MATHEMATICAL MODELING OF TURBULENT REACTING PLUMES

PART II: Computer Code Implementation

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TRPM - Computer Code

Demonstration Version - Release -1.1

A.R.B. Contract No. A0-044-32

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California Institute of Technology

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"Continued Development

of a Mathematical Modeling Capability

in Photochemical Air Pollution:

Reacting Plumes"

Disclaimer

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COMMENTS
on the Demonstration Version -1.1
of the TRPM Computer Code

The Turbulent Reacting Plume Model (TRPM) offers a general, versatile, description of atmospheric plume processes, that is highly modular in nature, allowing for the use of different levels of approximation of the phenomena involved (see Figure 1). This structural modularity is directly reflected in the practical implementation of the TRPM through computer coding. Thus (as it is explained in length in Part I of the present report) a great variety of alternative choices is possible, including both the character and the details of the numerical scheme that is applied for the solution of the fundamental evolution equations which describe the simultaneous mixing and chemical reaction inside the instantaneous plume (master module), and the complexity and sophistication of the information processed by the complementary and peripheral modules.

Here, rather than putting together a "random" collection of subroutines corresponding to some of the alternative choices of the various modules, we give a code that consists of a representative "serial" combination of single but "most typical" formulations of the various model components. This combination corresponds to the choices adopted for the fundamental version of the model that was tested and verified against experimental data; the particular choices of parameters correspond to the calculations presented in Chapter 3 of Part IA of the present report and the numerical results produced by this code are essentially equivalent to the results presented in the figures of that chapter.

The code presented here is in FORTRAN; to ensure portability the conventions employed in the most standard versions of FORTRAN IV are employed as far as

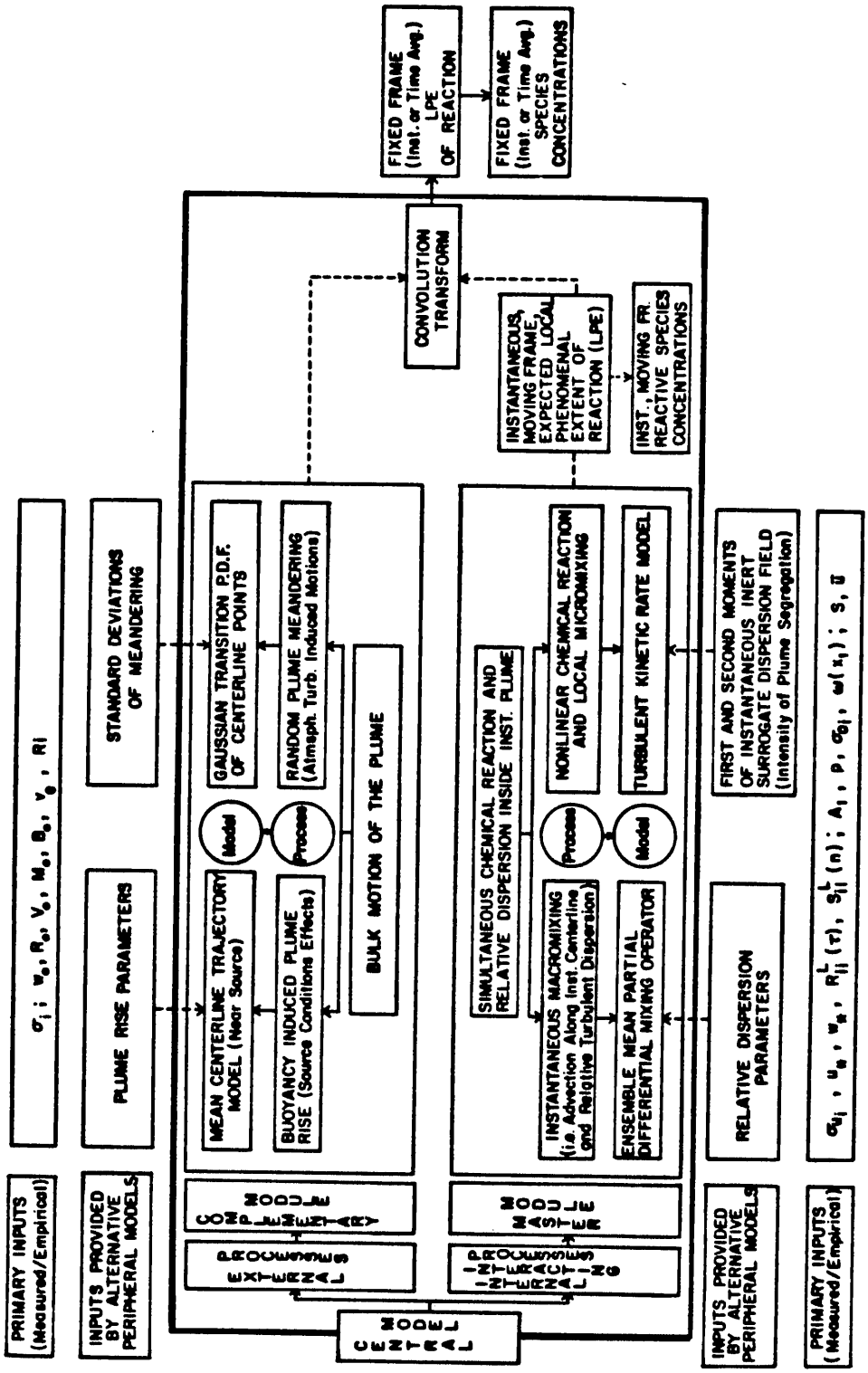

Figure 1

Structure of the TRPM

this is possible. Thus in this particular version there are no statements exclusively corresponding to either FORTRAN 77 or to special compilers. Moreover, in order to make this particular demonstration version readable (as much as this is possible for a computer program), a serial, "logical–order", presentation of all the calculations performed is adopted (instead of a – more flexible – multiple subroutine structure); furthermore extensive comments (including suggestions for allowable modifications of the code) have been added. Special, "immobilized," output routines provide the potential for examining intermediate results of the calculations that do not appear in the final outputs (a kind of a simple in-program debugger); similarly other such routines allow alternative outputs. As far as inputs are concerned, this special demonstration version is "closed," internally providing the parameters corresponding to the calculations of Chapter 3 (Part IA); however direct substitution of other input is completely straightforward (through replacement of the variables definitions statements by corresponding READ statements).

The present demonstration version of the code corresponds to a special situation of a plume with insignificant bulk motions. (Nevertheless both meandering and plume rise can be directly considered a posteriori). Thus the focus is on the "core" of the TRPM (master module). This core consists of the evolution equations for reaction progress variables appropriate for evolving, spatially varying systems ("local phenomenal extent of reaction"). These equations estimate the interaction of mixing and chemical reaction and require input parameters characterizing internal plume behavior, such as relative dispersion and fine scale plume segregation. Relative dispersion parameters are calculated through power law approximations of the form $\sigma_R = ax^b$ where x is the downwind distance and a, b are constants; the intensity of plume segregation is calculated from the "Localized Production of Fluctuations Model" (LPFM); the centerline intensity is estimated on the basis of empirical information.

TRPM DV-1.1

INPUTS

(Internally Defined)

Problem Parameters

Source Properties

QSTR: NO Source Strength (ppm m^3 s^{-1})

CSOUR: NO Source Concentration (ppm)

H: Source Height (m)

([Optional] D: Source Diameter (m))

Ambient Properties

CBO3: Background Ozone Concentration (ppm)

USP: Mean Wind Speed (m s^{-1})

HBL: A.B.L. Height (m)

ASIGY: a_y in $\sigma_{R_y} = a_y x^{b_y}$

BSIGY: b_y in $\sigma_{R_y} = a_y x^{b_y}$

ASIGZ: a_y in $\sigma_{R_z} = a_z x^{b_z}$

BSIGZ: b_z in $\sigma_{R_z} = a_z x^{b_z}$

TRPM DV-1.1

OUTPUTS (STANDARD)

A. LOGICAL UNIT 8

Quantities Downwind along

Plume Centerline

Every Output Line Contains (in order):

KK2: Even Step Counter

TIMOUT: Dispersion Time (s)

XOUT: Downwind Distance (m)

CEM2(8,1): NO_x Centerline Concentration (ppm)

V(8,1): NO_2 Centerline Concentration (ppm)

RAT1: NO/NO_x Concentration Centerline Ratio

RATO3: O_3/O_3^{env} Concentration Centerline Ratio

STHET(8,1): Centerline Square Root Segregation

FACT1: Segregation Self Similarity Factor

B. LOGICAL UNIT 9

Quantities in Cross-Wind Plane

at Source Height

XOUT: Downwind Distance (m)

ZZZ: Distance from the Centerline (m)

CEM2(8,I): NO_x Concentration (ppm)

SVAR(8,I): NO_x Concentration Standard Deviation (ppm)

THET(8,I): Intensity of Segregation

V(8,I): NO_2 Concentration (ppm)

```
      PROGRAM TRPM
C     DEMONSTRATION VERSION
C     RELEASE -1.1
C     (TESTED MARCH 1986)
C
C     ::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
C
C     THIS PROGRAM USES AN ALTERNATING DIRECTION IMPLICIT
C     FINITE DIFFERENCE METHOD
C     TO SOLVE THE CONVECTIVE DIFFUSION EQUATION
C     (FOR TRAVEL TIME T=X/U AND TWO SPACE DIMENSIONS Y,Z)
C     WITH SIMULTANEOUS NONLINEAR NON-TURBULENT OR TURBULENT
C     (DEPENDING ON THE VALUE OF A FLAG PARAMETER)
C     CHEMICAL REACTION
C     (WHICH CREATES A KINETIC TERM THAT IS A FUNCTION OF X,Y,Z)
C
C     THIS APPLICATION CONCERNS THE TURBULENT DIFFUSION
C     OF A NO PLUME IN A O3 RICH ATMOSPHERE
C     WHERE A 2ND ORDER REVERSIBLE REACTION TAKES PLACE
C
C     THE UNKNOWN VARIABLE IS THE LOCAL PHENOMENAL EXTENT OF REACTION
C
C     WE CONSIDER A STEADY "POINT" SOURCE
C
C     IN THIS VERSION
C     THE SOLUTION IS ASSUMED SYMMETRIC WITH RESPECT TO
C     THE Y AXIS AND THUS ONLY THE POSITIVE YOZ HALF-SPACE
C     OF A COORDINATE SYSTEM WITH THE SOURCE ON THE Z-AXIS
C     IS USED IN THE CONSTRUCTION OF THE FINITE DIFFERENCE GRID
C
C     ::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
C
C     PROGRAM SPECIFICATIONS.........................................
C
C     CHEMICAL KINETICS CONSTANTS
      REAL K1,K3
C
C     SPECIFICATIONS AND INITIAL DATA FOR THE A.D.I. FINITE DIFFERENCES
      DIMENSION UVLOD(22,3),UVLEV(22,3),BB(22),UVL1(22,3)
      DIMENSION U(23,23),V(23,23),RHS(23,23),SX(22,22)
      DIMENSION P(22,22),Q(22,22),S(22,22),PX(22,22),QX(22,22)
      DIMENSION CEM2(22,22),YY(22),LMN(22),RAT(22),THET(22,22)
      DIMENSION SVAR(22,22),STHET(22,22)
C
      DOUBLE PRECISION UVLOD,UVLEV,BB,RHS,U,V,P,Q,S,CEM,C2,CEM2,UVL1
      DOUBLE PRECISION THETA,THET,CVAR,PX,QX,SX
      DOUBLE PRECISION  RY ,RZ,RY1,RZ1,RY2,RZ2,RY3,RZ3,RYZ,RZY
C
      DATA U,V/1058*0.0/
      DATA UVLOD/66*-1.0/
      DATA UVLEV/66*-1.0/
      DATA DY,DZ,DT,TSTART,TMAX/0.020,0.020,0.0125,0.0350,13.00/
      DATA ASIGY,BSIGY/0.072,0.907/
      DATA ASIGZ,BSIGZ/0.036,0.907/
      DATA M/22/
C
C     TURBULENT/NON-TURBULENT KINETICS CHOICE
C     FLAG PARAMETER VALUE
C
      DATA TURB/1.0/
C
      MSIZE=M*M
```

```
0063            M2=M/2
0064            B1SIGY=2.*BSIGY-1.0
0065            B1SIGZ=2.*BSIGZ-1.0
0066      C
0067      C     PHYSICAL AND CHEMICAL DATA FOR THE PRESENT APPLICATION
0068      C
0069      C     SOURCE CHARACTERISTICS
0070      C
0071      C     SOURCE HEIGHT (M)
0072            H=0.14
0073      C
0074      CC     SOURCE DIAMETER (M)
0075      CC      D=0.003
0076      C
0077      C     SOURCE STRENGTH (PPM M3 /S)
0078            QSTR=0.011
0079      C
```

```
C       SOURCE CONCENTRATION (PPM)
        CSOUR=3900
C
C       ATMOSPHERIC BOUNDARY LAYER CHARACTERISTICS
C
CC       B.L. HEIGHT (M)
CC        HBL=0.8
C
C       MEAN WIND SPEED ASSUMED CONSTANT ACROSS AND ALONG THE PLUME
C       WITH DIRECTION THAT DEFINES THE PLUME AXIS  (M/S)
        USP=0.4
C
C       CONSTANTS OF THE RELATIVE DISPERSION PARAMETERS
        SRY0=ASIGY
        SRZ0=ASIGZ
C
CC       VARIANCE OF FLUCTUATIONS PARAMETERS
CC        A=0.6
CC        B=0.6
C
C       CHEMICAL DATA
C       CHEMICAL KINETICS CONSTANTS
        K1=0.000
        K3=0.430
C       BACKGROUND OZON CONCENTRATION
       CBO3=0.35
C
C      ..............................................................
C
C
C      TIME ITERATIONS
C
C      ..............................................................
C
C      INITIAL TIME:ADV=0.0
       XSTART=USP*TSTART
       TIME=TSTART
       KK=0
       KK1=0
       KK2=-1
       SS1=-1.0
C      TRAVEL TIME (S)
 777   CONTINUE
       IF (TIME.GT.TMAX) GOTO 7795
C      ..............................................................
C
       X=USP*TIME
       KK1=KK1+1
       KK2=KK2+1
       SS1=SS1+1.0
C
       LL1=KK2/5
       RLL1=LL1
       TT1=DD1/5.00
C
       LL2=KK2/25
       RLL2=LL2
       TT2=SS1/25.00
C
       TIMOUT=TIME-TSTART
       XOUT=X-XSTART
C
```

```
C
C
C       INITIALIZE
C
C
        DKY=USP*(ASIGY**2)*BSIGY*(X**B1SIGY)
        DKZ=USP*(ASIGZ**2)*BSIGZ*(X**B1SIGZ)
        RY=DKY*DT/DY**2
        RZ=DKZ*DT/DZ**2
        RZY=RZ/RY
        RYZ=RY/RZ
        RY1=1./RY+2.0
        RY2=1./RY-2.0*RZY
        RY3=DY**2/DKY
        RZ1=1./RZ+2.0
        RZ2=1./RZ-2.0*RYZ
        RZ3=DZ**2/DKZ
```

```
C
C       CONSTRUCTION OF THE UVLOD  MATRIX
C       (LHS COEFFICIENTS FOR THE ODD TRAVERSES)
C
C       DIAGONAL ELEMENTS
        DO 11 I=1,M
        UVLOD(I,2)=RY1
   11   CONTINUE
C
C       OFF-DIAGONAL ELEMENTS
        UVLOD(1,1)=0.0
        UVLOD(1,3)=-2.0
        UVLOD(M,3)=0.0
C
C       CONSTRUCTION OF THE UVLEV  MATRIX
C       (LHS COEFFICIENTS FOR THE EVEN TRAVERSES)
C
C       DIAGONAL ELEMENTS
        DO 112 I=L,M
        UVLEV(I,2)=RZ1
  112   CONTINUE
C
C       OFF-DIAGONAL ELEMENTS
        UVLEV(1,1)=0.0
        UVLEV(1,3)=-2.0
        UVLEV(M,3)=0.0
C
        IF (RLL1.EQ.TT1) GO TO 778
        GO TO 779
C
 778    CONTINUE
C
C       OPTIONAL OUTPUT.................................................
C
C       WRITE (6,393) KK1,TIMOUT,XOUT
C393    FORMAT (1H1,4X,15HTRAVERSE NUMBER,I3/
C      .4X,11HTRAVEL TIME,1X,F6.3,1X,7HSECONDS/
C      .4X,25H(DISTANCE FROM THE SOURCE,1X,F6.3,1X,7HMETERS)/)
C
C.................................................................
C
C       OUTPUT..........................................................
C
C       WRITE (6,552)
C       WRITE (6,1223) ((UVLOD(I,J),J=1,3),I=1,3)
C552    FORMAT (3X,33HUNIT DIAGONAL BLOCK OF UVLOD MATRIX)
C       WRITE (6,5521)
C       WRITE (6,1223) ((UVLEV(I,J),J=1,3),I=1,3)
C5521   FORMAT (3X,33HUNIT DIAGONAL BLOCK OF UVLEV MATRIX)
C
C1223   FORMAT (8(1X,F8.4))
C.................................................................
C
 779    CONTINUE
C
C       CONSTRUCTION OF THE P,Q,S MATRICES
C       (COEFFICIENTS OF NONLINEAR FORCING TERM)
C
        DO 33 I=1,M
        DO 33 J=1,M
        Y=(J-1)*DY
        Z=(I-1)*DZ
```

```
C
C
C     RELATIVE DISPERSION PARAMETERS
      SRY=SRY0*(X**BSIGY)
      SRZ=SRZ0*(X**BSIGZ)
C
C
C     CEM
C     ESTIMATION OF INERT RELEASED SURROGATE CONCENTRATION (PPM)
      SRY2=2.*SRY**2
      SRZ2=2.*SRZ**2
      SYZ=SRY*SRZ
      EX1=-Y*Y/SRY2
      EX2=-(Z-H)*(Z-H)/SRZ2
      EX3=-(Z+H)*(Z+H)/SRZ2
      CEM=QSTT*EXP(EX1)*(EXP(EX2)+EXP(EX3))/2./3.14159/USP/SYZ
C
```

```
      IF (CEM.GT.CSOUR) CEM=CSOUR
C
      CEM2(I,J)=CEM
C
      C2=CEM**2
      IF (C2.LT.0.0000001) GO TO 3456
      IF (TURB.EQ.0.0) GO TO 3456
C
C     CVAR
C     ESTIMATION OF VARIANCE OF INERT SURROGATE CONCENTRATION
C     THROUGH
C     THE LOCALIZED PRODUCTION OF FLUCTUATIONS MODEL
C
C     IF (X.LT.0.014) GO TO 3456
      IF (X.LT.2.774) GO TO 2222
      GO TO 3333
 2222 FACTR=1.57733*(1.00-EXP(-X/2.760))
      FACTOR=FACTR**2
      GO TO 5555
 3333 FACTOR=1.000
 5555 CONTINUE
      FACT1=0.702
      FACT2=1.33
      A1=2.721
      ALPHA=1.00
      XI=FACT1*X
      XD=X-XI
      S1Y=SRY0*(XI**BSIGY)
      SZZ=SRZ0*(XI**BSIGZ)
      S2Y=SRY0*(XD**BSIGY)
      S2Z=SRZ0*(XD**BSIGZ)
      AY=FACT2*S1Y
      BY=FACT2*S1Z
      QQ1=(QSTR/3.14159265/USP)**2
      QQ2=FACTOR*BSIGY*FACT1**(A1-1.0)/(2.0*S1Y*S1Z*S2Y*S2Z)
      QQ3A=-AY*BY/2.0/S2Y/S2Z
      QQ3=EXP(QQ3A)
      CCQ=QQ1*QQ2*QQ3
      EXY=-Y*Y/2./S2Y**2
      FY=EXP(EXY)
      EXZ1=-(Z-H)*(Z-H)/2./S2Z**2
      EXZ2=-(Z+H)*(Z+H)/2./S2Z**2
      FZ1=EXP(EXZ1)
      FZ2=EXP(EXZ2)
      BESS1=AY*AY*(Z-H)*(Z-H)+BY*BY*Y*Y
      BES1=SQRT(BESS1)/S2Y/S2Z
      ANS1=AI0(BES1)
      BESS2=AY*AY*(Z+H)*(Z+H)+BY*BY*Y*Y
      BES2=SQRT(BESS2)/S2Y/S2Z
      ANS2=AI0(BES2)
      CVAR=CCQ*FY*(FZ1*ANS1-ALPHA*FZ2*ANS2)
C
      IF (CVAR.LT.0.000) CVAR=0.000
      SVAR(I,J)=SQRT(CVAR)
C
C     INTENSITY OF PLUME SEGREGATION
C     (THETA FOR TURBULENT CHEMISTRY)
      THETA=CVAR/CEM**2
C               IF (THETA.GT.999999.999)  STOP
C
      GO TO 2345
C
```

```
C     (THETA FOR NON-TURBULENT CHEMISTRY)
 3456 THETA=0.0
C
 2345 CONTINUE
C
      THET(I,J)=THETA
      STHET(I,J)=SQRT(THETA)
      IF (THET(I,J).GT.9999.9999) THET(I,J)=9999.9999
C
C
      P(I,J)=K3*(1.+THETA)
      Q(I,J)=-K3*CEM*(1.+THETA)-K3*CBO3-K1
      S(I,J)=K3*CEM*CBO3
      PX(I,J)=P(I,J)
      IF(ABS(PX(I,J)).GT.9999.9999) PX(I,J)=9999.9999
      QX(I,J)=Q(I,J)
      IF(ABS(QX(I,J)).GT.999.9999) QX(I,J)=9999.9999
```

```
      SX(I,J)=S(I,J)
      IF(ABS(SX(I,J)).GT.9999.9999) SX(I,J)=9999.9999
C
   33 CONTINUE
C
      IF (RLL1.EQ.TT1) GO TO 7778
      GO TO 7779
C
 7778 CONTINUE
C     OPTIONAL OUTPUT.............................................
C
C     THIS SECTION PRINTS THE INERT SURROGATE CONCENTRATIONS
C     IN COORDINATE FORMAT (Z-AXIS DOWNWARDS)
C     (REMEMBER:THIS IS AN EXACT ANALYTICAL CALCULATION)
C
C     WRITE (6,4611) CEM2(M,1)
C     WRITE (6,461)
C     WRITE (6,661)
C     DO 1947 I=1,22
C     YY(I)=(I-1)*DY
C1947 CONTINUE
C     WRITE (6,566)
C     WRITE (6,877) (YY(I),I=1,11)
C     DO 947 I=1,22
C     ZZ=(I-1)*DZ
C     WRITE (6,876) (ZZ,(CEM2(I,J),J=1,11))
C947  CONTINUE
C     WRITE (6,461)
C     WRITE (6,661)
C     WRITE (6,567)
C     WRITE (6,877) (YY(I),I=12,22)
C     DO 946 I=1,22
C     ZZ=(I-1)*DZ
C     WRITE (6,876) (ZZ,(CEM2(I,J),J=12,22))
C946  CONTINUE
C661  FORMAT (4X,38HINERT RELEASED SURROGATE CONCENTRATION)
C.................................................................
C
 7779 CONTINUE
C
C     ODD TRAVERSES
C
C     ODD TRAVERSES:EVALUATION OF THE U-VECTOR
C     (IN FINAL VERSIONS THERE IS NO PRINTED OUTPUT FOR THESE ITERATIONS)
C
C     CONSTRUCTION OF THE RIGHT-HAND-SIDE MATRIX
C     FOR THE CALCULATION OF THE U-VECTOR
C
C     I=1
      DO 44 J=1,M
      RHS(1,J)=RY2*V(1,J)+2.*RZY*V(2,J)+
     .RY3*(P(1,J)*V(1,J)**2+Q(1,J)*V(1,J)+S(1,J))
   44 CONTINUE
      DO 45 I=2,M
      DO 45 J=1,M
      RHS(I,J)=RY2*V(I,J)+RZY*V(I+1,J)+RZY*V(I-1,J)+
     .RY3*(P(I,J)*V(I,J)*V(I,J)+Q(I,J)*V(I,J)+S(I,J))
   45 CONTINUE
C
C     OPTIONAL OUTPUT.............................................
C
C     THE ENTRIES OF THE RHS-VECTOR ARE PRINTED IN COORDINATE FORMAT
```

```
C     WRITE (6,472)
C     WRITE (6,474)
C     WRITE (6,566)
C     WRITE (6,877)  (YY(I),I=1,M2)
C     DO 996 I=1,M
C     ZZZ2=(I-1)*DZ
C     WRITE (6,876)  (ZZZ2,(RHS(I,J),J=1,M2))
C996  CONTINUE
C     WRITE (6,474)
C     WRITE (6,567)
C     WRITE (6,877)  (YY(I),I=M2+1,M)
C     DO 997 I=1,M
C     ZZZ3=(I-1)*DZ
C     WRITE (6,876)  (ZZZ3,(RHS(I,J),J=M2+1,M))
C997  CONTINUE
C.....................................................................
C
```

```
C     ENTRIES OF THE U-VECTOR:
C
      DO 9999 J=1,M
      DO 9998 I=1,M
      BB(I)=RHS(I,J)
 9998 CONTINUE
      DO 9991 I=1,M
      DO 9991 JJ=1,3
      UVL1(I,JJ)=UVLOD(I,JJ)
 9991 CONTINUE
      DO 9997 I=2,M
      UVL1(I,2)=UVL1(I,2)-UVL1(I,1)/UVL1(I-1,2)*UVL1(I-1,3)
      BB(I)=BB(I)-UVL1(I,1)/UVL1(I-1,2)*BB(I-1)
 9997 CONTINUE
      M1=M-1
      BB(M)=BB(M)/UVL1(M,2)
      DO 9996 I=1,M1
      MNUM=M-I
      BB(MNUM)=(BB(MNUM)-UVL1(MNUM,3)*BB(MNUM+1))/UVL1(MNUM,2)
 9996 CONTINUE
      DO 9995 I=1,M
      U(I,J)=BB(I)
 9995 CONTINUE
C
 9999 CONTINUE
C
      DO 6767 I=1,M
      DO 6767 J=1,M
      IF (U(I,J).LT.0.0) GO TO 7878
 6767 CONTINUE
      GO TO 6969
 7878 DO 7979 I=1,M
      DO 7979 J=1,M
      U(I,J)=0.0
 7979 CONTINUE
 6969 CONTINUE
C
C     OPTIONAL OUTPUT.............................................
C
C     THE ENTRIES OF THE U-VECTOR ARE PRINTED IN COORDINATE FORMAT
C     WRITE (6,472)
C     WRITE (6,383)
C     WRITE (6,566)
C     WRITE (6,877) (YY(I),I=1,M2)
C     DO 992 I=1,M
C     ZZZ2=(I-1)*DZ
C     WRITE (6,876) (ZZZ2,(U(I,J),J=1,M2))
C992  CONTINUE
C     WRITE (6,383)
C     WRITE (6,567)
C     WRITE (6,877) (YY(I),I=M2+1,M)
C     DO 993 I=1,M
C     ZZZ3=(I-1)*DZ
C     WRITE (6,876) (ZZZ3,(U(I,J),J=M2+1,M))
C993  CONTINUE
C
C
C     EVEN TRAVERSES
C     EVEN TIME STEP
      KK=KK+1
C
      X=TIME*USP
```

```
C
C
C     EVEN TRAVERSES:EVALUATION OF THE V-VECTOR
C
C
C     CONSTRUCTION OF THE RIGHT-HAND-SIDE VECTOR
C     FOR THE CALCULATION OF THE V-VECTOR
C
      J=1
      DO 441 I=1,M
      RHS(I,1)=RZ2*U(I,1)+2.*RYZ*U(I,2)+
     .RZ3*(P(I,1)*U(I,1)*U(I,1)+Q(I,1)*U(I,1)+S(I,1))
  441 CONTINUE
      DO 451 J=2,M
      DO 451 I=1,M
      RHS(I,J)=RZ2*U(I,J)+RYZ*U(I,J+1)+RYZ*U(I,J-1)+
     .RZ3*(P(I,J)*U(I,J)*U(I,J)+Q(I,J)*U(I,J)+S(I,J))
```

```
  451 CONTINUE
C
C     OPTIONAL OUTPUT
C     THE ENTRIES OF THE RHS-VECTOR ARE PRINTED IN COORDINATE FORMAT
C     WRITE (6,473)
C     WRITE (6,474)
C     WRITE (6,566)
C     WRITE (6,877) (YY(I),I=1,M2)
C     DO 89 I=1,M
C     ZZZ=(I-1)*DZ
C     WRITE (6,876) (ZZZ,(RHS(I,J),J=1,M2))
C 89  CONTINUE
C     WRITE (6,474)
C     WRITE (6,567)
C     WRITE (6,877) (YY(I),I=M2+1,M)
C     DO 898 I=1,M
C     ZZZ=(I-1)*DZ
C     WRITE (6,876) (ZZZ,(RHS(I,J),J=M2+1,M))
C898  CONTINUE
C474  FORMAT (//4X,25HENTRIES OF THE RHS-VECTOR/)
C.....................................................................
C
C     ENTRIES OF THE V-VECTOR
C
      DO 9989 I=1,M
      DO 9988 J=1,M
      BB(J)=RHS(I,J)
 9988 CONTINUE
      DO 9981 II=1,M
      DO 9981 JJ=1,3
      UVL1(II,JJ)=UVLEV(II,JJ)
 9981 CONTINUE
      DO 9987 J=2,M
      UVL1(J,2)=UVL1(J,2)-UVL1(J,1)/UVL1(J-1,2)*UVL1(J-1,3)
      BB(J)=BB(J)-UVL1(J,1)/UVL1(J-1,2)*BB(J-1)
 9987 CONTINUE
      M1=M-1
      BB(M)=BB(M)/UVL1(M,2)
      DO 9986 J=1,M1
      MNUM=M-J
      BB(MNUM)=(BB(MNUM)-UVL1(MNUM,3)*BB(MNUM+1))/UVL1(MNUM,2)
 9986 CONTINUE
      DO 9985 J=1,M
      V(I,J)=BB(J)
 9985 CONTINUE
C
 9989 CONTINUE
C
      DO 5656 I=1,M
      DO 5656 J=1,M
      IF (V(I,J).LT.0.0) GO TO 3434
 5656 CONTINUE
      GO TO 2323
 3434 DO 3535 I=1,M
      DO 3535 J=1,M
      V(I,J)=0.0
 3535 CONTINUE
 2323 CONTINUE
C
C
      IF (RLL1.EQ.TT1) GO TO 7788
      GO TO 7799
```

```
C
 7788 CONTINUE
C     OUTPUT ....................................................
C
C     THE ENTRIES OF THE V-VECTOR ARE PRINTED IN COORDINATE FORMAT
C     WRITE (6,461)
C     WRITE (6,473)
C     WRITE (6,383)
C     WRITE (6,566)
C     WRITE (6,877) (YY(I),I=1,11)
C    DO 99 I=1,22
C     ZZZ=(I-1)*DZ
C     WRITE (6,876) (ZZZ,(V(I,J),J=1,11))
C 99  CONTINUE
C     WRITE (6,461)
C     WRITE (6,383)
C     WRITE (6,567)
```

```
C      WRITE (8,877) (YY(I),I=12,22)
C      DO 999 I=1,22
C      ZZZ=(I-1)*DZ
C      WRITE (8,876) (ZZZ,(V(I,J),J=12,22))
C999  CONTINUE
C 383 FORMAT (//4X,23HADVANCEMENT OF REACTION/)
C.....................................................................
C
       CREAC=CEM2(8,1)-V(8,1)
       RAT1=CREAC/CEM2(8,1)
       RAT2=1.-RAT1
       CRO3=0.35-V(8,1)
       RATO3=CRO3/0.35
C
C
       WRITE (8,393) KK2,TIMOUT,XOUT,CEM2(8,1),V(8,1),RAT1,RATO3,
      *STHET(8,1),FACT1
  393 FORMAT (3X,I3,2X,F6.3,2X,F5.3,2X,F9.4,5(2X,F7.4))
       WRITE (8,394) KK2,XOUT
  394 FORMAT(3X,I4,2X,F5.3)
C
C       IF (XOUT-3.00) 7799,7798,7799
C 7798 DO 7799 I=1,22
C
 7799 CONTINUE
C
C      OUTPUT FORMATS
 4611 FORMAT (1H1,//4X,5(1H*)/4X,F12.8)
 461  FORMAT (1H1)
 472  FORMAT (1H0,4X,36HODD TRAVERSE (END OF HALF-TIME STEP))
 473  FORMAT (1H0,4X,32HEVEN TRAVERSE (END OF TIME STEP))
 566  FORMAT (1H0,4X,28HPART 1:LEFT HALF OF THE GRID)
 567  FORMAT (1H0,4X,29HPART 2:RIGHT HALF OF THE GRID)
 876  FORMAT (1H0,F8.4,1X,1H*,1X,11(1X,F9.4))
 877  FORMAT (1H0,12X,11(1X,F9.4)/16X,1H*,10(9X,1H*)//)
C
       IF (RLL2.EQ.TT2) GO TO 3663
       GO TO 7796
 3663 CONTINUE
 7797 DO 7796 I=1,22
       ZZZ=(I-1)*DZ
       WRITE (9,4621) XOUT,ZZZ,CEM2(8,I),SVAR(8,I),THET(8,I),V(8,I),
      *STHET(8,I)
 4621 FORMAT (3X,F5.3/3X,F5.3,7(1X,F9.4))
 7796 CONTINUE
       KK3=KK2/100
       KK4=KK3*100
       IF (KK4.NE.KK2) GO TO 3331
       WRITE (7,4623) 1,KK4, XOUT
 4623 FORMAT (I1,3X,I3,3X,F5.3///)
       DO 3332 I=1,22
       OZON=0.35000-V(8,I)
       ZZZ=(I-1)*DZ
       ZZZZ=-ZZZ
 3332 WRITE (7,4622) ZZZ,ZZZZ,OZON,CNO,V(8,I)
 4622 FORMAT (3X,F9.4,1X,F9.4,3(1X,F9.5))
 3331 CONTINUE
       TIME=TIME+2.*DT
       GO TO 777
 7795  STOP
        END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	2907	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	102	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	49700	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
	Total Space Allocated	52709	

ENTRY POINTS

Address	Type	Name
0-00000000		TRPM

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
**	R*4	A1	**	R*4	ALPHA	**	R*4	ANS1	**	R*4	ANS2
2-0000C1B4	R*4	ASIGY	2-0000C1B8	R*4	ASIGZ	2-0000C1EC	R*4	AY	**	R*4	B1SIGY
**	R*4	B1SIGZ	2-0000C1F8	R*4	BES1	2-0000C1FC	R*4	BES2	**	R*4	BESS1
**	R*4	BESS2	**	R*4	BSIGY	**	R*4	BSIGZ	2-0000C1F0	R*4	BY
**	R*8	C2	**	R*4	CBO3	**	R*4	CCQ	2-0000C1A0	R*8	CEM
2-0000C210	R*4	CNO	**	R*4	CREAC	**	R*4	CRO3	**	R*4	CSOUR
**	R*8	CVAR	2-0000C1D4	R*4	DD1	**	R*4	DKY	**	R*4	DKZ
2-0000C1A8	R*4	DT	**	R*4	DY	**	R*4	DZ	**	R*4	EX1
**	R*4	EX2	**	R*4	EX3	**	R*4	EXY	**	R*4	EXZ1
**	R*4	EXZ2	2-0000C1E8	R*4	FACT1	**	R*4	FACT2	**	R*4	FACTOR
**	R*4	FACTR	**	R*4	FY	**	R*4	FZ1	**	R*4	FZ2
**	R*4	H	2-0000C1D8	I*4	I	**	I*4	II	2-0000C1E0	I*4	J
**	I*4	JJ	**	R*4	K1	**	R*4	K3	2-0000C1C0	I*4	KK
2-0000C1C4	I*4	KK1	2-0000C1C8	I*4	KK2	**	I*4	KK3	**	I*4	KK4
2-0000C1DC	I*4	L	**	I*4	LL1	**	I*4	LL2	**	I*4	M
**	I*4	M1	**	I*4	M2	**	I*4	MNUM	**	I*4	MSIZE
**	R*4	OZON	**	R*4	QQ1	**	R*4	QQ2	**	R*4	QQ3
**	R*4	QQ3A	**	R*4	QSTR	2-0000C1E4	R*4	QSTT	**	R*4	RAT1
**	R*4	RAT2	**	R*4	RATO3	**	R*4	RLL1	**	R*4	RLL2
**	R*8	RY	**	R*8	RY1	**	R*8	RY2	**	R*8	RY3
**	R*8	RYZ	**	R*8	RZ	**	R*8	RZ1	**	R*8	RZ2
**	R*8	RZ3	**	R*8	RZY	**	R*4	S1Y	2-0000C1F4	R*4	S1Z
**	R*4	S2Y	**	R*4	S2Z	**	R*4	SRY	**	R*4	SRY0
**	R*4	SRY2	**	R*4	SRZ	**	R*4	SRZ0	**	R*4	SRZ2
2-0000C1CC	R*4	SS1	**	R*4	SYZ	**	R*4	SZZ	**	R*8	THETA
2-0000C1BC	R*4	TIME	**	R*4	TIMOUT	2-0000C1B0	R*4	TMAX	2-0000C1AC	R*4	TSTART
**	R*4	TT1	**	R*4	TT2	**	R*4	TURB	**	R*4	USP
2-0000C1D0	R*4	X	**	R*4	XD	**	R*4	XI	**	R*4	XOUT
**	R*4	XSTART	**	R*4	Y	**	R*4	Z	**	R*4	ZZZ
**	R*4	ZZZZ									

ARRAYS

Address	Type	Name	Bytes	Dimensions
2-00000420	R*8	BB	176	(22)
2-00009338	R*8	CEM2	3872	(22, 22)
2-00000058	I*4	LMN	88	(22)
2-00004798	R*8	P	3872	(22, 22)

2-000074F8	R*8	PX	3872	(22, 22)
2-000056B8	R*8	Q	3872	(22, 22)
2-00008418	R*8	QX	3872	(22, 22)
2-000000B0	R*4	RAT	88	(22)
2-000027F0	R*8	RHS	4232	(23, 23)
2-000065D8	R*8	S	3872	(22, 22)
2-0000BA10	R*4	STHET	1936	(22, 22)
2-0000B280	R*4	SVAR	1936	(22, 22)
2-00003878	R*8	SX	3872	(22, 22)
2-0000A258	R*8	THET	3872	(22, 22)
2-000006E0	R*8	U	4232	(23, 23)
2-000004D0	R*8	UVL1	528	(22, 3)
2-00000210	R*8	UVLEV	528	(22, 3)
2-00000000	R*8	UVLOD	528	(22, 3)
2-00001768	R*8	V	4232	(23, 23)
2-00000000	R*4	YY	88	(22)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
**	11	**	33	**	44	**	45	**	112	1-00000004	393'
1-00000022	394'	**	441	**	451	**	461'	**	472'	**	473'
**	566'	**	567'	0-00000028	777	0-0000017C	778	0-0000017C	779	**	876'
**	877'	0-000002AC	2222	0-0000090D	2323	0-0000045E	2345	0-00000B48	3331	**	3332
**	3333	0-000008EC	3434	0-0000045C	3456	**	3535	0-000009F4	3663	**	4611'
1-0000002C	4621'	1-00000051	4622'	1-00000042	4623'	0-000002CD	5555	**	5656	**	6767
0-00000731	6969	0-00000570	7778	0-00000570	7779	0-00000918	7788	0-00000B54	7795	0-00000A76	7796
**	7797	0-000009E7	7799	0-00000710	7878	**	7979	**	9981	**	9985
**	9986	**	9987	**	9988	**	9989	**	9991	**	9995
**	9996	**	9997	**	9998	**	9999				

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name	Type	Name	Type	Name
R*4	AI0	R*8	MTH$DSQRT	R*4	MTH$EXP	R*4	MTH$SQRT

COMMAND QUALIFIERS

```
FOR/LIS TRPM1

/CHECK=(NOBOUNDS,OVERFLOW,NOUNDERFLOW)
/DEBUG=(NOSYMBOLS,TRACEBACK)
/STANDARD=(NOSYNTAX,NOSOURCE_FORM)
/SHOW=(NOPREPROCESSOR,NOINCLUDE,MAP,NODICTIONARY,SINGLE)
/WARNINGS=(GENERAL,NODECLARATIONS)
/CONTINUATIONS=19  /NOCROSS_REFERENCE  /NOD_LINES  /NOEXTEND_SOURCE  /F77
/NOG_FLOATING  /I4  /NOMACHINE_CODE  /OPTIMIZE
```

COMPILATION STATISTICS

```
Run Time:          11.95 seconds
Elapsed Time:      14.91 seconds
Page Faults:       1019
Dynamic Memory:    702 pages
```