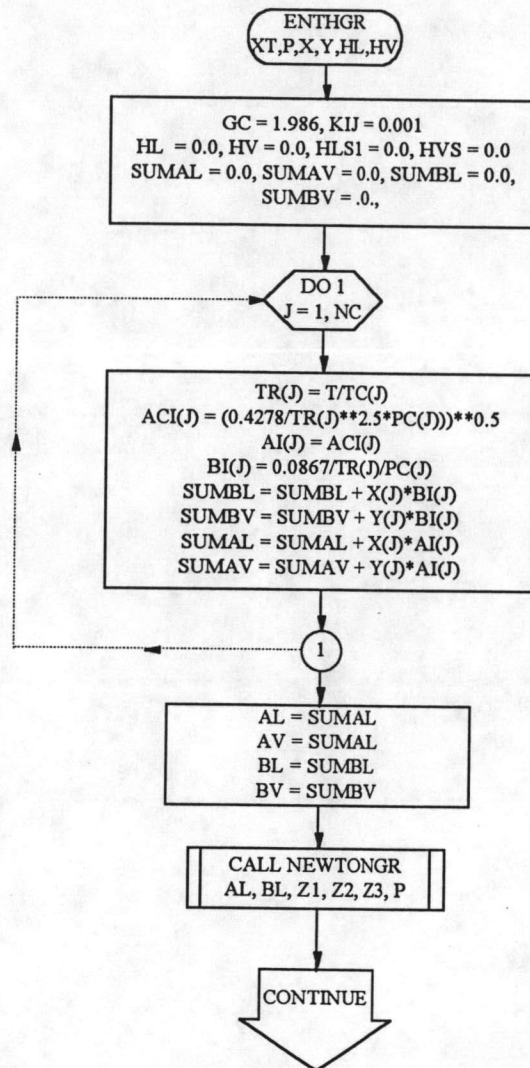
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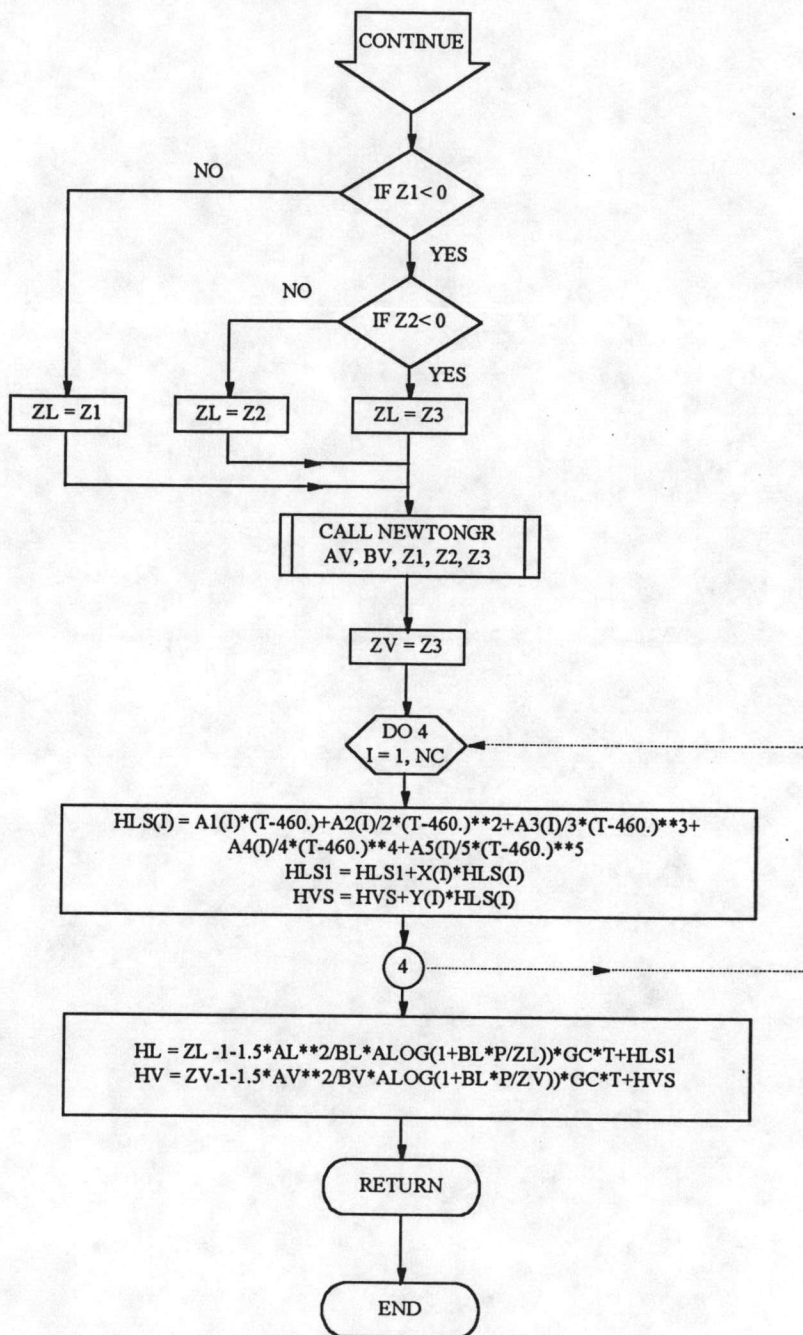
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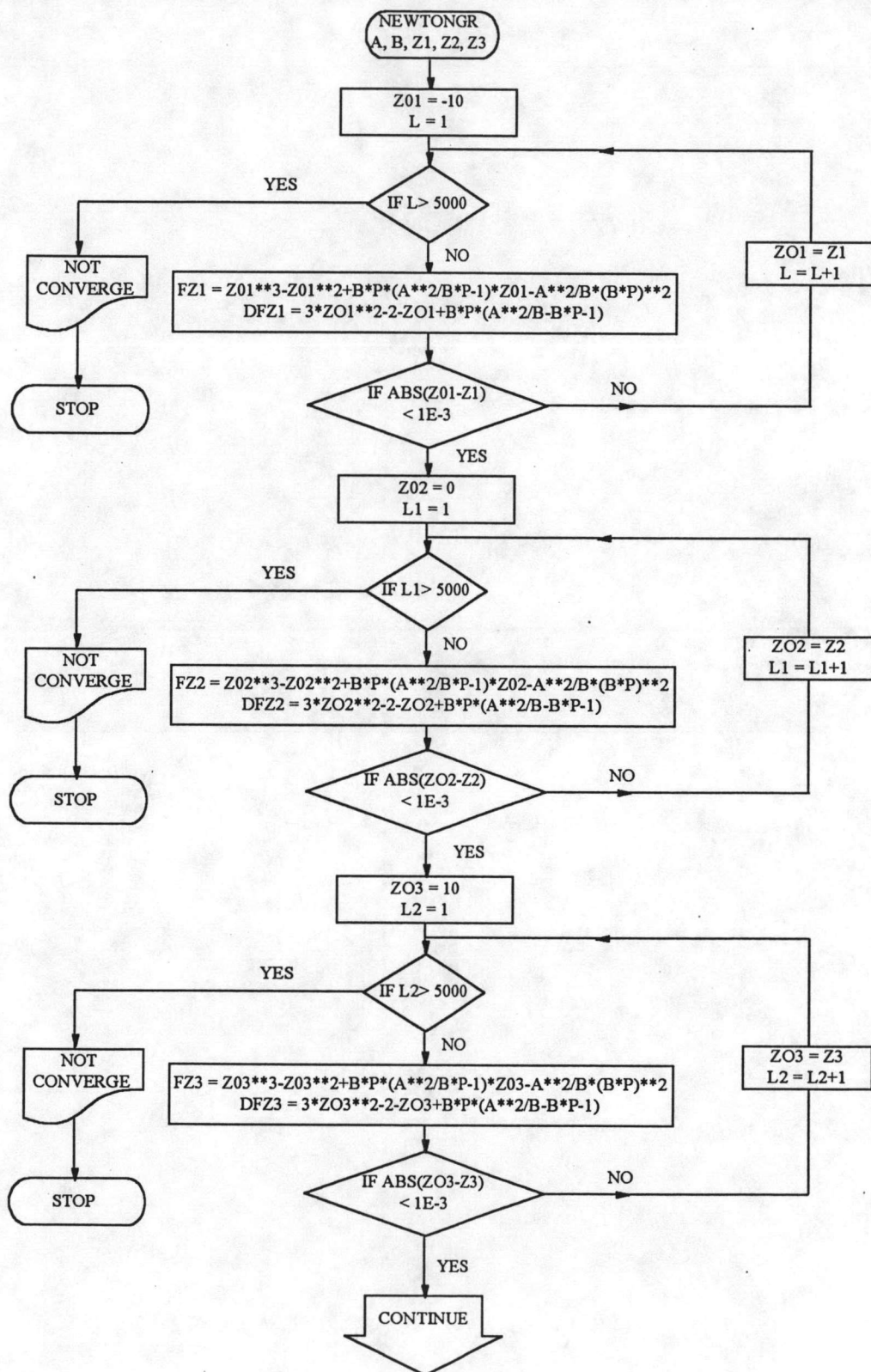
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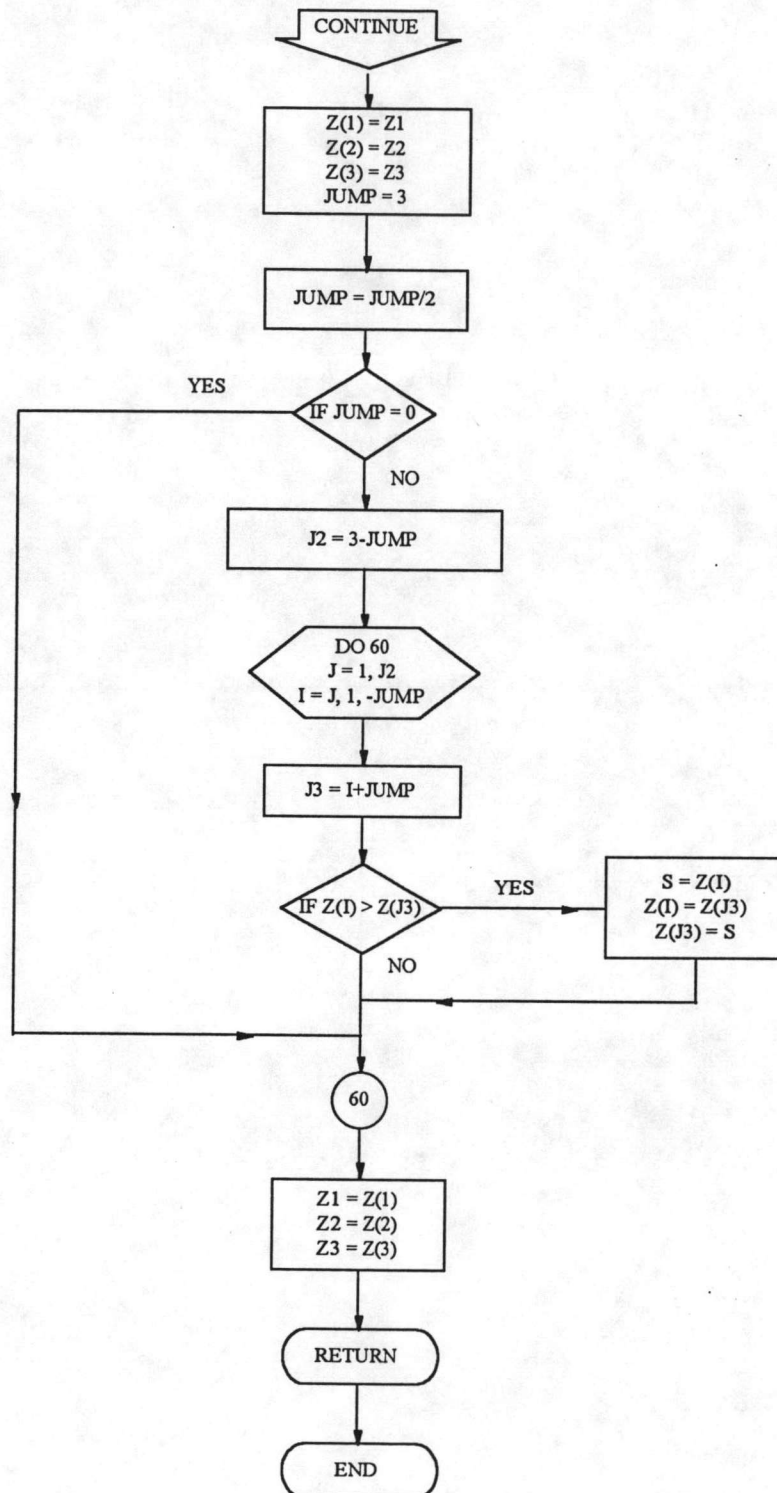
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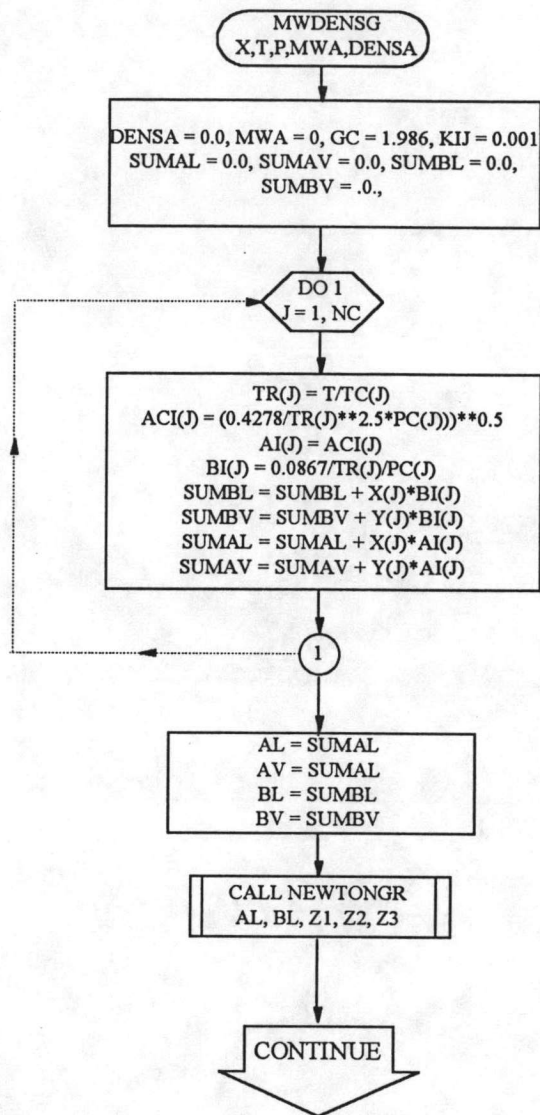
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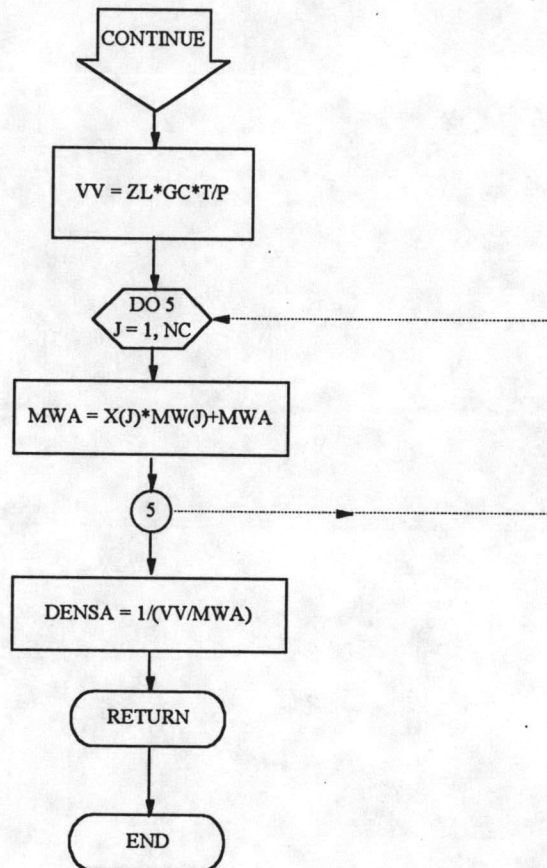
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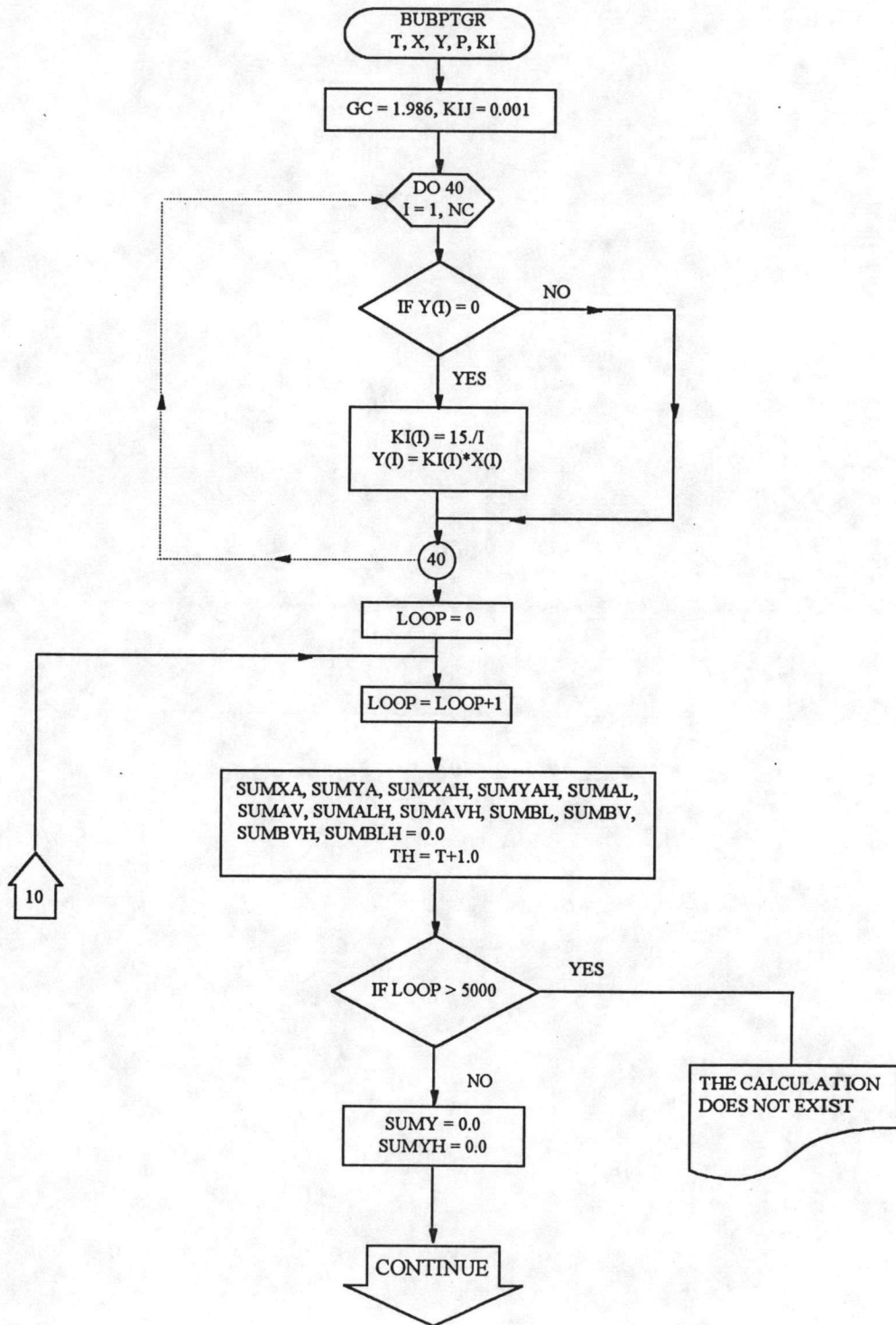
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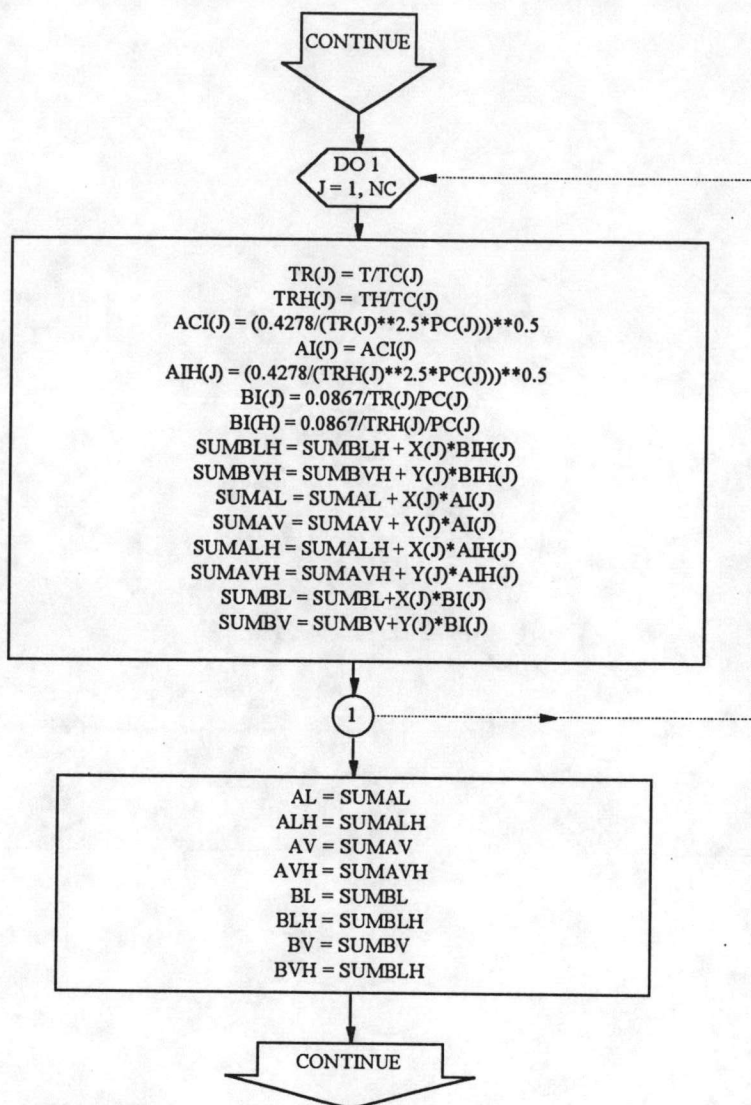
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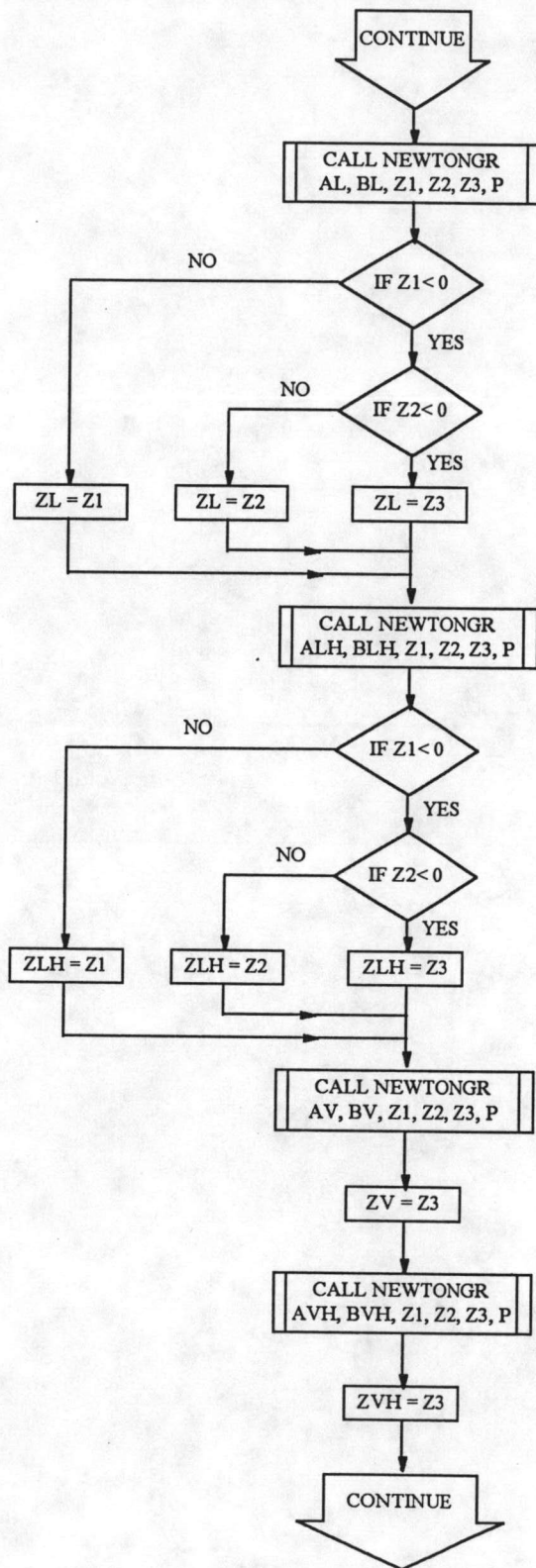
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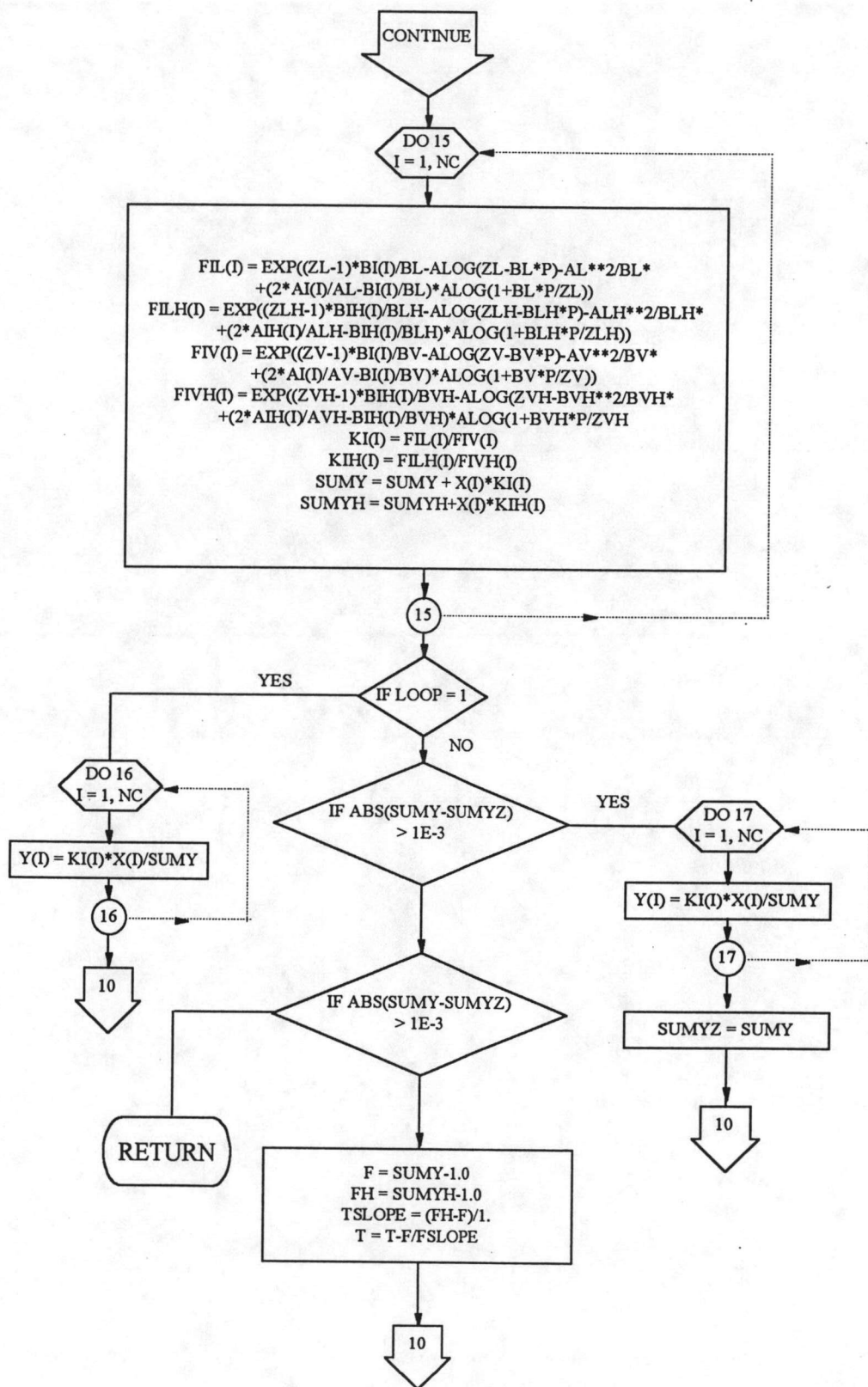
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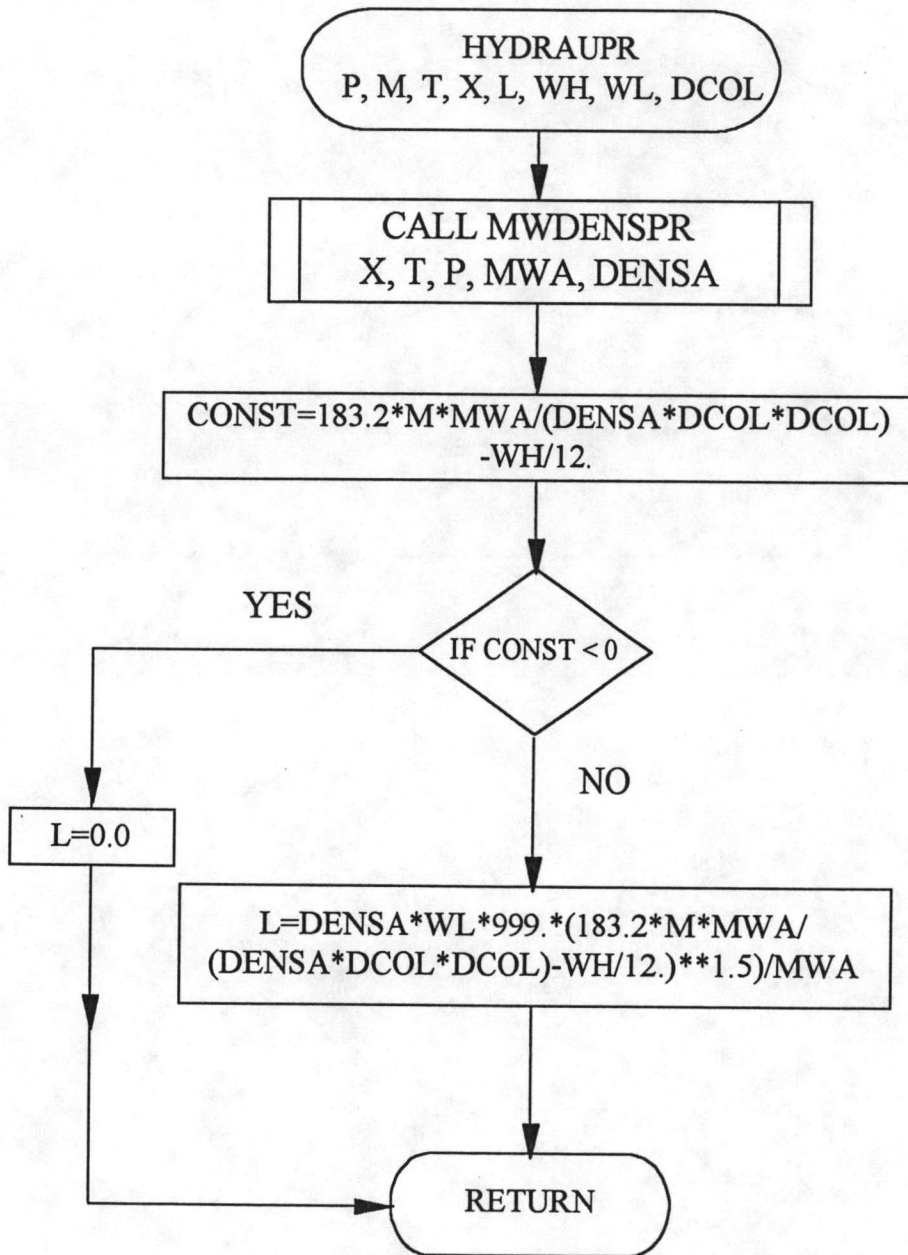
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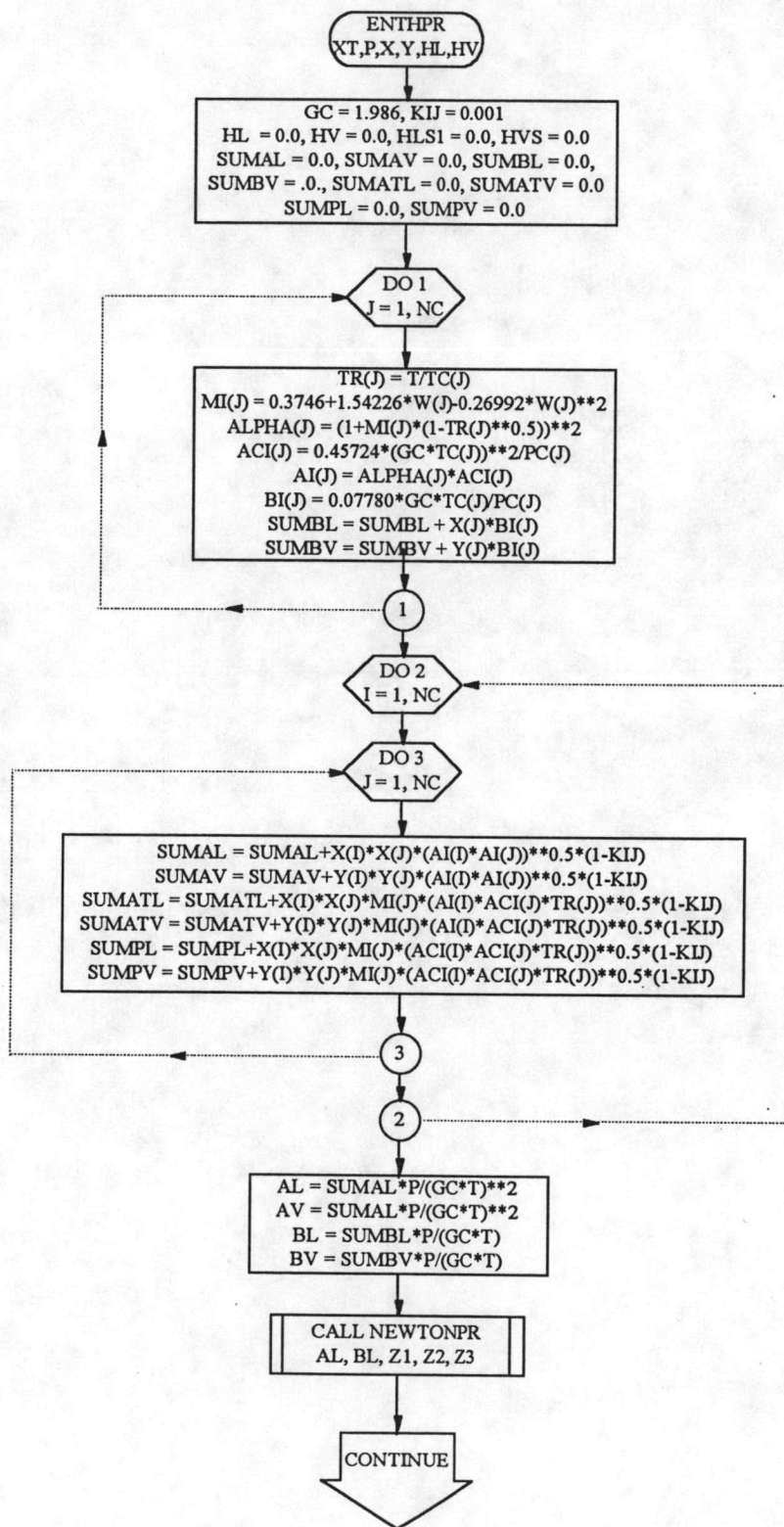
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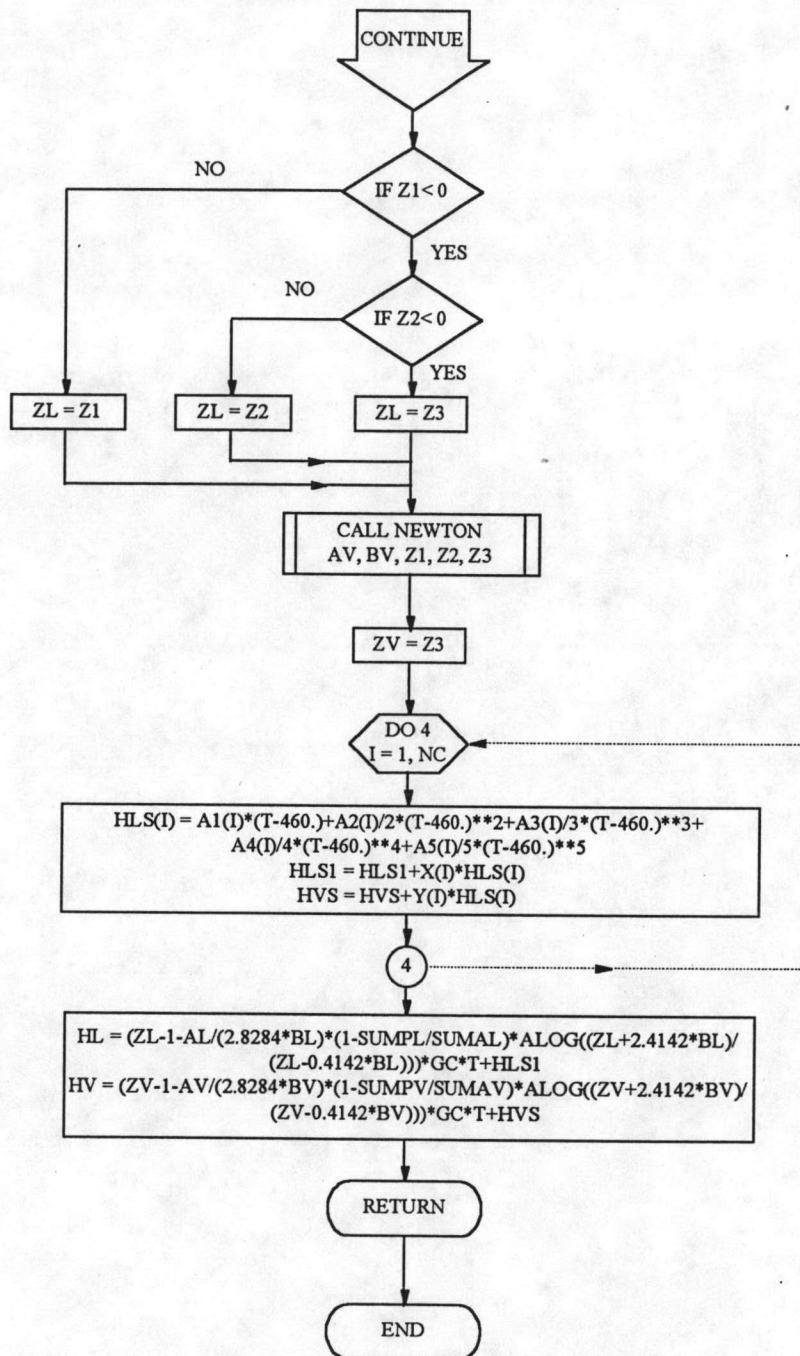
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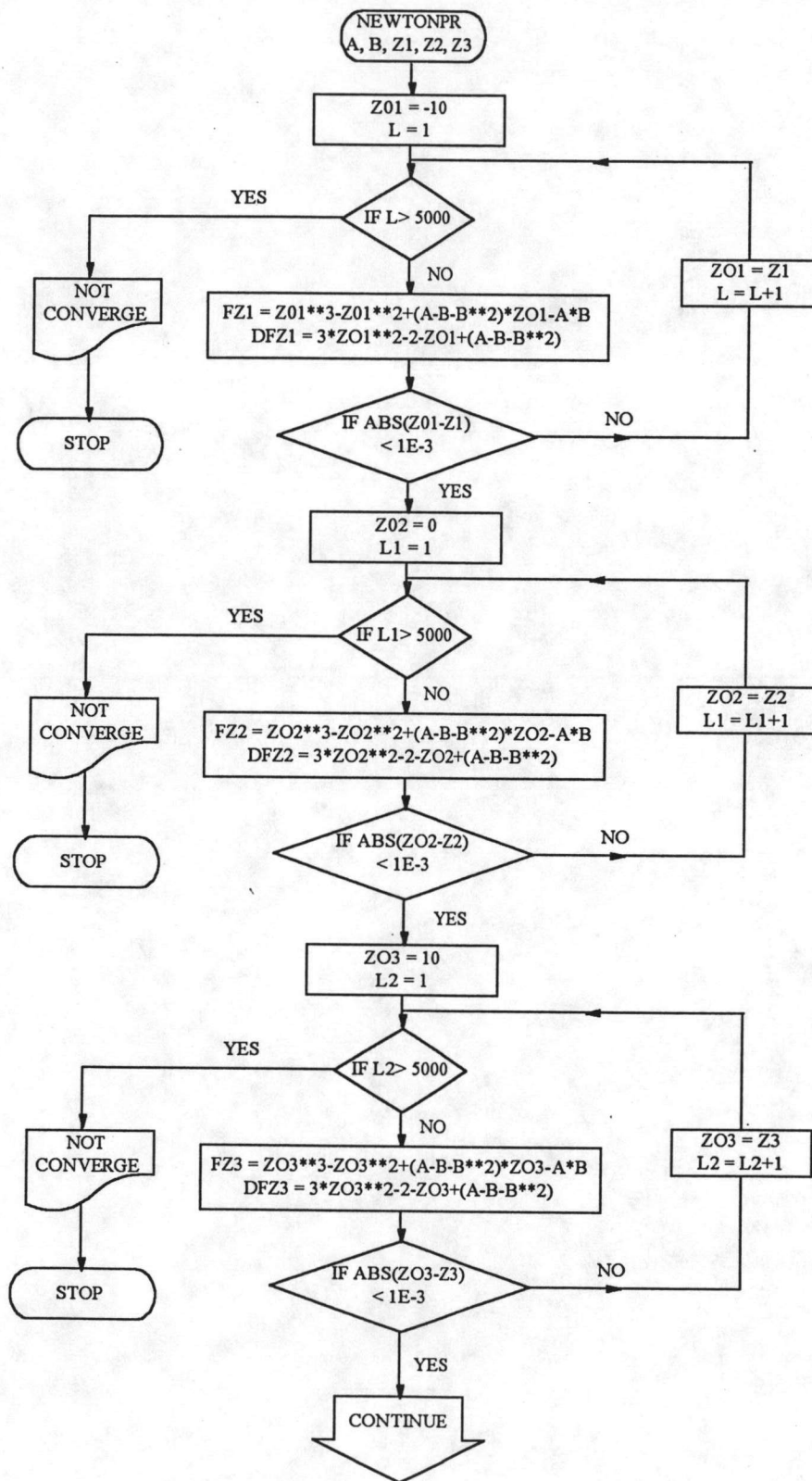
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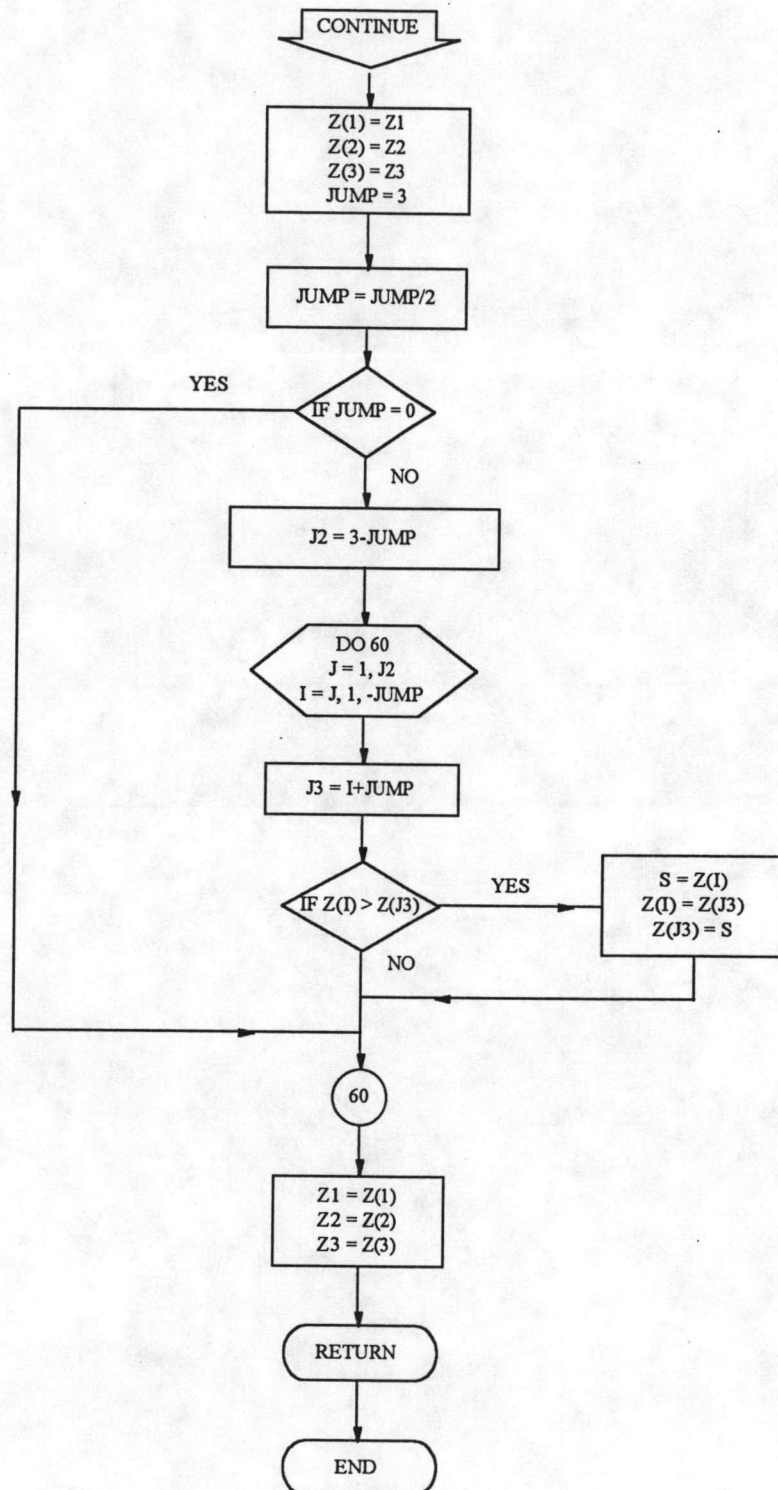
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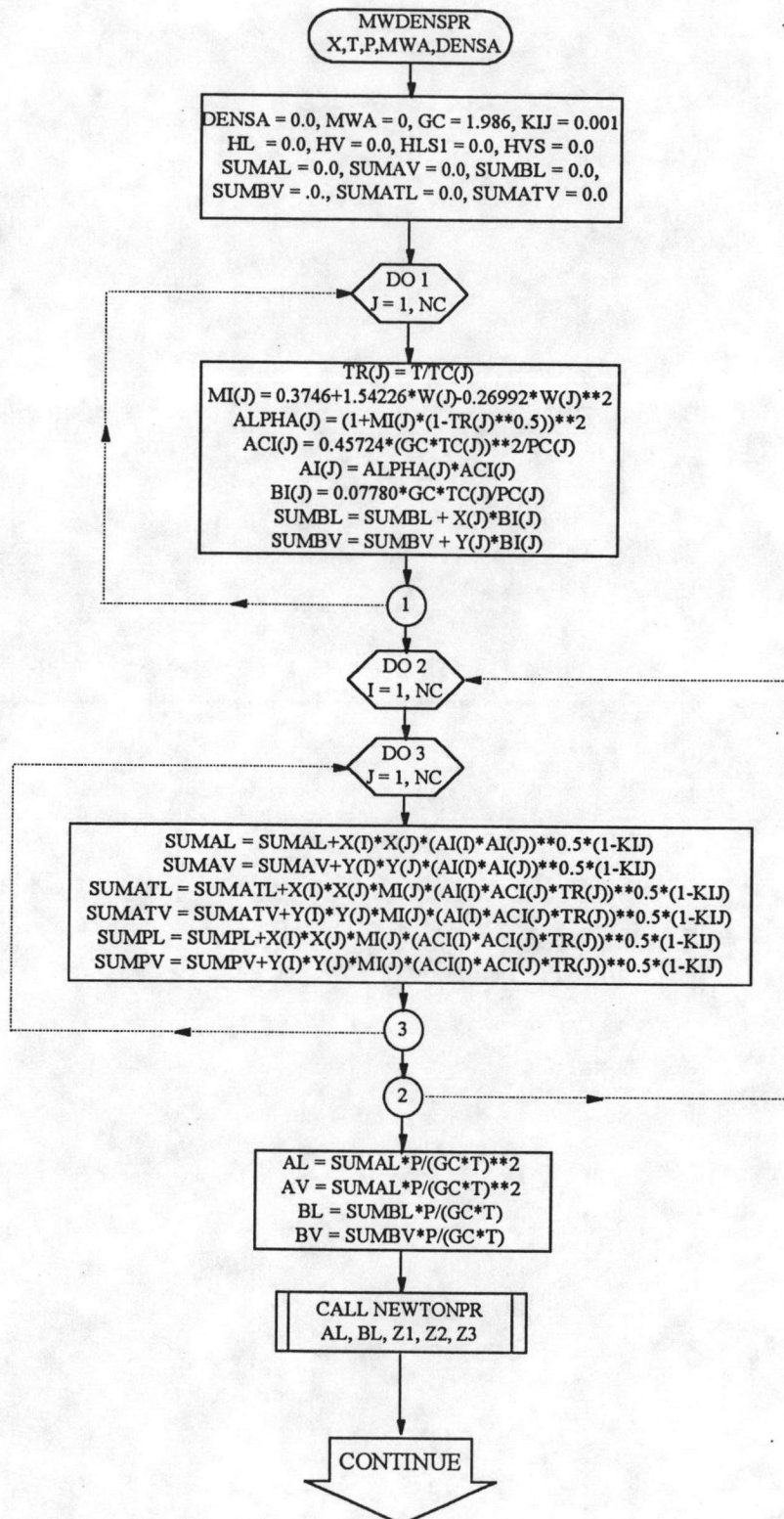
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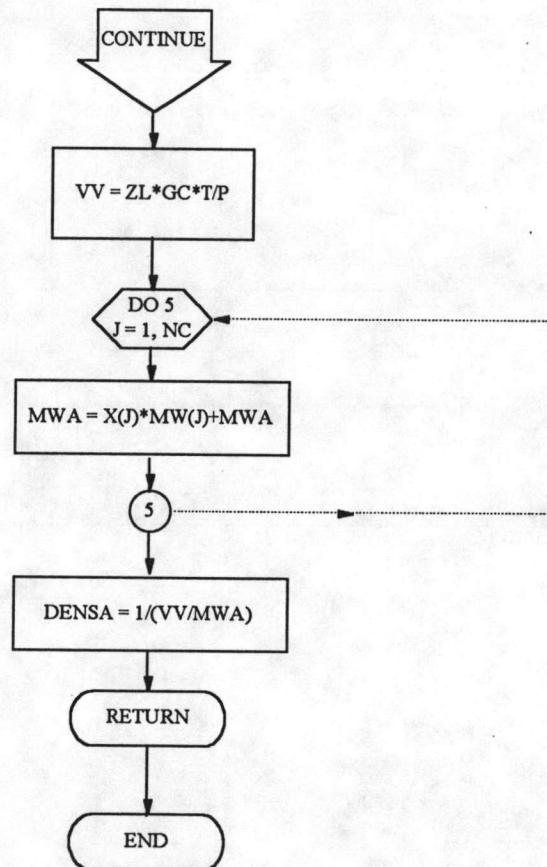
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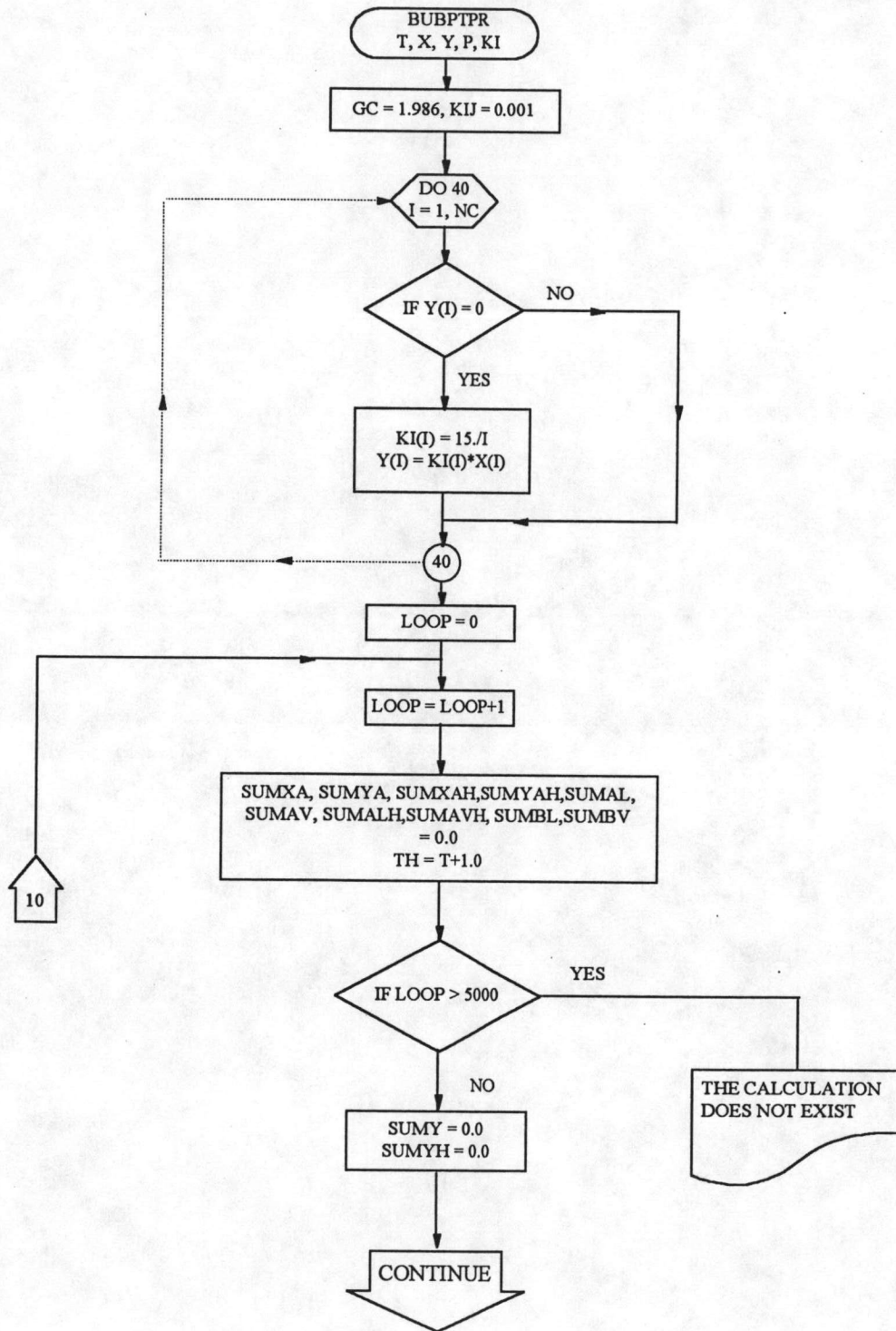
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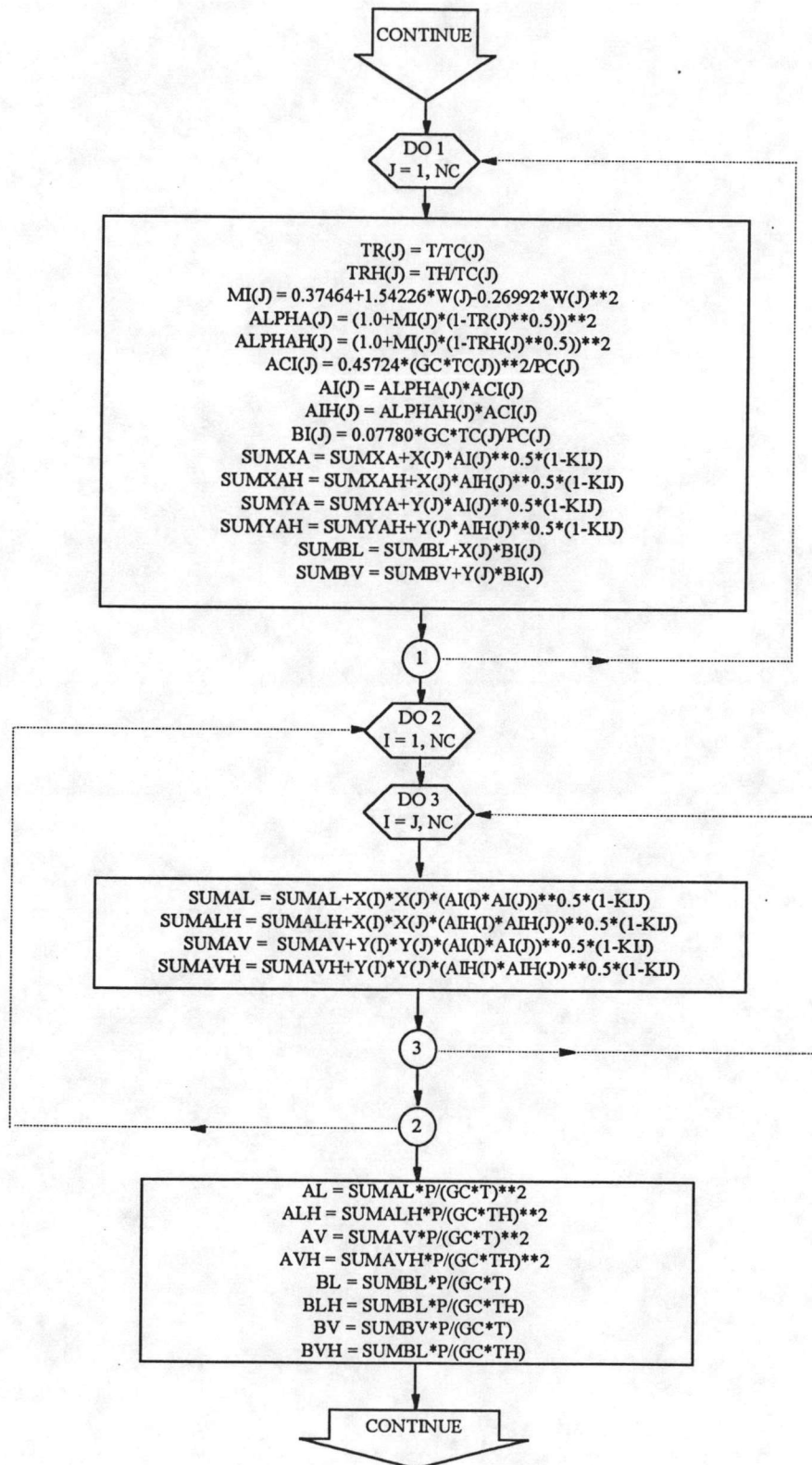
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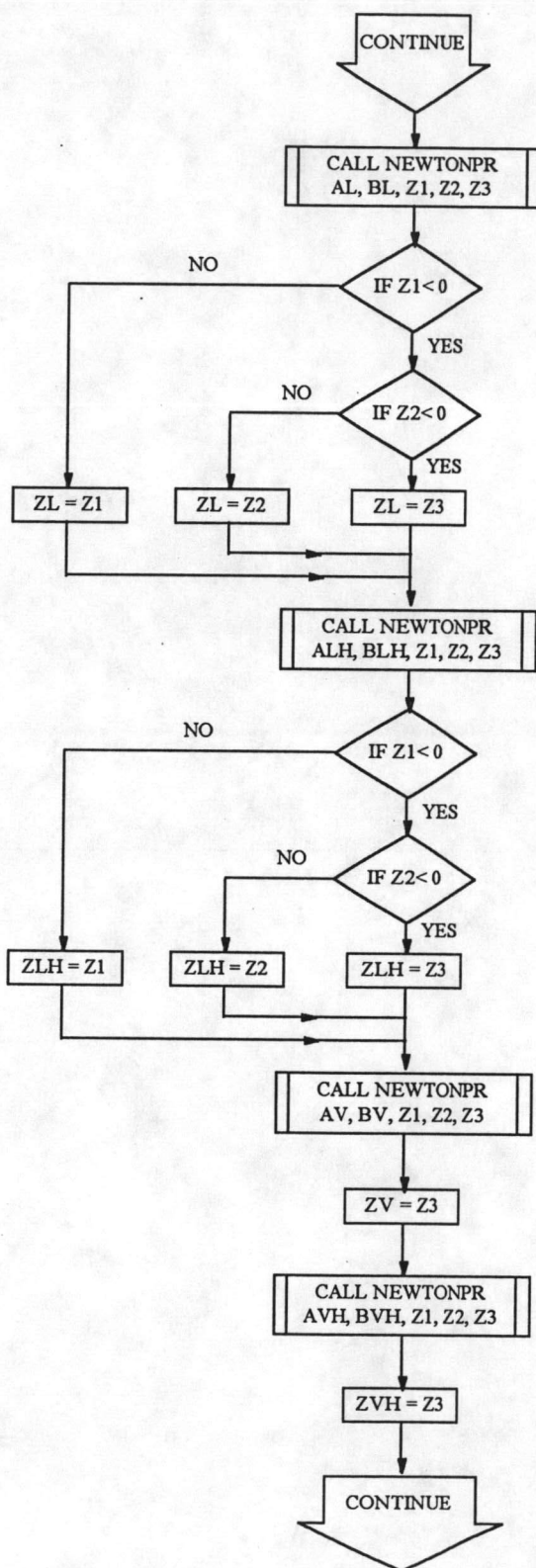
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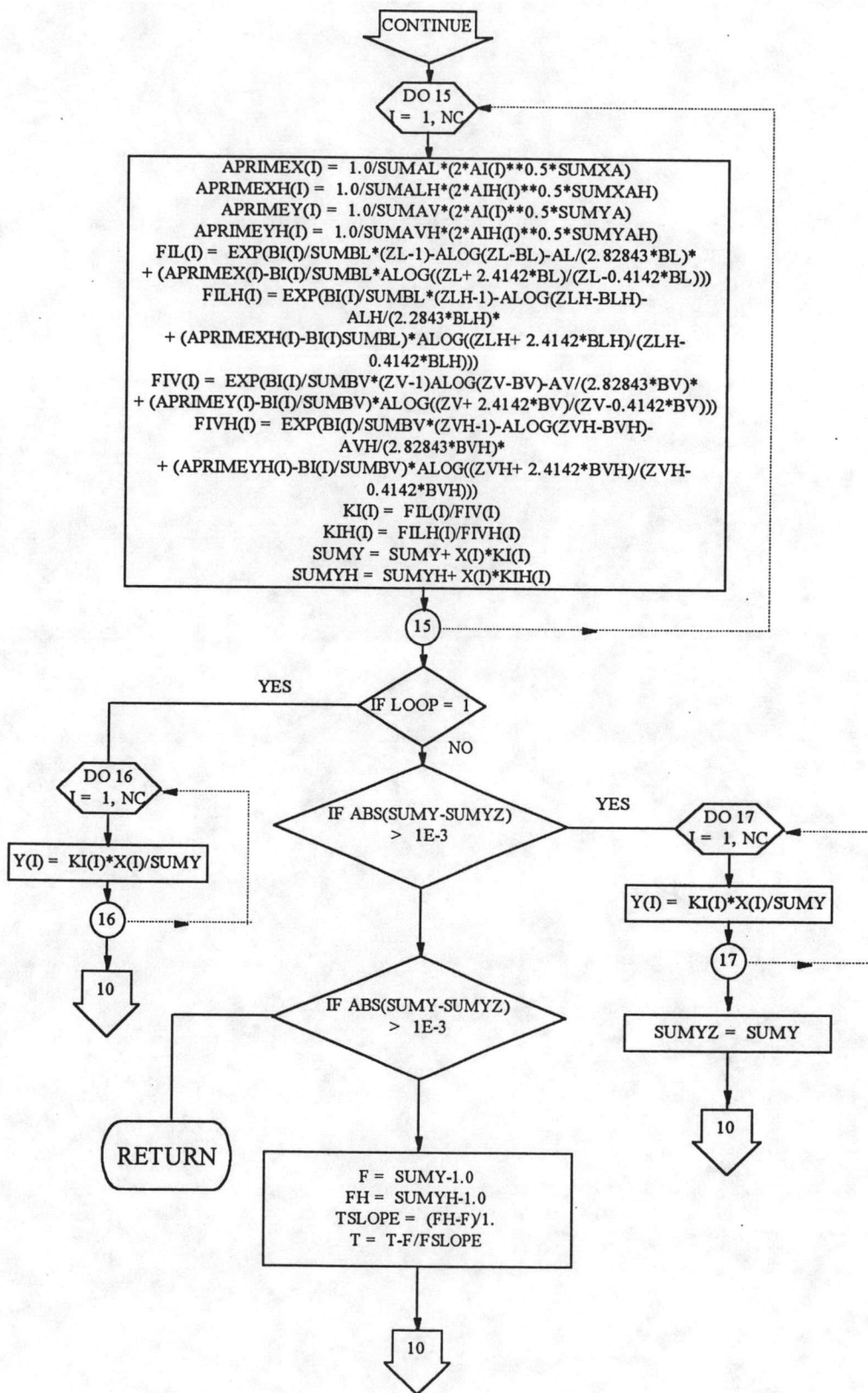
SUBROUTINE BUBPTR



SUBROUTINE BUBTPR (Continue)



SUBROUTINE BUBPTR (Continue)



SUBROUTINE BUBTPR (Continue)

Appendix B

List of computer program

CC Dynamics Simulation Program for Multicomponent Distillation
CC Created by Miss Kallaya Klaithong C 517152
CC Chemical Engineering Department
CC Chulalongkorn University @1994

```
INCLUDE 'FGRAPH.FT'  
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
```

```
CHARACTER*15 NAME,NAMEX,name1
```

```
CHARACTER str*2
```

```
COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),  
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),  
+a5(20)
```

```
DIMENSION LV(50),L(50),P(50),XF(20),YF(20),DXD(20),YAV(20),  
+YY(20),HL(50),HV(50),V(50),DM(50),DXM(50,20),XM(50,20),DXB(20)
```

```
DIMENSION NAME(20),T(50),XB(20),X(50,20),Y(50,20),LO(50),XD(20),  
+YB(20),YD(20),XX(20),MV(50),M(50)
```

```
INTEGER*2 dummy2, key
EXTERNAL printmenu
RECORD / rccoord / curpos
```

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

```
CC
CC
CC
```

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

```
dummy2 = settextrcolor( 14 )
CALL settextrposition( 11, 27, curpos )
CALL outtext( 'Dynamics Simulation Program' )
CALL settextrposition(13, 38, curpos )
CALL outtext( 'for' )
CALL settextrposition(15, 27, curpos )
CALL outtext( 'Multicomponent Distillation' )
```

```
dummy2 = settextrcolor( 15 )
CALL settextrposition(21, 35, curpos )
CALL outtext( 'Created by' )
CALL settextrposition( 22, 24, curpos )
CALL outtext( 'Miss Kallaya Klaithong C 517152' )
CALL settextrposition( 23, 32, curpos )
CALL outtext( 'M.Eng. Thesis @ 1994' )
```

```
READ (*,*)
```

```
CALL clearscreen( $VIEWPORT )
```

```
CC
```

```
CC 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    DO WHILE ( key .EQ. 9 )
CC    GOTO 9900
CC    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 settxtposition( 24, 5, curpos )
      CALL outtext( 'Component not exist !! ... Press ENTER' )
      READ(*,*)
      CALL drawlines()
      CALL drawlines1()
      dummy2 = settxtcolor( 14 )
      CALL settxtposition( 4, 27, curpos )
      CALL outtext( '*** Component Selection ***' )
      dummy2 = settxtcolor( 15 )
      CALL settxtposition( 5, 20, curpos )
      CALL outtext( 'The name must be typed in CAPITAL LETTER' )
      dummy2 = settxtcolor( 14 )
      CALL settxtposition( 9, 18, curpos )
      WRITE( str, '(I2)' ) NC
      CALL outtext( ' Total number of component ( NC ) = '// str )
      GOTO 2220

9130 CONTINUE
      CALL settxtposition( 24, 5, curpos )
      CALL outtext( 'Press ENTER to continue ...' )
      READ(*,*)

2095 kk2 = 0
      CALL drawlines()
      CALL drawlines3()
      dummy2 = settxtcolor( 14 )
      CALL settxtposition( 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 = settextrcolor( 15 )
      CALL settextrposition( 4, 23, curpos )
      CALL outtext( '**** Characteristic of Column ****' )
2000 dummy2 = settextrcolor( 14 )
      CALL settextrposition( 8, 14, curpos )
      CALL outtext( 'Total number of plates (NT) = ' )
      READ(*,*) NT
      CALL settextrposition( 10, 14, curpos )
      CALL outtext( 'Number of trays in stripping section (NF) = ' )
      READ(*,*) NF
      CALL settextrposition( 11, 14, curpos )
      CALL outtext( 'Weir height in stripping section (WHS) = ' )
      READ(*,*) WHS
      CALL settextrposition( 12, 14, curpos )
      CALL outtext( 'Weir height in rectifying section (WHR) = ' )
      READ(*,*) WHR
      CALL settextrposition( 13, 14, curpos )
      CALL outtext( 'Column diameter in stripping section (DS) = ' )
      READ(*,*) DS
      CALL settextrposition( 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( '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 = settextrcolor( 14 )
CALL settextrposition( 8, 14, curpos )
CALL outtext( 'Liquid Feed flow rate (moles/hr) = ' )
READ(*,*) FL
CALL settextrposition( 9, 14, curpos )
CALL outtext( 'Liquid Feed temperature (F) = ' )
READ(*,*) TFL
CALL settextrposition( 11, 14, curpos )
CALL outtext( 'Composition (mole fraction) : ' )
DO 310 J = 1,NC
CALL settextrposition( 11+J, 17, curpos )
namex = name(j)
CALL outtext( namex // ' = ' )
READ(*,*) XF(J)
310 CONTINUE
CALL drawlines()
CALL drawlines2()
dummy2 = settextrcolor( 15 )
CALL settextrposition( 4, 29, curpos )
CALL outtext( '**** Feed Data ****' )
dummy2 = settextrcolor( 14 )
CALL settextrposition( 8, 14, curpos )
CALL outtext( 'Vapor Feed flow rate (moles/hr) = ' )
READ(*,*) FV
CALL settextrposition( 9, 14, curpos )
CALL outtext( 'Vapor Feed temperature (F) = ' )
READ(*,*) TFV
CALL settextrposition( 11, 14, curpos )
CALL outtext( 'Composition (mole fraction) : ' )
DO 320 J = 1,NC
CALL settextrposition( 11+J, 17, curpos )
namex = name(j)
CALL outtext( namex // ' = ' )
READ(*,*) YF(J)
```

```
320 CONTINUE
CC    CALL ENTHS(TFL,P(NF),XF,YF,HLF,HVF)
      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 = settextrcolor( 15 )
CALL settextrposition( 4, 25, curpos )
CALL outtext( '**** Initial Conditions ****' )
dummy2 = settextrcolor( 14 )
WRITE( str, '(I2)' ) N
CALL settextrposition( 8, 14, curpos )
CALL outtext( 'Temperature in tray no.//str// (F) = ' )
READ(*,*) T(N)
CALL settextrposition( 9, 14, curpos )
CALL outtext( 'Liquid flow rate in tray no.//str// (moles/hr) =
+ ' )
READ(*,*) LO(N)
DO 520 J = 1,NC
CALL settextrposition( 10, 14, curpos )
CALL outtext( 'Composition in tray no.//str// :' )
CALL settextrposition( 11+J, 17, curpos )
namex = name(j)
CALL outtext( namex // ' = ' )
READ(*,*) X(N,J)
520 CONTINUE
BLANK=0.
CALL settextrposition( 24, 5, curpos )
CALL outtext( 'Press ENTER to continue ...' )
READ(*,*)
15 CONTINUE
CALL drawlines()
CALL drawlines2()
dummy2 = settextrcolor( 15 )
CALL settextrposition( 4, 25, curpos )
CALL outtext( '**** Initial Conditions ****' )
dummy2 = settextrcolor( 14 )
CALL settextrposition( 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(3,9640) 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)
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(4,9640) 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 SRK MODEL

CC

CC key = 8.1

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 ENTHS(TFL,P(NF),XF,YF,HLF,HVF)

CC

CC CALL INTTIAL HOLDUPS

CC

CALL MWDENSS(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 MWDENSS(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 MWDENSS(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 MWDENSS(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 Main Loop for each time step

CC

xxx=0

100 CONTINUE

write(*,*) xxx

CALL BUBPTS (TB,XB,YB,PB)

CALL ENTHS (TB,PB,XB,YB,HLB,HVB)

DO 105 J=1,NC

105 XX(J)=X(1,J)

CALL BUBPTS (T(1),XX,YY,P(1))

DO 106 J=1,NC

Y(1,J)=YB(J)+EFF*(YY(J)-YB(J))

106 YY(J)=Y(1,J)

CALL ENTHS(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 BUBPTS(T(N),XX,YY,P(N))

DO 112 J = 1,NC

```

      Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
112 YY(J)=Y(N,J)
      CALL ENTHS(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 BUBPTS(T(NF+1),XX,YY,P(NF+1))
      DO 114 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)
114 YY(J)=Y(NF+1,J)
      CALL ENTHS(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
116 XX(J)=X(N,J)
      CALL BUBPTS(T(N),XX,YY,P(N))
      DO 117 J=1,NC
      Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
117 YY(J)=Y(N,J)
      CALL ENTHS (T(N),P(N),XX,YY,HL(N),HV(N))
115 CONTINUE
      CALL BUBPTS (TD,XD,YD,PD)
      CALL ENTHS(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
CC   IF (B .LT. 0.) THEN
CC   WRITE(*,*) ' ***** B IS LESS THAN 0 *****'
CC   STOP

```

```

CC      END IF

      V(1)=(HL(2)*L(2)+HVB*VB-HL(1)*L(1))/HV(1)
      DO 120 N=2,NF-1
      V(N)=(HL(N+1)*L(N+1)+HV(N-1)*V(N-1)-HL(N)*L(N))/HV(N)
120 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      IF (DL .LT. 0) THEN
CC      WRITE(*,*) ' ***** DL IS LESS THAN 0 *****'
CC      STOP
CC      END IF

CC
CC      EVALUATE DERIVATIVES
CC

      DM(1)=L(2)+VB-V(1)-L(1)
      DO 140 N=2,NF-1
140 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 150 N=NF+2,NT-1
150 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)=(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 165 N=2,NF-1

```



```

165 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 170 N=NF+2,NT-1
170 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
160 CONTINUE
IF (TIME .GT. 4e-2) GOTO 9000
IF (TIME .LT. TPRINT) GOTO 210

CALL drawlines()
WRITE(5,201)
201 FORMAT (5X,'TIME T X1 X2 X3 X4
+ X5 L')
WRITE(5,202) TIME,TB,(XB(J),J=1,NC),B
202 FORMAT (1X,F5.4,3X,F7.2,8F14.6,F10.1)
DO 203 N=1,NT
203 WRITE(5,204) N,T(N),(X(N,J),J=1,NC),L(N)
204 FORMAT (3X,I3,3X,F7.2,8F14.6,F10.1)
WRITE(5,205) TD,(XD(J),J=1,NC),R
205 FORMAT (9X,F7.2,8F14.6,F10.1)
WRITE(5,206) (YD(J),J=1,NC),DL
206 FORMAT(16X,8F14.6,F10.1)
TPRINT = TPRINT + .001
cc CALL settextposition( 24, 5, curpos )
cc CALL outtext( 'Press ENTER to continue ...' )
cc READ(*,*)

CC
CC INTEGRATION ALA EULER
CC

```



```

210 TIME = TIME + DELTA
cc WRITE(*,*) TIME
cc READ(*,*)

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 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
225 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 HYDRAUS(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 HYDRAUS(P(N),M(N),T(N),XX,L(N),WHR,WLR,DR)
```

```
273 CONTINUE
```

```
xxx=xxx+1.0
```

```
GOTO 100
```

```
400 STOP
```

```
END
```

```
CC
```

```
CC Calculate Liquid tray holdup by Francis Wier equation
```

```
CC
```

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

```
REAL M,L,MW,MWA
```

```
COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),  
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),  
+a5(20)
```

```
DIMENSION X(20)
```

```
CALL MWDENSS(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 ENTHSalpy calculation
```

```
CC
```

```
SUBROUTINE ENTHS(T,P,X,Y,HL,HV)
```

REAL GC,MI

COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)

DIMENSION X(20),Y(20),TR(20),MI(20),ALPHA(20),ACI(20),AI(20),
+BI(20),HLS(20)

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))**.5*(1-KIJ)
SUMAV = SUMAV+Y(I)*Y(J)*(AI(I)*AI(J))**.5*(1-KIJ)
SUMATL = SUMATL+X(I)*X(J)*MI(J)*(AI(I)*ACI(J)*TR(J))**.5*(1-KIJ)
SUMATV = SUMATV+Y(I)*Y(J)*MI(J)*(AI(I)*ACI(J)*TR(J))**.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 NEWTONS(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 NEWTONS(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 NEWTONS's technique

CC

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

DIMENSION Z(3)

ZO1 = -10

L = 1

10 IF (L .GT. 8000) 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. 8000) 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. 8000 ) 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 MWDENSS(X,T,P,MWA,DENSA)
```

```
COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)
```

```
DIMENSION X(20),TR(20),MI(20),ALPHA(20),ACI(20),AI(20),BI(20)
```

```
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 NEWTONS(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 BUBPTS(T,X,Y,P)

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

COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)

DIMENSION X(20),Y(20),TR(20),MI(20),ALPHA(20),ACI(20),
+AI(20),BI(20),FIL(20),FIV(20),KI(20),APRIMEX(20),APRIMEY(20)

DIMENSION FILH(20),FIVH(20),APRIMEXH(20),APRIMEYH(20),KIH(20),
```


+ALPHAH(20),AIH(20),TRH(20)

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) = 1.

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. 8000) 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 NEWTONS(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 NEWTONS(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 NEWTONS(AV,BV,Z1,Z2,Z3)
ZV = Z3
CALL NEWTONS(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

```

```
1000 WRITE(*,*) ' ***** Converged !!'  
    read(*,*)  
    WRITE(*,*) '      TEMP      SUMY      LOOP '  
    WRITE(*,*)  
    WRITE(*,*) T, SUMY, LOOP  
    READ(*,*)  
    WRITE(*,*)  
    WRITE(*,*) '   yi      ki'  
    write(*,*)  
    DO 1010 I = 1,NC  
    WRITE(*,*) Y(I),KI(I)  
    READ(*,*)  
1010 CONTINUE  
    stop
```

```
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      Data Menu
```

```
CC
```

```
SUBROUTINE datamenu(dat)
```

```
INCLUDE 'FGRAPH.FD'
```

```
RECORD / rccoord / curpos
```

```
100 key2 = -1
```

```
DO WHILE ((key2 .LT. 0) .OR. (key2 .GT. 4))
```

```
CALL drawlines()
```

```
CALL drawlines1()
```

```
dummy2 = settextcolor( 14 )
```

```
CALL settextposition( 4, 30, curpos )
```

```
CALL outtext( '**** Data Menu ****' )
```

```
dummy2 = settextcolor( 15 )
```

```
CALL settextposition( 10, 25, curpos )
```

```
CALL outtext( '0) Return to Main Menu' )
```

```
CALL settextposition( 12, 25, curpos )
```

```
CALL outtext( '1) New Data' )
```

```
CALL settextposition( 14, 25, curpos )
```

```
CALL outtext( '2) Old Data' )
CALL settextposition( 16, 25, curpos )
CALL outtext( '3) Save Data' )
dummy2 = settextcolor( 14 )
CALL settextposition( 22, 25, curpos )
CALL outtext( 'Please ENTER your selection : ' )
READ(*,*,ERR = 100) key2
dat = key2
END DO
dummy2 = setvideomode( $DEFAULTMODE )
```

```
DO WHILE (key2 .EQ. 0)
    RETURN
END DO
```

```
DO WHILE (key2 .EQ. 1)
    RETURN
END DO
```

```
DO WHILE (key2 .EQ. 2)
    CALL old()
    RETURN
END DO
```

```
DO WHILE (key2 .EQ. 3)
    CALL save()
    RETURN
END DO
```

```
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
```

CC RUN GRK MODEL

CC

CC key = 8.2

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 ENTHGR(TFL,P(NF),XF,YF,HLF,HVF)

CC

CC CALL INTTIAL HOLDUPS

CC

CALL MWDENSG(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 MWDENSG(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 MWDENSG(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 MWDENSG(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   Main Loop for each time step
CC
```

```
xxx=0
```

```
100 CONTINUE
```

```
write(*,*) xxx
```

```
CALL BUBPTGR (TB, XB, YB, PB)
```

```
CALL ENTHGR (TB, PB, XB, YB, HLB, HVB)
```

```
DO 105 J=1, NC
```

```
105 XX(J)=X(1,J)
```

```
CALL BUBPTGR (T(1), XX, YY, P(1))
```

```
DO 106 J=1, NC
```

```
Y(1,J)=YB(J)+EFF*(YY(J)-YB(J))
```

```
106 YY(J)=Y(1,J)
```

```
CALL ENTHGR (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 BUBPTGR (T(N), XX, YY, P(N))
```

```
DO 112 J = 1, NC
```

```
Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
```

```
112 YY(J)=Y(N,J)
```

```
CALL ENTHGR(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 BUBPTGR(T(NF+1),XX,YY,P(NF+1))
      DO 114 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)
114 YY(J)=Y(NF+1,J)
      CALL ENTHGR(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
116 XX(J)=X(N,J)
      CALL BUBPTGR(T(N),XX,YY,P(N))
      DO 117 J=1,NC
      Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
117 YY(J)=Y(N,J)
      CALL ENTHGR (T(N),P(N),XX,YY,HL(N),HV(N))
115 CONTINUE
      CALL BUBPTGR (TD,XD,YD,PD)
      CALL ENTHGR(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
CC   IF (B .LT. 0.) THEN
CC   WRITE(*,*) '***** B IS LESS THAN 0 *****'
CC   STOP
CC   END IF

      V(1)=(HL(2)*L(2)+HVB*VB-HL(1)*L(1))/HV(1)
      DO 120 N=2,NF-1

```




```
V(N)=(HL(N+1)*L(N+1)+HV(N-1)*V(N-1)-HL(N)*L(N))/HV(N)
120 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 IF (DL .LT. 0) THEN
CC WRITE(*,*) '***** DL IS LESS THAN 0 *****'
CC STOP
CC END IF

CC
CC EVALUATE DERIVATIVES
CC

DM(1)=L(2)+VB-V(1)-L(1)
DO 140 N=2,NF-1
140 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 150 N=NF+2,NT-1
150 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)=(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 165 N=2,NF-1
165 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 170 N=NF+2,NT-1
170 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
160 CONTINUE
IF (TIME .GT. 3e-2) GOTO 9000
IF (TIME .LT. TPRINT) GOTO 210

CALL drawlines()
WRITE(5,201)
201 FORMAT (5X,'TIME   T   X1   X2   X3   X4
+   X5   L')
WRITE(5,202) TIME,TB,(XB(J),J=1,NC),B
202 FORMAT (1X,F5.4,3X,F7.2,8F14.6,F10.1)
DO 203 N=1,NT
203 WRITE(5,204) N,T(N),(X(N,J),J=1,NC),L(N)
204 FORMAT (3X,I3,3X,F7.2,8F14.6,F10.1)
WRITE(5,205) TD,(XD(J),J=1,NC),R
205 FORMAT (9X,F7.2,8F14.6,F10.1)
WRITE(5,206) (YD(J),J=1,NC),DL
206 FORMAT(16X,8F14.6,F10.1)
TPRINT = TPRINT + .001
cc CALL settxtposition( 24, 5, curpos )
cc CALL outtext( 'Press ENTER to continue ...' )
cc READ(*,*)

CC
CC   INTEGRATION ALA EULER
CC

210 TIME = TIME + DELTA
cc WRITE(*,*) TIME
cc READ(*,*)

```

```
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 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
225 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+1.0
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(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)

DIMENSION X(20)

CALL MWDENSG(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 ENTHGR(T,P,X,Y,HL,HV)

REAL GC,MI

COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),

+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)

DIMENSION X(20),Y(20),TR(20),MI(20),ALPHA(20),ACI(20),AI(20),
+BI(20),HLS(20)

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)

ACI(J) = (0.4278/(TR(J)**2.5*PC(J)))**0.5

AI(J) = ACI(J)

BI(J) = 0.0867/TR(J)/PC(J)

SUMBL = SUMBL + X(J)*BI(J)

SUMBV = SUMBV + Y(J)*BI(J)

SUMAL = SUMAL + X(J)*AI(J)

SUMAV = SUMAV + Y(J)*AI(J)

1 CONTINUE


```

AL = SUMAL
AV = SUMAV
BL = SUMBL
BV = SUMBV
CALL NEWTON(AL,BL,P,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,P,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-1-1.5*AL**2/BL*ALOG(1+BL*P/ZL))*GC*T+HLS1
HV = (ZV-1-1.5*AV**2/BV*ALOG(1+BV*P/ZV))*GC*T+HVS
RETURN
END

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

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

```

```
DIMENSION Z(3)

ZO1 = -10
L = 1
10 IF ( L .GT. 8000 ) THEN
    WRITE(*,*) ' ***** NOT CONVERGE !! *****'
    STOP
END IF
FZ1 = ZO1**3-ZO1**2+B*P*(A**2/B-B*P-1)*ZO1-A**2/B*(B*P)**2
DFZ1 = 3*ZO1**2-2*ZO1+B*P*(A**2/B-B*P-1)
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. 8000 ) THEN
    WRITE(*,*) ' ***** NOT CONVERGE !! *****'
    STOP
END IF
FZ2 = ZO2**3-ZO2**2+B*P*(A**2/B-B*P-1)*ZO2-A**2/B*(B*P)**2
DFZ2 = 3*ZO2**2-2*ZO2+B*P*(A**2/B-B*P-1)
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. 8000 ) THEN
        WRITE(*,*) ' ***** NOT CONVERGE !! *****'
        STOP
    END IF
    FZ3 = ZO3**3-ZO3**2+B*P*(A**2/B-B*P-1)*ZO3-A**2/B*(B*P)**2
    DFZ3 = 3*ZO3**2-2*ZO3+B*P*(A**2/B-B*P-1)
    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
            END DO
        END DO
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 MWDENSG(X,T,P,MWA,DENSA)

COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)

DIMENSION X(20),TR(20),MI(20),ALPHA(20),ACI(20),AI(20),BI(20)

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)
ACI(J) = (0.42748/(TR(J)**2.5*PC(J)))**0.5
AI(J) = ACI(J)
BI(J) = 0.0867/TR(J)/PC(J)
SUMBL = SUMBL + X(J)*BI(J)
SUMAL = SUMAL + X(J)*AI(J)
1 CONTINUE
```

```
AL = SUMAL
BL = SUMBL
```

```
CALL NEWTON(AL,BL,P,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 BUBPTGR(T,X,Y,P)

REAL GC,MI,KI,KIH,FSLOPE,F,y

COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
 +BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
 +a5(20)

DIMENSION X(20),Y(20),TR(20),MI(20),ALPHA(20),ACI(20),
 +AI(20),BI(20),BIH(20),FIL(20),FIV(20),KI(20)

DIMENSION FILH(20),FIVH(20),APRIMEXH(20),APRIMEYH(20),KIH(20),
 +ALPHAH(20),AIH(20),TRH(20)

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) = 1.

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
 SUMBLH = 0.0
 SUMBVH = 0.0

TH = T+1.0

IF(LOOP .GT. 8000),GOTO 30

SUMY=0.0

SUMYH = 0.0

DO 1 J=1,NC

TR(J) = T/TC(J)

TRH(J) = TH/TC(J)

ACI(J) = (0.4278/(TR(J)**2.5*PC(J)))**0.5

AI(J) = ACI(J)

AIH(J) = (0.4278/(TRH(J)**2.5*PC(J)))**0.5

BI(J) = 0.0867/TR(J)/PC(J)

BIH(J) = 0.0867/TRH(J)/PC(J)

SUMBL = SUMBL + X(J)*BI(J)

SUMBV = SUMBV + Y(J)*BI(J)

SUMBLH = SUMBLH + X(J)*BIH(J)

SUMBVH = SUMBVH + Y(J)*BIH(J)

SUMAL = SUMAL + X(J)*AI(J)

SUMAV = SUMAV + Y(J)*AI(J)

SUMALH = SUMALH + X(J)*AIH(J)

SUMAVH = SUMAVH + Y(J)*AIH(J)

1 CONTINUE

```
AL = SUMAL
ALH = SUMALH
AV = SUMAV
AVH = SUMAVH
BL = SUMBL
BLH = SUMBLH
BV = SUMBV
BVH = SUMBLH

CALL NEWTON(AL,BL,P,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,P,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,P,Z1,Z2,Z3)
ZV = Z3

CALL NEWTON(AVH,BVH,P,Z1,Z2,Z3)
ZVH = Z3
```

```
DO 15 I=1,NC
```

```
FIL(I) = EXP((ZL-1)*BI(I)/BL-ALOG(ZL-BL*P)-AL**2/BL*  
+(2*AI(I)/AL-BI(I)/BL)*ALOG(1+BL*P/ZL))
```

```
FILH(I) = EXP((ZLH-1)*BIH(I)/BLH-ALOG(ZLH-BLH*P)-ALH**2/BLH*  
+(2*AIH(I)/ALH-BIH(I)/BLH)*ALOG(1+BLH*P/ZLH))
```

```
FIV(I) = EXP((ZV-1)*BI(I)/BV-ALOG(ZV-BV*P)-AV**2/BV*  
+(2*AI(I)/AV-BI(I)/BV)*ALOG(1+BV*P/ZV))
```

```
FIVH(I) = EXP((ZVH-1)*BIH(I)/BVH-ALOG(ZVH-BVH*P)-AVH**2/BVH*  
+(2*AIH(I)/AVH-BIH(I)/BVH)*ALOG(1+BVH*P/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
```

```
1000 WRITE(*,*) ' ***** Converged !!'
```

```
read(*,*)
```

```
WRITE(*,*) '      TEMP      SUMY      LOOP '
```

```
WRITE(*,*)
```

```
WRITE(*,*) T, SUMY, LOOP
```

```
READ(*,*)
```

```
WRITE(*,*)
```

```
WRITE(*,*) '   yi           ki'
```

```
write(*,*)
```

```
DO 1010 I = 1,NC
```

```
WRITE(*,*) Y(I),KI(I)
```

```
READ(*,*)
```

```
1010 CONTINUE
```

```
stop
```

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

```
STOP
```

```
END
```




CC RUN PR MODEL

CC

CC key = 8.3

CC

CC

CC Assign temperature in Degree Rangin

CC

9800 TFL = TFL + 460.

TFV = TFV + 460.

TB = TB + 460.

TD = TD + 460.+115.0

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 ENTHPR(TFL,P(NF),XF,YF,HLF,HVF)

CC

CC CALL INTITIAL HOLDUPS

CC

```
CALL MWDENSPR(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 MWDENSPR(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 MWDENSPR(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 MWDENSPR(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   Main Loop for each time step
CC
```

```
xxx=0
```

```
100 CONTINUE
```

```
write(*,*) xxx
```

```
CALL BUBTPR (TB, XB, YB, PB)
```

```
CALL ENTHPR (TB, PB, XB, YB, HLB, HVB)
```

```
DO 105 J=1, NC
```

```
105 XX(J)=X(1,J)
```

```
CALL BUBTPR (T(1), XX, YY, P(1))
```

```
DO 106 J=1, NC
```

```
Y(1,J)=YB(J)+EFF*(YY(J)-YB(J))
```

```
106 YY(J)=Y(1,J)
```

```
CALL ENTHPR(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 BUBTPR(T(N), XX, YY, P(N))
```

```
DO 112 J = 1, NC
```

```
Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
```

```
112 YY(J)=Y(N,J)
```

```
CALL ENTHPR(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 BUBTPR(T(NF+1),XX,YY,P(NF+1))
    DO 114 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)
114 YY(J)=Y(NF+1,J)
    CALL ENTHPR(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
116 XX(J)=X(N,J)
    CALL BUBTPR(T(N),XX,YY,P(N))
    DO 117 J=1,NC
    Y(N,J)=(YY(J)-Y(N-1,J))*EFF+Y(N-1,J)
117 YY(J)=Y(N,J)
    CALL ENTHPR (T(N),P(N),XX,YY,HL(N),HV(N))
115 CONTINUE
    CALL BUBTPR (TD,XD,YD,PD)
    CALL ENTHPR(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
CC    IF (B .LT. 0.) THEN
CC    WRITE(*,*) ' ***** B IS LESS THAN 0 *****'
CC    STOP
CC    END IF

V(1)=(HL(2)*L(2)+HVB*VB-HL(1)*L(1))/HV(1)
DO 120 N=2,NF-1

```

```

V(N)=(HL(N+1)*L(N+1)+HV(N-1)*V(N-1)-HL(N)*L(N))/HV(N)
120 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 IF (DL .LT. 0) THEN
CC WRITE(*,*) '***** DL IS LESS THAN 0 *****'
CC STOP
CC END IF

CC
CC EVALUATE DERIVATIVES
CC

DM(1)=L(2)+VB-V(1)-L(1)
DO 140 N=2,NF-1
140 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 150 N=NF+2,NT-1
150 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)=(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 165 N=2,NF-1
165 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 170 N=NF+2,NT-1
170 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
160 CONTINUE
IF (TIME .GT. 4e-2) GOTO 9000
IF (TIME .LT. TPRINT) GOTO 210

CALL drawlines()
WRITE(5,201)
201 FORMAT (5X,'TIME T X1 X2 X3 X4
+ X5 L')
WRITE(5,202) TIME,TB,(XB(J),J=1,NC),B
202 FORMAT (1X,F5.4,3X,F7.2,8F14.6,F10.1)
DO 203 N=1,NT
203 WRITE(5,204) N,T(N),(X(N,J),J=1,NC),L(N)
204 FORMAT (3X,I3,3X,F7.2,8F14.6,F10.1)
WRITE(5,205) TD,(XD(J),J=1,NC),R
205 FORMAT (9X,F7.2,8F14.6,F10.1)
WRITE(5,206) (YD(J),J=1,NC),DL
206 FORMAT(16X,8F14.6,F10.1)
TPRINT = TPRINT + .001
cc CALL settextposition( 24, 5, curpos )
cc CALL outtext( 'Press ENTER to continue ...' )
cc READ(*,*)

CC
CC INTEGRATION ALA EULER
CC

210 TIME = TIME + DELTA
cc WRITE(*,*) TIME
cc READ(*,*)

```

```
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 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
225 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+1.0
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(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)

DIMENSION X(20)

CALL MWDENSPR(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 ENTHPR(T,P,X,Y,HL,HV)

REAL GC,MI

COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),

```
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)
```

```
DIMENSION X(20),Y(20),TR(20),MI(20),ALPHA(20),ACI(20),AI(20),
+BI(20),HLS(20)
```

```
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
```

```
SUMPL = 0.0
```

```
SUMPV = 0.0
```

```
DO 1 J=1,NC
```

```
TR(J) = T/TC(J)
```

```
MI(J) = 0.37464+1.54226*W(J)-0.26992*W(J)**2
```

```
ALPHA(J) = (1.0+MI(J)*(1-TR(J)**(0.5)))**2
```

```
ACI(J) = 0.45724*(GC*TC(J))**2/PC(J)
```

```
AI(J) = ALPHA(J)*ACI(J)
```

```
BI(J) = 0.07780*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)

SUMPL = SUMPL+X(I)*X(J)*MI(J)*(ACI(I)*ACI(J)*TR(J))**0.5*(1-KIJ)

SUMPV = SUMPV+Y(I)*Y(J)*MI(J)*(ACI(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

$$HL = (ZL-1-AL/(2.8284*BL))*(1-SUMPL/SUMAL)*ALOG((ZL+2.4142*BL)/$$

$$+(ZL-0.4142*BL))*GC*T+HLS1$$

$$HV = (ZV-1-AV/(2.8284*BV))*(1-SUMPV/SUMAV)*ALOG((ZV+2.4142*BV)/$$

$$+(ZV-0.4142*BV))*GC*T+HVS$$

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. 8000) 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. 8000 ) 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. 8000 ) 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 MWDENSPR(X,T,P,MWA,DENSA)

      COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),
+BV(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),
+a5(20)

      DIMENSION X(20),TR(20),MI(20),ALPHA(20),ACI(20),AI(20),BI(20)
```

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) = 0.37464+1.54226*W(J)-0.26992*W(J)**2

ALPHA(J) = (1.0+MI(J)*(1-TR(J)**(0.5)))**2

ACI(J) = 0.45724*(GC*TC(J))**2/PC(J)

AI(J) = ALPHA(J)*ACI(J)

BI(J) = 0.07780*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 BUBTPR(T,X,Y,P)
```

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

```
COMMON NC,MW(20),DENS(20),C1(20),C2(20),C3(20),BPT(20),AVP(20),  
+BVP(20),tc(20),pc(20),zc(20),w(20),a1(20),a2(20),a3(20),a4(20),  
+a5(20)
```

```
DIMENSION X(20),Y(20),TR(20),MI(20),ALPHA(20),ACI(20),  
+AI(20),BI(20),FIL(20),FIV(20),KI(20),APRIMEX(20),APRIMEY(20)
```



```
DIMENSION FILH(20),FIVH(20),APRIMEXH(20),APRIMEYH(20),KIH(20),  
+ALPHAH(20),AIH(20),TRH(20)
```

```
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) = 1.
```

```
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. 8000) 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) = 0.37464+1.54226*W(J)-0.26992*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) = 0.45724*(GC*TC(J))**2/PC(J)
AI(J) = ALPHA(J)*ACI(J)
AIH(J) = ALPHAH(J)*ACI(J)
BI(J) = 0.07780*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/(2.82843*BL))*
+(APRIMEX(I)-BI(I)/SUMBL)*ALOG((ZL+2.4142*BL)/(ZL-0.4142*BL)))
FILH(I) = EXP(BI(I)/SUMBL*(ZLH-1)-ALOG(ZLH-BLH)-ALH/(2.82843*BLH))*
+(APRIMEXH(I)-BI(I)/SUMBL)*ALOG((ZLH+2.4142*BLH)/(ZLH-0.4142*BLH)))
FIV(I) = EXP(BI(I)/SUMBV*(ZV-1)-ALOG(ZV-BV)-AV/(2.82843*BV))*
+(APRIMEY(I)-BI(I)/SUMBV)*ALOG((ZV+2.4142*BV)/(ZV-0.4142*BV)))
FIVH(I) = EXP(BI(I)/SUMBV*(ZVH-1)-ALOG(ZVH-BVH)-AVH/(2.82843*BVH))*
+(APRIMEYH(I)-BI(I)/SUMBV)*ALOG((ZVH+2.4142*BVH)/(ZVH-0.4142*BVH)))
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

1000 WRITE(*,*) ' ***** Converged !!'
      read(*,*)
      WRITE(*,*) '      TEMP      SUMY      LOOP '
      WRITE(*,*)
      WRITE(*,*) T, SUMY, LOOP
      READ(*,*)
      WRITE(*,*)
      WRITE(*,*) '      yi      ki'
      write(*,*)
      DO 1010 I = 1,NC
      WRITE(*,*) Y(I),KI(I)
      READ(*,*)
1010 CONTINUE

      stop

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




VITA

Miss Kallaya Klaithong graduated high school from Benchama Ratrungrarit school in 1986 and received Bachelor Degree in Chemical Engineering from the Department of Chemical Technology, Faculty of Science, Chulalongkorn University in 1990. After then she 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.

She also has an experience in working as process engineer at The Bangchak Petroleum Public Company Limited in 1990 until the present.