# 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*

*Pasadena, California 91125*

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*"Continued Development*
*of a Mathematical Modeling Capability*
*in Photochemical Air Pollution:*
*Reacting Plumes"*

## Disclaimer

## 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

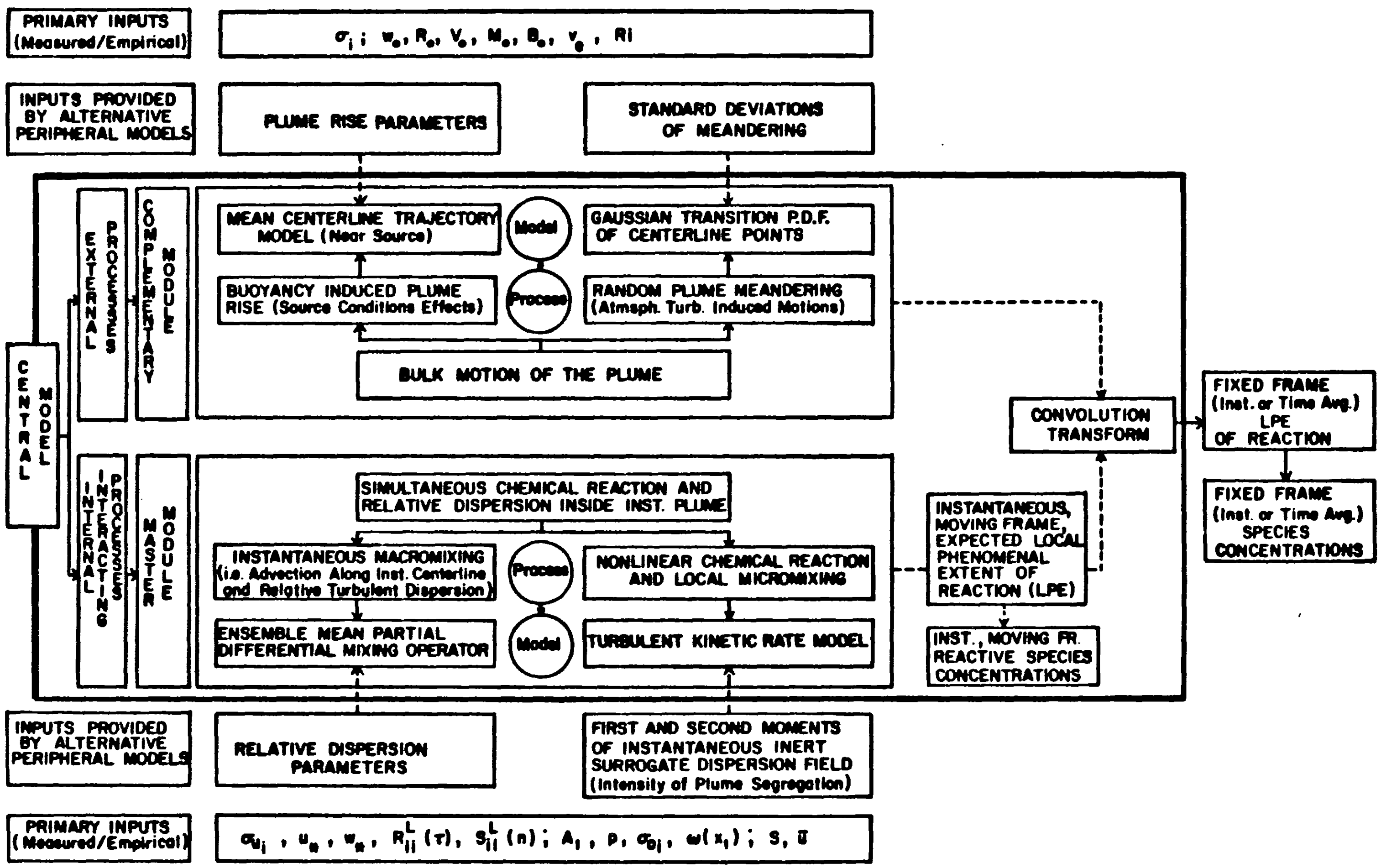


**Figure 1**

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
```

```
      M2=M/2
      B1SIGY=2.*BSIGY-1.0
      B1SIGZ=2.*BSIGZ-1.0
C
C     PHYSICAL AND CHEMICAL DATA FOR THE PRESENT APPLICATION
C
C     SOURCE CHARACTERISTICS
C
C     SOURCE HEIGHT (M)
      H=0.14
C
CC     SOURCE DIAMETER (M)
CC      D=0.003
C
C     SOURCE STRENGTH (PPM M3 /S)
      QSTR=0.011
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
       CB03=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 (6(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=SRYØ*(X**BSIGY)
      SRZ=SRZØ*(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*CB03-K1
      S(I,J)=K3*CEM*CB03
      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 (6,877) (YY(I),I=12,22)
C      DO 999 I=1,22
C      ZZZ=(I-1)*DZ
C      WRITE (6,876) (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 (6,393) 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 (6,394) 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 |