NUREG/CR-1391
SAND80-0822
R7
Printed December 1982

MAEROS User Manual

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Prepared by
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Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-76DP00789

Prepared for
U. S. NUCLEAR REGULATORY COMMISSION

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NUREG/CR-1391

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MAEROS

User Manual

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Albuquerque, NM 87185

Operated by
Sandia Corporation
for the
U. S. Department of Energy

Prepared for
Division of Reactor Safety Research
Office of Nuclear Regulatory Research
U. S. Nuclear Regulatory Commission
Washington, DC 20555

Under Memorandum of Understanding DOE 40-550-75
NRC FIN. NO. A1198

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ABSTRACT

This manual discusses the capabilities and implementation procedures for MAERIOS, the stand-alone multicomponent aerosol module of CONTAIN. The module calculates aerosol composition and mass concentration as a function of particle size and time. The processes that may be incorporated are 1) coagulation due to Brownian motion, gravity and turbulence; 2) particle deposition due to gravitational settling, diffusion and thermophoresis; 3) particle growth due to condensation of a gas, typically water vapor; and 4) time varying sources of particles of different sizes and chemical compositions. The capabilities of the code are illustrated through simulating an aerosol released in a hypothetical situation.

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I. INTRODUCTION

For assessing health consequences due to inhalation of an aerosol, much effort has been devoted to modeling the physical and chemical processes that govern the evolution of a spatially homogeneous aerosol. Although particle size is generally considered to be the single most important variable characterizing the respirability of an aerosol,[2] different substances usually do not have similar biological effects and thus studies restricted to size distribution dynamics alone cannot fully assess aerosol health effects. Therefore, in this work, a general code for simulating the evolution of the distribution of chemical species with respect to particle size is presented. The physical phenomena included are: 1) coagulation, 2) deposition, 3) particle growth due to condensation or what is often called gas-to-particle conversion and 4) time varying sources of particles with different sizes and chemical compositions. A complete discussion for implementing the above processes is given by Gelbard and Seinfeld.[3]

To make the code modular, all interfacing is achieved through a common block and a call statement in a subroutine supplied by the user. This eliminates the reading of input data and facilitates incorporation of MAEROS into codes requiring an aerosol model. To implement this simplified interfacing procedure, one need only read Chapters I, II III and V of this manual. However, since an extensive study of the basic coefficients used to specify the processes governing aerosol

evolution was not made, the user may wish to change some or all of the three basic coefficient specification routines. A discussion of these routines is therefore given in Chapter IV of this manual. The functional forms of the basic coefficients used in MAEROS are given in Appendix A.

Although this is the first officially released version of MAEROS, many suggestions have already been made for future developments. The author would be interested in any additional comments on MAEROS.

II. NUMERICAL METHOD

The numerical technique is based upon dividing the particle size domain into m sections and imposing the condition of mass conservation for each chemical component for the processes given above. Therefore, aerosol mass concentrations are grouped into sections (i.e., size classes) for which an average composition is determined. Although the complete technique[3] places virtually no restrictions on the size or number of sections, the code is limited to geometrically spaced sections in particle mass (i.e. $v_{i+1} \geq 2v_i$, where v_i is the largest particle mass in section i). Thus the maximum number of sections is given by

$$\frac{\log(v_m/v_o)}{\log 2}$$

where v_o and v_m are the smallest and largest particle masses in the computational domain, respectively. The code is also restricted to coagulation, deposition and condensation mechanisms which are only dependent on particle mass and not chemical composition. Only the source mechanisms may be particle size and composition dependent. Since intra-particle chemical reactions and condensation of more than one component were not of significant interest for reactor safety studies, the code does not currently simulate these processes but a discussion for incorporating them is given by Gelbard and Seinfeld.[3] Incorporating these processes into the code is being considered for the next version of MAEROS. However, for the mechanisms that can be simulated by the code, the error in computing the aerosol

mass concentration of each component as a function of particle size can be made arbitrarily small by increasing the number of sections with the restriction that $v_{i+1} \geq 2v_i$.

For m sections, a set of $2m^2+4m$ "sectional" coefficients must be calculated before integrating in time. These coefficients are determined from the basic coagulation, condensation and deposition coefficients discussed in Chapter IV and tabulated in Appendix A. Since the sectional coefficients depend on the physical properties of the containment chamber (e.g., temperature, pressure, chamber volume and deposition surface area), one will generally have to recalculate them for a particular application. Unfortunately, computing the sectional coefficients usually requires a significant computational effort. However, for a given containment chamber, the sectional coefficients will probably vary only with temperature and pressure. Therefore, the code has been developed such that the sectional coefficients are stored at a user specified upper and lower bound for both temperature and pressure. Thus, linear interpolation from the four sets of sectional coefficients is used to determine the sectional coefficients at a particular temperature and pressure, without requiring recalculation of the sectional coefficients for each time step. If the same sectional coefficients are used for all simulations, to save computer time it is highly recommended that these coefficients be "hard wired" into the code. The procedure for hard wiring sectional coefficients is given in Chapter IV. The code as supplied, automatically defaults all coefficients to

zero unless they are requested to be calculated in the call to MAEROS.

III. INTERFACING MAEROS

Given the initial state of the aerosol in a chamber, one calls the MAEROS routine to calculate the aerosol concentrations after a specified time step. Thus by calling MAEROS recursively, the evolution of the aerosol can be calculated. For the users' convenience, a subroutine called PRAERO is supplied with the code to print the aerosol concentrations after each time step. Thus, as shown in the sample problem in Chapter V, PRAERO is called after each call to MAEROS. Clearly one is not restricted to using PRAERO and may substitute one's own output routine. One must dimension the following arrays in the program that calls MAEROS: Q(160), SRATE(160), DEPSIT(3,8), DIAM(21).

MAEROS must be called as follows:

```
CALL MAEROS(M,KCOMP,TIME,DELTIM,Q,SRATE,TGAS,PGAS,DEPSIT,DIAM,
  TGAS1,TGAS2,PGAS1,PGAS2,ROUND,IPRNT,IFLAG,NEWCOF).
```

where,

<u>Input to MAEROS (to be supplied by the user)</u>

M = Number of sections (must be an integer from 5 to 20). For more than 20 sections, array dimensions must be changed as discussed in Appendix B. One may use initially 10 sections and check for convergence by repeating the calculations with 20 sections.

KCOMP = number of components (must be an integer from 1 to 8). For more than 8 components, array dimensions must be changed as discussed in Appendix B.

TIME = initial time (real variable in seconds).

DELTIM = time step (real variable in seconds), such that MAEROS will integrate in time from TIME to TIME+DELTIM.

Q = array of suspended mass concentrations at the beginning of the time step, where Q(K+(L-1)*KCOMP) is the suspended mass concentration of component K in section L. Q is a real array in kg/m^3.

SRATE = array of concentration generation rates to be used over the time step, where SRATE(K+(L-1)*KCOMP) is the concentration generation rate of component K in section L. SRATE is a real array in $kg/(s\ m^3)$. Note that if any element of SRATE is changed from the previous call to MAEROS, IFLAG should be reset to -1, but NEWCOF need not be reassigned a positive value.

TGAS = gas temperature to be used over the time step. TGAS is a real variable in K. Note that if TGAS is changed from the previous call to MAEROS, IFLAG should be reset to -1, but NEWCOF need not be reassigned a positive value.

PGAS = gas pressure to be used over the time step. PGAS is a real variable in Pa. Note that if PGAS is changed from the previous call to MAEROS, IFLAG should be reset to -1, but NEWCOF need not be reassigned a positive value.

DIAM = (M+1) dimensional array of particle diameters at the section boundaries. DIAM is a real array in meters and may not be changed after the first call to MAEROS.

TGAS1 = lowest gas temperature in K.

TGAS2 = highest gas temperature in K. Note that TGAS2 must be greater than TGAS1 and both TGAS1 and TGAS2 are real variables which should not be changed after the first call to MAEROS.

PGAS1 = lowest gas pressure in Pa.

PGAS2 = highest gas pressure in Pa. Note that PGAS2 must be greater than PGAS1 and both PGAS1 and PGAS2 are real variables which should not be changed after the first call to MAEROS.

ROUND = machine unit round-off error. This is the smallest number added to 1.0 which the machine will distinguish from 1.0.

Machine	ROUND
IBM 360/370	9.6E-7
DEC 10	7.7E-9
DEC VAX	6.0E-8
CDC 6600/7600	7.7E-15
UNIVAC 1108	1.5E-8

IPRNT = logical unit number of printer. IPRNT must be an integer.

IFLAG = time integration flag. Set IFLAG to 1 for the first call to MAEROS. If SRATE, TGAS, or PGAS are changed from their previous values or NEWCOF $\geq$ 1, reset IFLAG to -1. IFLAG must be an integer variable.

NEWCOF = Flag to indicate which coefficients are to be recalculated. For |NEWCOF| < 10, condensation of the last component is assumed. For |NEWCOF| $\geq$ 11, condensation is neglected. If NEWCOF is negative, coefficients are not recalculated and all variables passed through the common block PHYSPT are ignored, and M, KCOMP, and Q may not be changed from the previous call to MAEROS. Interpolation is always performed to determine the sectional coefficients based on TGAS, PGAS, TGAS1, TGAS2, PGAS1, and PGAS2, regardless of the value of NEWCOF. However, as noted previously, one should use a negative value of NEWCOF to avoid the excessive computational cost of

recomputing sectional coefficients. One of the following positive integer values of NEWCOF may be passed to MAEROS to indicate which sectional coefficients are to be recalculated. NEWCOF must be an integer variable.

NEWCOF	Meaning
1	Recalculate coefficients at the four combinations of temperature and pressure given by TGAS1, TGAS2, PGAS1, and PGAS2.
2	Recalculate coefficients only at TGAS1 and PGAS1.
3	Recalculate coefficients for PGAS1 at TGAS1 and TGAS2.
4	Recalculate coefficients for TGAS1 at PGAS1 and PGAS2.
5	Same as 1, except recalculate only deposition coefficients.
6	Same as 1, except recalculate only condensation coefficients.

7 Same as 1, except recalculate only deposition and condensation coefficients.

8 Modify condensation coefficients by multiplying sectional condensation coefficients by DELSAT. DELSAT will now be used as a multiplicative factor on the previous value of the condensation coefficient.

9 Recalculate only condensation coefficients at TGAS1 and PGAS1.

11 Same as 1, except no condensation.

12 Same as 2, except no condensation.

13 Same as 3, except no condensation.

14 Same as 4, except no condensation.

15 Same as 5, except no condensation.

NEWCOF must be positive on the first call to MAEROS. Since the code automatically changes NEWCOF to -|NEWCOF| on returning from MAEROS, the user need not specify NEWCOF for subsequent calls to MAEROS.

Output from MAEROS

TIME = final time equal to the initial time plus the time step (seconds).

Q = array of suspended mass concentrations at end of the time step (kg/m^3)

DEPSIT(J,K) = mass of K-th component deposited on the J-th deposition surface over the time step (real variable in kg).

where J = 1 ceiling
2 vertical walls
3 floor

NOTE: This is not the cumulative mass for the entire simulation.

IFLAG = The code will automatically reset IFLAG for the next call to MAEROS.

NEWCOF = -|NEWCOF|

Before calling MAEROS, if coefficients are to be recalculated (i.e. NEWCOF > 0), the following parameters must be set in the common block PHYSPT.

```
COMMON/PHYSPT/ACELOV,AFLROV,AWALOV,CHI,DELDIF,
$DELSAT,DENSTY,FSLIP,FTHERM,GAMMA,PSAT,STICK,TGRADC,TGRADF,
$TGRADW,TKGOP,TURBDS,VOLUME,WTCONM,WTMOL
```

where

ACELOV = ratio of surface area of ceiling to chamber volume (1/meters).

AFLROV = ratio of surface area of floor to chamber volume (1/meters).

AWALOV = ratio of surface area of vertical walls to chamber volume (1/meters). Note that if ACELOV,AFLROV and AWALOV are set to zero, all deposition mechanisms are ignored.

CHI = dynamic shape factor (~1).

DELDIF = diffusion boundary layer thickness (meters). This variable is used only for calculating diffusive deposition.

DELSAT = saturation ratio minus 1 (may not be negative). The current version of the code assumes that there is an infinite source of condensing gas such that DELSAT is constant. In the next version of MAEROS,

removal of condensible species from the gas phase will be accounted for. If NEWCOF = 8, the condensation coefficient will be multiplied by DELSAT.

DENSTY = particle material density (kg/m^3). If the material density is a function of particle size, see Chapter IV.E.

FSLIP = particle slip coefficient (~1.37).

FTHERM = a constant associated with the thermal accommodation coefficient (~1).

GAMMA = agglomeration shape factor (~1).

PSAT = equilibrium vapor pressure of condensing gas (Pa). Note that for rapid condensation of a vapor, the equations solved by MAEROS become stiff and difficult to solve using the current version of the code. This problem should be resolved in the next version of the code. The user may encounter stiffness for large values of DELSAT and PSAT.

STICK = particle sticking probability (~1).

TGRADC = temperature gradient from ceiling to gas (positive for gas hotter than surface) (K/m).

TGRADF = temperature gradient from floor to gas (K/m).

TGRADW = temperature gradient from wall to gas (K/m). TGRADC, TGRADF and TGRADDW are used only for calculating thermophoretic deposition.

TKGOP = thermal conductivity of gas over that for particle.

TURBDS = turbulence dissipation rate (m^2/s^3).

VOLUME = chamber volume (m^3).

WTCONM = mass of condensing molecule (kg).

WTMOL = molecular weight of gas (kg/kg-mole)

Note that if CHI and GAMMA are functions of particle mass, they may be changed in the routines BETA and DEPOST as discussed in Chapters IV.B and IV.C. If DENSTY is a function of particle mass, the subroutine RHODD should be changed as discussed in Chapter IV.E.

III.A. Output

For the user's convenience, the routine PRAERO may be used to print and plot the section concentrations. The routine is set up for an arbitrary number of sections and a maximum of 8 components. However, unless the DIMENSION statement is changed, only a maximum of 20 sections may be printed. To initialize PRAERO, PRAERO should be called with IFLAG=1, before calling MAEROS. To print the results at the end of each time step, one only needs to call PRAERO using the calling sequence.

```
CALL PRAERO(Q,DEPSIT,DIAM,TIME,VOLUME,M,KCOMP,IFLAG,
IPRNT,IPLOT,QMINPL,QMAXPL,ISCAL,NROW,NCOL)
```

PRAERO calls the routine PPLOT which prints a plot suitable for output on either an alphanumeric computer terminal or a line printer. The size and type of plots are controlled by the last six input variables to PRAERO. Thus the following must be supplied by the user as input to PRAERO.

<u>Input to PRAERO (to be supplied by user)</u>

Q,DEPSIT,DIAM,TIME,VOLUME,M,KCOMP,IFLAG and IPRNT are inputs to PRAERO and they are the output variables from MAEROS as defined above.

IPLOT = the logical unit number to print the plot. If one is using a time sharing system, it may be useful to have the tabulated results printed on the line printer and have the plots appear on the terminal screen. IPLOT may be set equal to IPRNT for the

plots to be printed on the same device. IPLOT must be an integer.

QMINPL = minimum mass concentration in kg/m^3 to be plotted. If |ISCAL|<2, QMINPL is ignored. QMINPL must be a real number.

QMAXPL = maximum mass concentration to be plotted. If |ISCAL|<2, QMAXPL is ignored. QMAXPL must be a real number.

ISCAL = scaling parameter. The mass concentration axis may be plotted linearly or logarithmically by specifying ISCAL to be positive or negative, respectively. However, as shown in the example problem, if the mass concentration in any section is zero, the code will switch from logarithmic to linear scaling. If |ISCAL| = 1, the code will ignore QMINPL and QMAXPL and choose appropriate bounds for the mass concentration axis. The user may insist on using QMINPL and QMAXPL by setting |ISCAL| = 3. If |ISCAL|=2, the code will use QMINPL and QMAXPL, unless any section concentration is below QMINPL or above QMAXPL. In this case the code will rescale the appropriate bound. In general when one does not know the range of the results, it is best to use ISCAL = -1. In summary, the values of ISCAL may be

-3 user logarithmic scaling

-2 user or automatic logarithmic scaling

-1 automatic logarithmic scaling

0 do not print any plot

1 automatic linear scaling

2 user or automatic linear scaling

3 user linear scaling

ISCAL must be an integer

NROW = number of rows for plotting. NROW must be an integer. Note that since a maximum of 50 rows may be used, the resolution of the plot is not good and one can not expect slight differences in section concentrations to be displayed on a printed plot. However, printed plots provide a very fast and convenient sketch of the results and are extremely useful for quick qualitative analysis. If NROW is less than 13 the code will automatically reset NROW to 13.

NCOL = number of columns for plotting. NCOL must be an integer with a maximum value of 101. Since the code uses the first 18 columns for labelling the y-axis, NCOL+18 columns are required to print a plot. Thus if NCOL = 90, the code will use 108 columns to print a plot. If NCOL is greater than 101, the code will automatically reset NCOL=101. If NCOL is less than two times the number of

sections plus one, the code will automatically increase NCOL to this value. The number of columns used to represent a section will be roughly proportional to the section size based on the logarithm of particle diameter.

IV. COEFFICIENT SPECIFICATION ROUTINES

For those cases in which the existing basic coefficients given in Appendix A do not adequately represent the phenomena of interest, one should change the coefficient specification routines discussed in this chapter. However, if only the parameters need to be changed, that can be accomplished by specifying new values for the parameters through the common block PHYSPT in the MAEROS calling routine, as discussed in the previous Chapter. The user is cautioned that many of the basic coefficients were obtained from those reported in another code[4]. Little research was done on the accuracy of the reported coefficients and one may decide to change some of the existing coefficient specification routines for a particular application.

IV. A. Coefficient Storage

For cases with identical particle size domains (i.e., v_o and v_m), number of sections and basic coefficients, the sectional coefficients should be stored in the routine BLOCK DATA for subsequent use in other simulations. This will avoid the expensive and redundant calculation of recomputing sectional coefficients. One may access the new sectional coefficients after calling MAEROS with a positive value of NEWCOF through the common block,

```
COMMON/DBLK/CT1P1(880),CT1P2(880),CT2P1(880),CT2P2(880)
```

where the arrays CT(I)P(J) contain the sectional coefficients for the I-th temperature (i.e., I=1 for TGAS1 or I=2 for TGAS2) and the J-th pressure (i.e., J=1 for PGAS1 or J=2 for PGAS2). All four arrays in the common block DBLK should be replaced in the BLOCK DATA routine with the new values such that MAEROS may always be called with a negative value of NEWCOF.

IV. B. Coagulation

Any mechanism which results in the collision and subsequent coalescence of particles may be classified as a coagulation process. A compilation of the coagulation coefficient for various mechanisms is given by Drake[5]. The three mechanisms of primary interest are 1)Brownian motion, 2) turbulence and 3) gravity. The functional forms of the coagulation coefficient for each of these mechanisms is given in Appendix A and the sum of the three coefficients is used as the basic coagulation coefficient in the code.

The coagulation coefficient is specified by the subroutine BETA(Y,X,TGAS,PGAS,NBTYPE) where Y and X are the natural logarithms of the masses (in kilograms), of the coagulating particles. TGAS and PGAS are the gas temperature (in K) and pressure (in Pa), respectively. NBTYPE is a flag used in the last part of the routine to convert the coagulation coefficient for sectionalization. Before this conversion, BETA has the units of

m^3/s. The material density of a particle can be determined by calling the routine RHODD, as discussed in Chapter IV.E.

IV. C. Deposition

The three mechanisms considered for aerosol removal are 1) gravitational settling, 2) diffusive wall deposition and 3) thermophoretic wall deposition. The deposition coefficient is specified by the routine DEPOST(X,DUM,TGAS,PGAS,NBTYPE), where X is the natural logarithm of the particle mass (in kilograms), DUM is a dummy argument and TGAS and PGAS are the gas temperature and pressure, respectively. NBTYPE is used to specify the deposition surface, such that the deposition coefficient on the ceiling, vertical walls or floor, is returned for NBTYPE equal to 1, 2 or 3, respectively. The common block PHYSPT discussed in Chapter III may also be used in this routine.

IV. D. Condensation

Condensation of a vapor on to a particle results in particle growth. For isothermal condensation, the growth rate given by Fuchs and Sutugin[7] (as tabulated in Appendix A), is often used to calculate particle growth. The user is cautioned that this expression may not be appropriate for many reactor safety studies. The expression has been used to demonstrate the capabilities of the code and the possible effects of condensation.

To incorporate other expressions for particle growth in MAEROS, the rate at which a particle of mass V increases mass divided by the particle mass should be used for GROWTH(V, DUM,TGAS,PGAS,NDUM) where V is the natural logarithm of the particle mass (in kilograms), DUM is a dummy argument, TGAS and PGAS are the gas temperature and pressure respectively, and NDUM is an integer dummy argument. The user may also incorporate the common block PHYSPT discussed Chapter III. Note that condensation of the last component is calculated only if |NEWCOF| < 10 in the MAEROS calling routine and the growth rate is in units of s^{-1}.

IV. E. Physical Properties

The function routine RHODD(V,D,RHO) is used to specify the material density of the particle RHO (in kg/m^3), given either the mass of the particle V (in kg) or the particle diameter D (in meters). If the particle mass is zero, this flags the routine that the particle diameter must be used to calculate the particle

mass. However, if the particle mass is positive, the particle diameter must be calculated from the particle mass. This routine should be modified only if the material density is a function of particle size. If the material density is constant, it may be specified by assigning the appropriate value to DENSTY in the common block PHYSPT and thus the user avoids modifications to RHODD.

V. SAMPLE PROBLEM

A sample problem is included with the code in the main program. A listing of the main program and the output it produces are given in the following pages. In the sample problem, there are 20 sections logarithmically spaced in particle diameter from 0.01 to 20 microns. The initial aerosol is composed entirely of component 1, for which the aerosolized mass concentration in section I is $1.0 \times 10^{-6} \exp[-(8(I-1)+1)/4]$ kg/m^3. The other 7 components are not contained in the initial aerosol. Components 2 through 7 are generated in section 1 at a rate of $1.0 \times 10^{-9}/I^2$ kg/m^3, where I is the component number. This choice of initial mass concentration and source generation rate is arbitrary. Component 8 is condensing on the aerosol since $|NEWCOF|<10$. By specifying NEWCOF = 2, the sectional coefficients are computed only for a gas temperature and pressure of TGAS1 and PGAS1, respectively. Thus the temperature and pressure for the simulation was set at TGAS1 and PGAS1, respectively.

To print the initial conditions and initialize the cumulative mass deposited, the routine PRAERO is called with IFLAG=1. If $1 \leq |ISCAL| \leq 3$, PRAERO will call the plotting routine PPLOT, which prints on logical unit number IPLOT. In this example, IPLOT and IPRNT are both set at 6, and thus the tabulated results and plots will both be sent to logical unit number 6. By calling MAEROS in the do-loop for ITIME equal 1 to 4, four time steps are taken for output after 1, 10, 60 and 200 seconds of simulation. In general, it is best to request very small initial time steps such that the

code can get an idea of the time scales of the problem. After each call to MAEROS, PRAERO is called to print and plot the results at the end of a time step. Clearly the user may replace PRAERO with another output routine, but it is recommended that PRAERO initially be used until the user is familiar with MAEROS.

For this example, we note that there is no source of component 1. Therefore, after 200 seconds of simulation, the total suspended and deposited mass of component 1 is equal to the initial suspended mass of component 1. Due to condensational growth and scavenging by coagulation, all the mass of component 1 has been removed from section 1 after 200 seconds of simulation. Finally we note that the total suspended and deposited masses of components 2 to 7 are equal to the generation rate of that component multiplied by time and the chamber volume.

```
      PROGRAM MAIN(OUTPUT,INPUT,TAPE6=OUTPUT)
      DIMENSION Q(160),SRATE(160),DEPSIT(3,8),TOUT(4),DIAM(21)
      COMMON/PHYSPT/ACELOV,AFLROV,AWALOV,CHI,DELDIF,DELSAT,DENSTY,FSLIP,
     $FTHERM,GAMMA,PSAT,STICK,TGRADC,TGRADF,TGRADW,TKGOP,TURBDS,VOLUME,
     $WTCONM,WTMOL
C
C       FOR CDC 6600/7600 AND DEC/VAX COMPUTERS A DATA STATEMENT MAY
C      BE USED FOR INITIALIZING THE VARIABLES IN THE COMMON BLOCK PHYSPT
C
C     DATA ACELOV,AFLROV,AWALOV,CHI,DELDIF,DELSAT,DENSTY,FSLIP,FTHERM,
C    $GAMMA,PSAT,STICK,TGRADC,TGRADF,TGRADW,TKGOP,TURBDS,VOLUME,WTCONM,
C    $WTMOL/
C    $ 1.07,1.07,2.29,1.,1.E-5,1.E-11,1.E3,1.37,1.,1.,3.16E3,1.,0.,0.,
C    $0.,.05,.001,2.86,3.0E-26,28.8/
      DATA M,KCOMP,IPRNT,IPLOT,ISCAL,NROW,NCOL,QMINPL,QMAXPL,TGAS1,
     $TGAS2,PGAS1,PGAS2,TOUT
     $/20,8,6,6,0,45,101,1.E-6,1.,298.,450.,1.01E5,7.E5,1.,10.,60.,200./
C
C     SET VARIABLES IN COMMON BLOCK PHYSPT
C
      ACELOV=1.07
      AFLROV=1.07
      AWALOV=2.29
      CHI=1.
      DELDIF=1.E-5
      DELSAT=1.E-11
      DENSTY=1.E3
      FSLIP=1.37
      FTHERM=1.
      GAMMA=1.
      PSAT=3.16E3
      STICK=1.
      TGRADC=0.
      TGRADF=0.
      TGRADW=0.
      TKGOP=.05
      TURBDS=.001
      VOLUME=2.86
      WTCONM=3.0E-26
      WTMOL=28.8
C
C      SET SECTION BOUNDARIES
C
      DIAM(1)=.01E-6
      DIAM(M+1)=20.E-6
      DO 2 I=2,M
    2 DIAM(I)=DIAM(1)*(DIAM(M+1)/DIAM(1))**(FLOAT(I-1)/FLOAT(M))
C
C      INITIALIZE ALL SOURCES AND SECTION CONCENTRATIONS TO ZERO
C
      MKCOMP=M*KCOMP
      DO 4 I=1,MKCOMP
      Q(I)=0.
    4 SRATE(I)=0.
C
C     DETERMINE INITIAL CONCENTRATIONS OF THE FIRST COMPONENT AND THE
C     SOURCE RATE IN SECTION 1 FOR COMPONENTS 2-7
C
      DO 1 I=1,MKCOMP,8
    1 Q(I)=1.E-6*EXP(-.25*FLOAT(I))
      DO 6 I=2,7
    6 SRATE(I)=1.E-9/FLOAT(I*I)
C
```

```
C     SET TGAS=TGAS1 AND PGAS=PGAS1 TO USE SECTIONAL COEFFICIENTS
C     AT THESE TEMPERATURES AND PRESSURES
C
      TGAS=TGAS1
      PGAS=PGAS1
      TIME=0.
      ROUND=7.7E-15
      IFLAG=1
      NEWCOF=2
C
C     CALL THE ROUTINE PRAERO TO PRINT THE INITIAL CONCENTRATIONS
C     BEFORE CALLING MAEROS TO INTEGRATE IN TIME TO TOUT(1). CALL MAEROS
C     FOR EACH TIME OUTPUT IS REQUIRED FOLLOWED BY A CALL TO PRAERO.
C     NOTE THAT BY SETTING ISCAL TO -1 FOR ITIME=4, PLOTS WILL BE
C     GENERATED ONLY ON THE LAST CALL TO MAEROS, SINCE ISCAL WAS
C     INITIALIZED TO ZERO IN THE DATA STATEMENT.
C
      CALL PRAERO(Q,DEPSIT,DIAM,TIME,VOLUME,M,KCOMP,IFLAG,IPRNT,IPLOT,
     $QMINPL,QMAXPL,ISCAL,NROW,NCOL)
      DO 3 ITIME=1,4
      IF(ITIME.EQ.4)ISCAL=-1
      DELTIM=TOUT(ITIME)-TIME
      CALL MAEROS(M,KCOMP,TIME,DELTIM,Q,SRATE,TGAS,PGAS,DEPSIT,DIAM,
     $ TGAS1,TGAS2,PGAS1,PGAS2,ROUND,IPRNT,IFLAG,NEWCOF)
    3 CALL PRAERO(Q,DEPSIT,DIAM,TIME,VOLUME,M,KCOMP,IFLAG,IPRNT,IPLOT,
     $QMINPL,QMAXPL,ISCAL,NROW,NCOL)
C
      STOP
      END
```

TIME =0. SECONDS

SECTION	DIAMETER RANGE (M)	KG/M**3	NUMBER/M**3	KG
1	.1000E-07 -- .1462E-07	.7788E-06	.8874E+15	.2227E-05
2	.1462E-07 -- .2138E-07	.1054E-06	.3840E+14	.3014E-06
3	.2138E-07 -- .3127E-07	.1426E-07	.1662E+13	.4080E-07
4	.3127E-07 -- .4573E-07	.1930E-08	.7193E+11	.5521E-08
5	.4573E-07 -- .6687E-07	.2613E-09	.3113E+10	.7472E-09
6	.6687E-07 -- .9779E-07	.3536E-10	.1347E+09	.1011E-09
7	.9779E-07 -- .1430E-06	.4785E-11	.5830E+07	.1369E-10
8	.1430E-06 -- .2091E-06	.6476E-12	.2523E+06	.1852E-11
9	.2091E-06 -- .3058E-06	.8764E-13	.1092E+05	.2507E-12
10	.3058E-06 -- .4472E-06	.1186E-13	.4725E+03	.3392E-13
11	.4472E-06 -- .6540E-06	.1605E-14	.2045E+02	.4591E-14
12	.6540E-06 -- .9564E-06	.2172E-15	.8850E+00	.6213E-15
13	.9564E-06 -- .1399E-05	.2940E-16	.3830E-01	.8409E-16
14	.1399E-05 -- .2045E-05	.3979E-17	.1658E-02	.1138E-16
15	.2045E-05 -- .2991E-05	.5385E-18	.7173E-04	.1540E-17
16	.2991E-05 -- .4373E-05	.7288E-19	.3104E-05	.2084E-18
17	.4373E-05 -- .6396E-05	.9863E-20	.1343E-06	.2821E-19
18	.6396E-05 -- .9352E-05	.1335E-20	.5814E-08	.3818E-20
19	.9352E-05 -- .1368E-04	.1806E-21	.2516E-09	.5166E-21
20	.1368E-04 -- .2000E-04	.2445E-22	.1089E-10	.6992E-22
	TOTAL	.9007E-06	.9275E+15	.2576E-05

COMPONENT (KG/M**3)

DIAMETER RANGE (M)	1	2	3	4	5	6	7	8
.1000E-07 -- .1462E-07	.7788E-06	0.	0.	0.	0.	0.	0.	0.
.1462E-07 -- .2138E-07	.1054E-06	0.	0.	0.	0.	0.	0.	0.
.2138E-07 -- .3127E-07	.1426E-07	0.	0.	0.	0.	0.	0.	0.
.3127E-07 -- .4573E-07	.1930E-08	0.	0.	0.	0.	0.	0.	0.
.4573E-07 -- .6687E-07	.2613E-09	0.	0.	0.	0.	0.	0.	0.
.6687E-07 -- .9779E-07	.3536E-10	0.	0.	0.	0.	0.	0.	0.
.9779E-07 -- .1430E-06	.4785E-11	0.	0.	0.	0.	0.	0.	0.
.1430E-06 -- .2091E-06	.6476E-12	0.	0.	0.	0.	0.	0.	0.
.2091E-06 -- .3058E-06	.8764E-13	0.	0.	0.	0.	0.	0.	0.
.3058E-06 -- .4472E-06	.1186E-13	0.	0.	0.	0.	0.	0.	0.
.4472E-06 -- .6540E-06	.1605E-14	0.	0.	0.	0.	0.	0.	0.
.6540E-06 -- .9564E-06	.2172E-15	0.	0.	0.	0.	0.	0.	0.
.9564E-06 -- .1399E-05	.2940E-16	0.	0.	0.	0.	0.	0.	0.
.1399E-05 -- .2045E-05	.3979E-17	0.	0.	0.	0.	0.	0.	0.
.2045E-05 -- .2991E-05	.5385E-18	0.	0.	0.	0.	0.	0.	0.
.2991E-05 -- .4373E-05	.7288E-19	0.	0.	0.	0.	0.	0.	0.
.4373E-05 -- .6396E-05	.9863E-20	0.	0.	0.	0.	0.	0.	0.
.6396E-05 -- .9352E-05	.1335E-20	0.	0.	0.	0.	0.	0.	0.
.9352E-05 -- .1368E-04	.1806E-21	0.	0.	0.	0.	0.	0.	0.
.1368E-04 -- .2000E-04	.2445E-22	0.	0.	0.	0.	0.	0.	0.
TOTAL (KG/M**3)	.9007E-06	0.	0.	0.	0.	0.	0.	0.
TOTAL (KG)	.2576E-05	0.	0.	0.	0.	0.	0.	0.

TIME = .1000E+01 SECONDS

SECTION	DIAMETER RANGE (M)	KG/M**3	NUMBER/M**3	KG
1	.1000E-07 -- .1462E-07	.2618E-06	.2983E+15	.7488E-06
2	.1462E-07 -- .2138E-07	.4230E-06	.1541E+15	.1210E-05
3	.2138E-07 -- .3127E-07	.1830E-06	.2132E+14	.5234E-06
4	.3127E-07 -- .4573E-07	.2101E-07	.7828E+12	.6009E-07
5	.4573E-07 -- .6687E-07	.1018E-08	.1213E+11	.2911E-08
6	.6687E-07 -- .9779E-07	.5759E-10	.2194E+09	.1647E-09
7	.9779E-07 -- .1430E-06	.5785E-11	.7048E+07	.1654E-10
8	.1430E-06 -- .2091E-06	.7075E-12	.2756E+06	.2023E-11
9	.2091E-06 -- .3058E-06	.9147E-13	.1140E+05	.2616E-12
10	.3058E-06 -- .4472E-06	.1211E-13	.4824E+03	.3463E-13
11	.4472E-06 -- .6540E-06	.1621E-14	.2065E+02	.4636E-14
12	.6540E-06 -- .9564E-06	.2183E-15	.8891E+00	.6242E-15
13	.9564E-06 -- .1399E-05	.2946E-16	.3838E-01	.8427E-16
14	.1399E-05 -- .2045E-05	.3983E-17	.1659E-02	.1139E-16
15	.2045E-05 -- .2991E-05	.5386E-18	.7175E-04	.1541E-17
16	.2991E-05 -- .4373E-05	.7286E-19	.3104E-05	.2084E-18
17	.4373E-05 -- .6396E-05	.9855E-20	.1342E-06	.2818E-19
18	.6396E-05 -- .9352E-05	.1332E-20	.5803E-08	.3810E-20
19	.9352E-05 -- .1368E-04	.1799E-21	.2506E-09	.5145E-21
20	.1368E-04 -- .2000E-04	.2423E-22	.1079E-10	.6929E-22
	TOTAL	.8899E-06	.4746E+15	.2545E-05

COMPONENT (KG/M**3)

DIAMETER RANGE (M)	1	2	3	4	5	6	7	8
.1000E-07 -- .1462E-07	.2615E-06	.1579E-09	.7016E-10	.3946E-10	.2526E-10	.1754E-10	.1289E-10	.7931E-11
.1462E-07 -- .2138E-07	.4228E-06	.6895E-10	.3065E-10	.1724E-10	.1103E-10	.7661E-11	.5629E-11	.1006E-10
.2138E-07 -- .3127E-07	.1830E-06	.1972E-10	.8765E-11	.4930E-11	.3155E-11	.2191E-11	.1610E-11	.3588E-11
.3127E-07 -- .4573E-07	.2101E-07	.1573E-11	.6993E-12	.3934E-12	.2517E-12	.1748E-12	.1284E-12	.3339E-12
.4573E-07 -- .6687E-07	.1018E-08	.4089E-13	.1817E-13	.1022E-13	.6542E-14	.4543E-14	.3338E-14	.1113E-13
.6687E-07 -- .9779E-07	.5759E-10	.6384E-15	.2837E-15	.1596E-15	.1021E-15	.7093E-16	.5211E-16	.3039E-15
.9779E-07 -- .1430E-06	.5785E-11	.1914E-16	.8509E-17	.4786E-17	.3063E-17	.2127E-17	.1563E-17	.1510E-16
.1430E-06 -- .2091E-06	.7075E-12	.1065E-17	.4732E-18	.2662E-18	.1704E-18	.1183E-18	.8692E-19	.1012E-17
.2091E-06 -- .3058E-06	.9147E-13	.6655E-19	.2958E-19	.1664E-19	.1065E-19	.7394E-20	.5433E-20	.7073E-19
.3058E-06 -- .4472E-06	.1211E-13	.4250E-20	.1889E-20	.1062E-20	.6799E-21	.4722E-21	.3469E-21	.4895E-20
.4472E-06 -- .6540E-06	.1621E-14	.2725E-21	.1211E-21	.6811E-22	.4359E-22	.3027E-22	.2224E-22	.3324E-21
.6540E-06 -- .9564E-06	.2183E-15	.1745E-22	.7755E-23	.4362E-23	.2792E-23	.1939E-23	.1424E-23	.2215E-22
.9564E-06 -- .1399E-05	.2946E-16	.1115E-23	.4954E-24	.2786E-24	.1783E-24	.1238E-24	.9099E-25	.1454E-23
.1399E-05 -- .2045E-05	.3983E-17	.7103E-25	.3157E-25	.1776E-25	.1136E-25	.7892E-26	.5798E-26	.9439E-25
.2045E-05 -- .2991E-05	.5386E-18	.4518E-26	.2008E-26	.1129E-26	.7228E-27	.5020E-27	.3688E-27	.6078E-26
.2991E-05 -- .4373E-05	.7286E-19	.2869E-27	.1275E-27	.7172E-28	.4590E-28	.3187E-28	.2342E-28	.3892E-27
.4373E-05 -- .6396E-05	.9855E-20	.1819E-28	.8086E-29	.4548E-29	.2911E-29	.2021E-29	.1485E-29	.2482E-28
.6396E-05 -- .9352E-05	.1332E-20	.1152E-29	.5122E-30	.2881E-30	.1844E-30	.1281E-30	.9408E-31	.1578E-29
.9352E-05 -- .1368E-04	.1799E-21	.7293E-31	.3241E-31	.1823E-31	.1167E-31	.8103E-32	.5953E-32	.1000E-30
.1368E-04 -- .2000E-04	.2423E-22	.4610E-32	.2049E-32	.1153E-32	.7376E-33	.5122E-33	.3763E-33	.6318E-32
TOTAL (KG/M**3)	.8893E-06	.2481E-09	.1103E-09	.6203E-10	.3970E-10	.2757E-10	.2026E-10	.2193E-10
TOTAL (KG)	.2543E-05	.7097E-09	.3154E-09	.1774E-09	.1135E-09	.7885E-10	.5793E-10	.6271E-10

TOTAL DEPOSITED MASS = .3251E-07 KG CUMULATIVE = .3251E-07 KG

CEILING (KG)	.7848E-08	.1286E-11	.5717E-12	.3216E-12	.2058E-12	.1429E-12	.1050E-12	.4797E-12
VERTICAL WALLS (KG)	.1680E-07	.2753E-11	.1224E-11	.6883E-12	.4405E-12	.3059E-12	.2248E-12	.1027E-11
FLOOR (KG)	.7849E-08	.1286E-11	.5718E-12	.3216E-12	.2058E-12	.1429E-12	.1050E-12	.4798E-12
TOTAL (KG)	.3249E-07	.5326E-11	.2367E-11	.1332E-11	.8522E-12	.5918E-12	.4348E-12	.1986E-11
CUMULATIVE (KG)	.3249E-07	.5326E-11	.2367E-11	.1332E-11	.8522E-12	.5918E-12	.4348E-12	.1986E-11

TIME = .1000E+02 SECONDS

SECTION	DIAMETER RANGE (M)	KG/M**3	NUMBER/M**3	KG
1	.1000E-07 -- .1462E-07	.6077E-08	.6924E+13	.1738E-07
2	.1462E-07 -- .2138E-07	.5706E-07	.2079E+14	.1632E-06
3	.2138E-07 -- .3127E-07	.2746E-06	.3200E+14	.7854E-06
4	.3127E-07 -- .4573E-07	.3851E-06	.1435E+14	.1101E-05
5	.4573E-07 -- .6687E-07	.1237E-06	.1474E+13	.3537E-06
6	.6687E-07 -- .9779E-07	.9341E-08	.3559E+11	.2671E-07
7	.9779E-07 -- .1430E-06	.2157E-09	.2627E+09	.6168E-09
8	.1430E-06 -- .2091E-06	.2700E-11	.1052E+07	.7721E-11
9	.2091E-06 -- .3058E-06	.1145E-12	.1426E+05	.3275E-12
10	.3058E-06 -- .4472E-06	.1309E-13	.5215E+03	.3744E-13
11	.4472E-06 -- .6540E-06	.1679E-14	.2139E+02	.4803E-14
12	.6540E-06 -- .9564E-06	.2218E-15	.9036E+00	.6344E-15
13	.9564E-06 -- .1399E-05	.2968E-16	.3866E-01	.8488E-16
14	.1399E-05 -- .2045E-05	.3993E-17	.1663E-02	.1142E-16
15	.2045E-05 -- .2991E-05	.5385E-18	.7173E-04	.1540E-17
16	.2991E-05 -- .4373E-05	.7262E-19	.3094E-05	.2077E-18
17	.4373E-05 -- .6396E-05	.9775E-20	.1331E-06	.2796E-19
18	.6396E-05 -- .9352E-05	.1309E-20	.5701E-08	.3743E-20
19	.9352E-05 -- .1368E-04	.1732E-21	.2412E-09	.4953E-21
20	.1368E-04 -- .2000E-04	.2234E-22	.9952E-11	.6390E-22
	TOTAL	.8561E-06	.7557E+14	.2448E-05

COMPONENT (KG/M**3)

DIAMETER RANGE (M)	1	2	3	4	5	6	7	8
.1000E-07 -- .1462E-07	.4597E-08	.7220E-09	.3209E-09	.1805E-09	.1155E-09	.8023E-10	.5894E-10	.1501E-11
.1462E-07 -- .2138E-07	.5656E-07	.2391E-09	.1063E-09	.5977E-10	.3825E-10	.2656E-10	.1952E-10	.1238E-10
.2138E-07 -- .3127E-07	.2733E-06	.6363E-09	.2828E-09	.1591E-09	.1018E-09	.7070E-10	.5194E-10	.4608E-10
.3127E-07 -- .4573E-07	.3837E-06	.6256E-09	.2781E-09	.1564E-09	.1001E-09	.6951E-10	.5107E-10	.5355E-10
.4573E-07 -- .6687E-07	.1233E-06	.1562E-09	.6942E-10	.3905E-10	.2499E-10	.1736E-10	.1275E-10	.1483E-10
.6687E-07 -- .9779E-07	.9320E-08	.9403E-11	.4179E-11	.2351E-11	.1504E-11	.1045E-11	.7676E-12	.9702E-12
.9779E-07 -- .1430E-06	.2153E-09	.1670E-12	.7421E-13	.4174E-13	.2671E-13	.1855E-13	.1363E-13	.1873E-13
.1430E-06 -- .2091E-06	.2697E-11	.1152E-14	.5122E-15	.2881E-15	.1844E-15	.1281E-15	.9408E-16	.1452E-15
.2091E-06 -- .3058E-06	.1145E-12	.7789E-17	.3462E-17	.1947E-17	.1246E-17	.8654E-18	.6358E-18	.1355E-17
.3058E-06 -- .4472E-06	.1309E-13	.2871E-18	.1276E-18	.7177E-19	.4593E-19	.3190E-19	.2344E-19	.6073E-19
.4472E-06 -- .6540E-06	.1679E-14	.1717E-19	.7629E-20	.4292E-20	.2747E-20	.1907E-20	.1401E-20	.3843E-20
.6540E-06 -- .9564E-06	.2218E-15	.1070E-20	.4755E-21	.2674E-21	.1712E-21	.1189E-21	.8733E-22	.2485E-21
.9564E-06 -- .1399E-05	.2968E-16	.6745E-22	.2998E-22	.1686E-22	.1079E-22	.7494E-23	.5506E-23	.1607E-22
.1399E-05 -- .2045E-05	.3993E-17	.4269E-23	.1897E-23	.1067E-23	.6830E-24	.4743E-24	.3485E-24	.1035E-23
.2045E-05 -- .2991E-05	.5385E-18	.2704E-24	.1202E-24	.6759E-25	.4326E-25	.3004E-25	.2207E-25	.6631E-25
.2991E-05 -- .4373E-05	.7262E-19	.1710E-25	.7601E-26	.4276E-26	.2737E-26	.1900E-26	.1396E-26	.4228E-26
.4373E-05 -- .6396E-05	.9775E-20	.1079E-26	.4795E-27	.2697E-27	.1726E-27	.1199E-27	.8808E-28	.2682E-27
.6396E-05 -- .9352E-05	.1309E-20	.6768E-28	.3008E-28	.1692E-28	.1083E-28	.7520E-29	.5525E-29	.1688E-28
.9352E-05 -- .1368E-04	.1732E-21	.4199E-29	.1866E-29	.1050E-29	.6718E-30	.4665E-30	.3428E-30	.1048E-29
.1368E-04 -- .2000E-04	.2234E-22	.2547E-30	.1132E-30	.6367E-31	.4075E-31	.2830E-31	.2079E-31	.6348E-31
TOTAL (KG/M**3)	.8510E-06	.2389E-08	.1062E-08	.5972E-09	.3822E-09	.2654E-09	.1950E-09	.1293E-09
TOTAL (KG)	.2434E-05	.6832E-08	.3036E-08	.1708E-08	.1093E-08	.7591E-09	.5577E-09	.3699E-09

TOTAL DEPOSITED MASS = .1102E-06 KG CUMULATIVE = .1427E-06 KG

CEILING (KG)	.2645E-07	.7554E-10	.3357E-10	.1888E-10	.1209E-10	.8393E-11	.6166E-11	.1462E-10
VERTICAL WALLS (KG)	.5661E-07	.1617E-09	.7186E-10	.4042E-10	.2587E-10	.1796E-10	.1320E-10	.3129E-10
FLOOR (KG)	.2645E-07	.7555E-10	.3358E-10	.1889E-10	.1209E-10	.8395E-11	.6167E-11	.1463E-10
TOTAL (KG)	.1095E-06	.3128E-09	.1390E-09	.7819E-10	.5004E-10	.3475E-10	.2553E-10	.6054E-10
CUMULATIVE (KG)	.1420E-06	.3181E-09	.1414E-09	.7952E-10	.5089E-10	.3534E-10	.2597E-10	.6252E-10

TIME = .6000E+02 SECONDS

SECTION	DIAMETER RANGE (M)	KG/M**3	NUMBER/M**3	KG
1	.1000E-07 -- .1462E-07	.4275E-08	.4871E+13	.1223E-07
2	.1462E-07 -- .2138E-07	.7829E-09	.2853E+12	.2239E-08
3	.2138E-07 -- .3127E-07	.1448E-07	.1687E+13	.4140E-07
4	.3127E-07 -- .4573E-07	.1421E-06	.5296E+13	.4065E-06
5	.4573E-07 -- .6687E-07	.3909E-06	.4657E+13	.1118E-05
6	.6687E-07 -- .9779E-07	.2329E-06	.8875E+12	.6662E-06
7	.9779E-07 -- .1430E-06	.2847E-07	.3469E+11	.8143E-07
8	.1430E-06 -- .2091E-06	.8579E-09	.3342E+09	.2454E-08
9	.2091E-06 -- .3058E-06	.8340E-11	.1039E+07	.2385E-10
10	.3058E-06 -- .4472E-06	.4444E-13	.1770E+04	.1271E-12
11	.4472E-06 -- .6540E-06	.1840E-14	.2344E+02	.5262E-14
12	.6540E-06 -- .9564E-06	.2284E-15	.9303E+00	.6531E-15
13	.9564E-06 -- .1399E-05	.3001E-16	.3909E-01	.8582E-16
14	.1399E-05 -- .2045E-05	.3997E-17	.1665E-02	.1143E-16
15	.2045E-05 -- .2991E-05	.5343E-18	.7117E-04	.1528E-17
16	.2991E-05 -- .4373E-05	.7111E-19	.3029E-05	.2034E-18
17	.4373E-05 -- .6396E-05	.9331E-20	.1271E-06	.2669E-19
18	.6396E-05 -- .9352E-05	.1185E-20	.5161E-08	.3389E-20
19	.9352E-05 -- .1368E-04	.1402E-21	.1952E-09	.4009E-21
20	.1368E-04 -- .2000E-04	.1424E-22	.6343E-11	.4073E-22
	TOTAL	.8148E-06	.1772E+14	.2330E-05

COMPONENT (KG/M**3)

DIAMETER RANGE (M)	1	2	3	4	5	6	7	8
.1000E-07 -- .1462E-07	.1832E-11	.2087E-08	.9275E-09	.5217E-09	.3339E-09	.2319E-09	.1704E-09	.1011E-11
.1462E-07 -- .2138E-07	.4035E-09	.1850E-09	.8221E-10	.4624E-10	.2959E-10	.2055E-10	.1510E-10	.6691E-12
.2138E-07 -- .3127E-07	.1347E-07	.4837E-09	.2150E-09	.1209E-09	.7738E-10	.5374E-10	.3948E-10	.1219E-10
.3127E-07 -- .4573E-07	.1365E-06	.2710E-08	.1204E-08	.6775E-09	.4336E-09	.3011E-09	.2212E-09	.8983E-10
.4573E-07 -- .6687E-07	.3804E-06	.5020E-08	.2231E-08	.1255E-08	.8032E-09	.5578E-09	.4098E-09	.1989E-09
.6687E-07 -- .9779E-07	.2282E-06	.2269E-08	.1008E-08	.5672E-09	.3630E-09	.2521E-09	.1852E-09	.1011E-09
.9779E-07 -- .1430E-06	.2801E-07	.2218E-09	.9856E-10	.5544E-10	.3548E-10	.2464E-10	.1810E-10	.1079E-10
.1430E-06 -- .2091E-06	.8466E-09	.5377E-11	.2390E-11	.1344E-11	.8603E-12	.5974E-12	.4389E-12	.2835E-12
.2091E-06 -- .3058E-06	.8253E-11	.4137E-13	.1839E-13	.1034E-13	.6619E-14	.4597E-14	.3377E-14	.2362E-14
.3058E-06 -- .4472E-06	.4418E-13	.1239E-15	.5505E-16	.3097E-16	.1982E-16	.1376E-16	.1011E-16	.7704E-17
.4472E-06 -- .6540E-06	.1839E-14	.4786E-18	.2127E-18	.1196E-18	.7657E-19	.5318E-19	.3907E-19	.3522E-19
.6540E-06 -- .9564E-06	.2283E-15	.2037E-19	.9052E-20	.5092E-20	.3259E-20	.2263E-20	.1663E-20	.1612E-20
.9564E-06 -- .1399E-05	.3001E-16	.1248E-20	.5548E-21	.3121E-21	.1997E-21	.1387E-21	.1019E-21	.1013E-21
.1399E-05 -- .2045E-05	.3997E-17	.7795E-22	.3464E-22	.1949E-22	.1247E-22	.8661E-23	.6363E-23	.6430E-23
.2045E-05 -- .2991E-05	.5343E-18	.4884E-23	.2171E-23	.1221E-23	.7814E-24	.5426E-24	.3987E-24	.4075E-24
.2991E-05 -- .4373E-05	.7111E-19	.3046E-24	.1354E-24	.7614E-25	.4873E-25	.3384E-25	.2486E-25	.2561E-25
.4373E-05 -- .6396E-05	.9331E-20	.1872E-25	.8321E-26	.4680E-26	.2995E-26	.2080E-26	.1528E-26	.1582E-26
.6396E-05 -- .9352E-05	.1185E-20	.1114E-26	.4951E-27	.2785E-27	.1782E-27	.1238E-27	.9093E-28	.9444E-28
.9352E-05 -- .1368E-04	.1402E-21	.6184E-28	.2748E-28	.1546E-28	.9894E-29	.6871E-29	.5048E-29	.5248E-29
.1368E-04 -- .2000E-04	.1424E-22	.2965E-29	.1318E-29	.7413E-30	.4745E-30	.3295E-30	.2421E-30	.2509E-30
TOTAL (KG/M**3)	.7878E-06	.1298E-07	.5769E-08	.3245E-08	.2077E-08	.1442E-08	.1060E-08	.4148E-09
TOTAL (KG)	.2253E-05	.3713E-07	.1650E-07	.9282E-08	.5940E-08	.4125E-08	.3031E-08	.1186E-08

TOTAL DEPOSITED MASS = .1922E-06 KG CUMULATIVE = .3349E-06 KG

CEILING (KG)	.4364E-07	.1317E-08	.5854E-09	.3293E-09	.2108E-09	.1464E-09	.1075E-09	.4645E-10
VERTICAL WALLS (KG)	.9348E-07	.2820E-08	.1253E-08	.7050E-09	.4512E-09	.3133E-09	.2302E-09	.9953E-10
FLOOR (KG)	.4372E-07	.1318E-08	.5858E-09	.3295E-09	.2109E-09	.1465E-09	.1076E-09	.4656E-10
TOTAL (KG)	.1808E-06	.5455E-08	.2425E-08	.1364E-08	.8729E-09	.6061E-09	.4453E-09	.1925E-09
CUMULATIVE (KG)	.3229E-06	.5773E-08	.2566E-08	.1443E-08	.9238E-09	.6415E-09	.4713E-09	.2551E-09

TIME = .2000E+03 SECONDS

SECTION	DIAMETER RANGE (M)	KG/M**3	NUMBER/M**3	KG
1	.1000E-07 -- .1462E-07	.6671E-08	.7601E+13	.1908E-07
2	.1462E-07 -- .2138E-07	.1791E-08	.6526E+12	.5122E-08
3	.2138E-07 -- .3127E-07	.6757E-09	.7873E+11	.1933E-08
4	.3127E-07 -- .4573E-07	.1497E-07	.5577E+12	.4281E-07
5	.4573E-07 -- .6687E-07	.1546E-06	.1842E+13	.4423E-06
6	.6687E-07 -- .9779E-07	.3907E-06	.1489E+13	.1117E-05
7	.9779E-07 -- .1430E-06	.2022E-06	.2463E+12	.5783E-06
8	.1430E-06 -- .2091E-06	.2132E-07	.8307E+10	.6098E-07
9	.2091E-06 -- .3058E-06	.5615E-09	.6996E+08	.1606E-08
10	.3058E-06 -- .4472E-06	.4729E-11	.1884E+06	.1353E-10
11	.4472E-06 -- .6540E-06	.1649E-13	.2101E+03	.4716E-13
12	.6540E-06 -- .9564E-06	.2556E-15	.1041E+01	.7309E-15
13	.9564E-06 -- .1399E-05	.3039E-16	.3959E-01	.8691E-16
14	.1399E-05 -- .2045E-05	.3974E-17	.1655E-02	.1137E-16
15	.2045E-05 -- .2991E-05	.5205E-18	.6934E-04	.1489E-17
16	.2991E-05 -- .4373E-05	.6691E-19	.2850E-05	.1914E-18
17	.4373E-05 -- .6396E-05	.8184E-20	.1115E-06	.2341E-19
18	.6396E-05 -- .9352E-05	.8966E-21	.3906E-08	.2564E-20
19	.9352E-05 -- .1368E-04	.7750E-22	.1080E-09	.2217E-21
20	.1368E-04 -- .2000E-04	.4036E-23	.1798E-11	.1154E-22
	TOTAL	.7935E-06	.1248E+14	.2270E-05

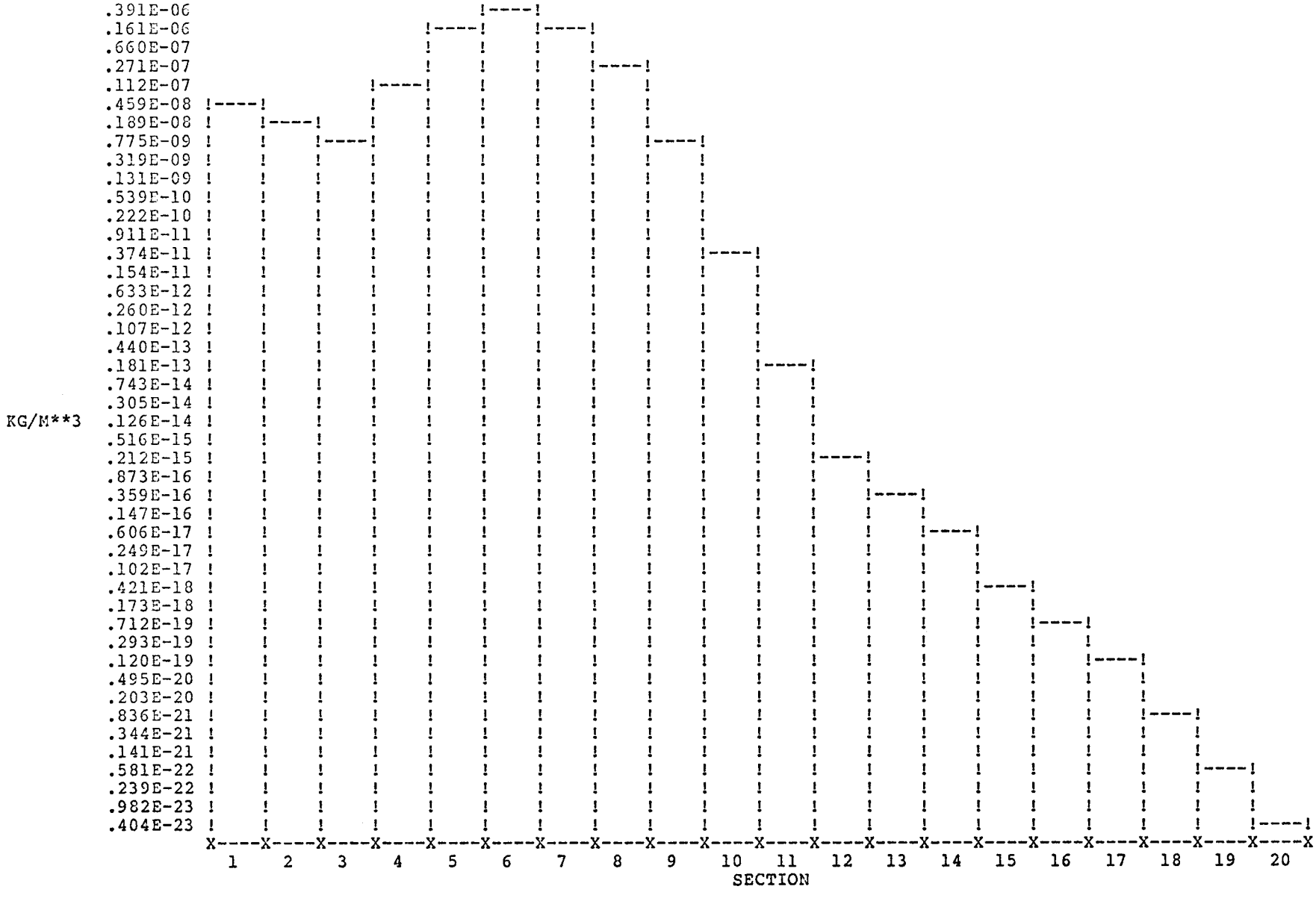
COMPONENT (KG/M**3)

DIAMETER RANGE (M)	1	2	3	4	5	6	7	8
.1000E-07 -- .1462E-07	0.	.3257E-08	.1448E-08	.8143E-09	.5212E-09	.3619E-09	.2659E-09	.2585E-11
.1462E-07 -- .2138E-07	.3873E-12	.8739E-09	.3884E-09	.2185E-09	.1398E-09	.9710E-10	.7134E-10	.1437E-11
.2138E-07 -- .3127E-07	.2382E-09	.2131E-09	.9473E-10	.5329E-10	.3410E-10	.2368E-10	.1740E-10	.1158E-11
.3127E-07 -- .4573E-07	.1195E-07	.1461E-08	.6493E-09	.3652E-09	.2337E-09	.1623E-09	.1193E-09	.2619E-10
.4573E-07 -- .6687E-07	.1357E-06	.9138E-08	.4062E-08	.2285E-08	.1462E-08	.1015E-08	.7460E-09	.2071E-09
.6687E-07 -- .9779E-07	.3575E-06	.1600E-07	.7111E-08	.4000E-08	.2560E-08	.1778E-08	.1306E-08	.4241E-09
.9779E-07 -- .1430E-06	.1889E-06	.6387E-08	.2839E-08	.1597E-08	.1022E-08	.7097E-09	.5214E-09	.1876E-09
.1430E-06 -- .2091E-06	.2019E-07	.5455E-09	.2424E-09	.1364E-09	.8728E-10	.6061E-10	.4453E-10	.1731E-10
.2091E-06 -- .3058E-06	.5371E-09	.1174E-10	.5219E-11	.2936E-11	.1879E-11	.1305E-11	.9586E-12	.3998E-12
.3058E-06 -- .4472E-06	.4561E-11	.8077E-13	.3590E-13	.2019E-13	.1292E-13	.8975E-14	.6594E-14	.2944E-14
.4472E-06 -- .6540E-06	.1606E-13	.2072E-15	.9210E-16	.5181E-16	.3316E-16	.2303E-16	.1692E-16	.8071E-17
.6540E-06 -- .9564E-06	.2549E-15	.3360E-18	.1493E-18	.8401E-19	.5376E-19	.3734E-19	.2743E-19	.1436E-19
.9564E-06 -- .1399E-05	.3037E-16	.7762E-20	.3450E-20	.1941E-20	.1242E-20	.8625E-21	.6337E-21	.3565E-21
.1399E-05 -- .2045E-05	.3973E-17	.4681E-21	.2080E-21	.1170E-21	.7489E-22	.5201E-22	.3821E-22	.2186E-22
.2045E-05 -- .2991E-05	.5205E-18	.2866E-22	.1274E-22	.7165E-23	.4585E-23	.3184E-23	.2340E-23	.1354E-23
.2991E-05 -- .4373E-05	.6691E-19	.1724E-23	.7661E-24	.4309E-24	.2758E-24	.1915E-24	.1407E-24	.8205E-25
.4373E-05 -- .6396E-05	.8184E-20	.9871E-25	.4387E-25	.2468E-25	.1579E-25	.1097E-25	.8058E-26	.4723E-26
.6396E-05 -- .9352E-05	.8966E-21	.5068E-26	.2253E-26	.1267E-26	.8109E-27	.5631E-27	.4137E-27	.2432E-27
.9352E-05 -- .1368E-04	.7750E-22	.2059E-27	.9153E-28	.5148E-28	.3295E-28	.2288E-28	.1681E-28	.9886E-29
.1368E-04 -- .2000E-04	.4036E-23	.5089E-29	.2262E-29	.1272E-29	.8142E-30	.5654E-30	.4154E-30	.2432E-30
TOTAL (KG/M**3)	.7151E-06	.3789E-07	.1684E-07	.9472E-08	.6062E-08	.4210E-08	.3093E-08	.8678E-09
TOTAL (KG)	.2045E-05	.1084E-06	.4816E-07	.2709E-07	.1734E-07	.1204E-07	.8846E-08	.2482E-08

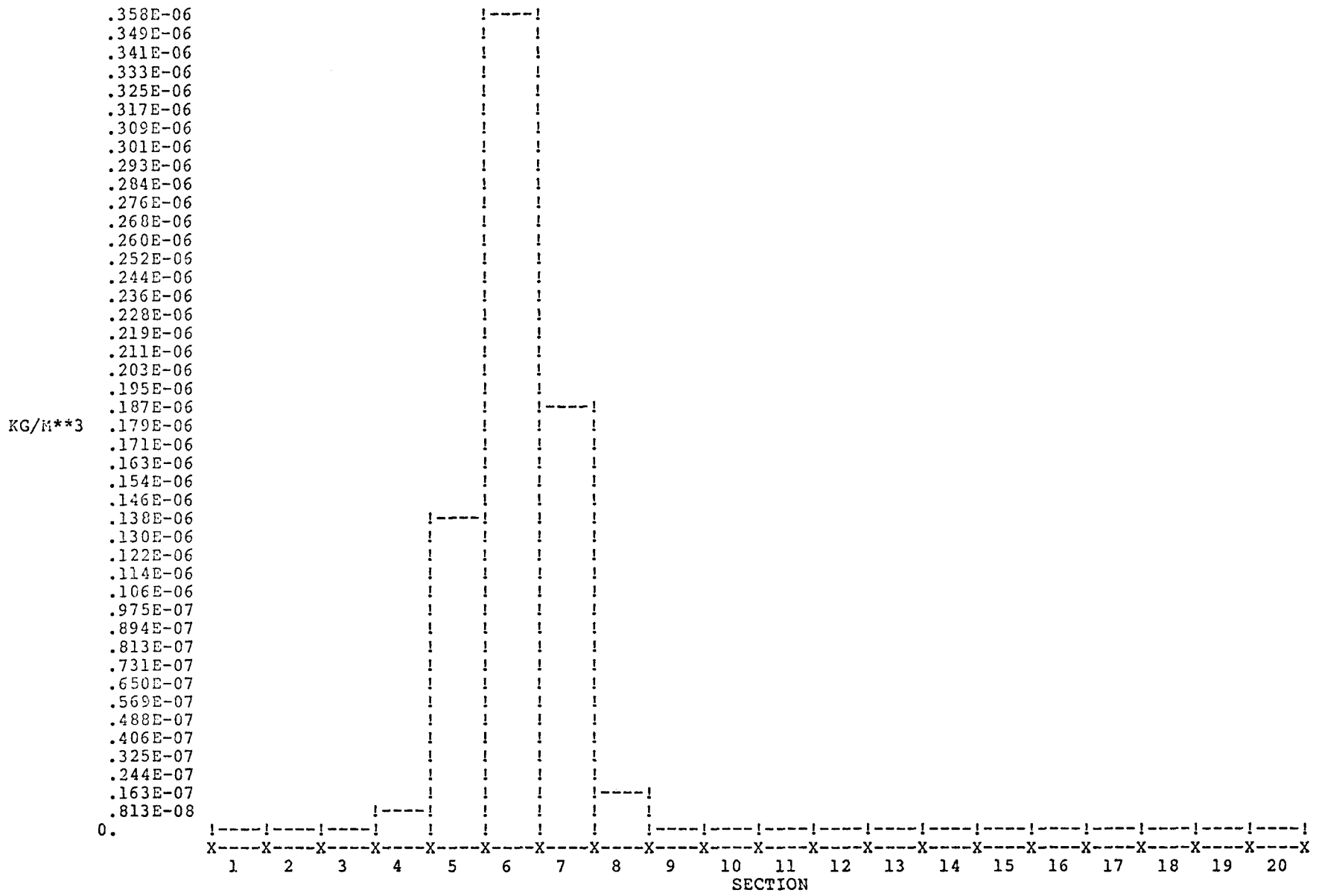
TOTAL DEPOSITED MASS = .2673E-06 KG CUMULATIVE = .6022E-06 KG

CEILING (KG)	.5003E-07	.6965E-08	.3096E-08	.1741E-08	.1114E-08	.7739E-09	.5686E-09	.7283E-10
VERTICAL WALLS (KG)	.1075E-06	.1492E-07	.6632E-08	.3730E-08	.2387E-08	.1658E-08	.1218E-08	.1564E-09
FLOOR (KG)	.5040E-07	.6978E-08	.3102E-08	.1745E-08	.1117E-08	.7754E-09	.5697E-09	.7335E-10
TOTAL (KG)	.2079E-06	.2886E-07	.1283E-07	.7216E-08	.4618E-08	.3207E-08	.2356E-08	.3026E-09
CUMULATIVE (KG)	.5308E-06	.3464E-07	.1539E-07	.8659E-08	.5542E-08	.3849E-08	.2828E-08	.5577E-09

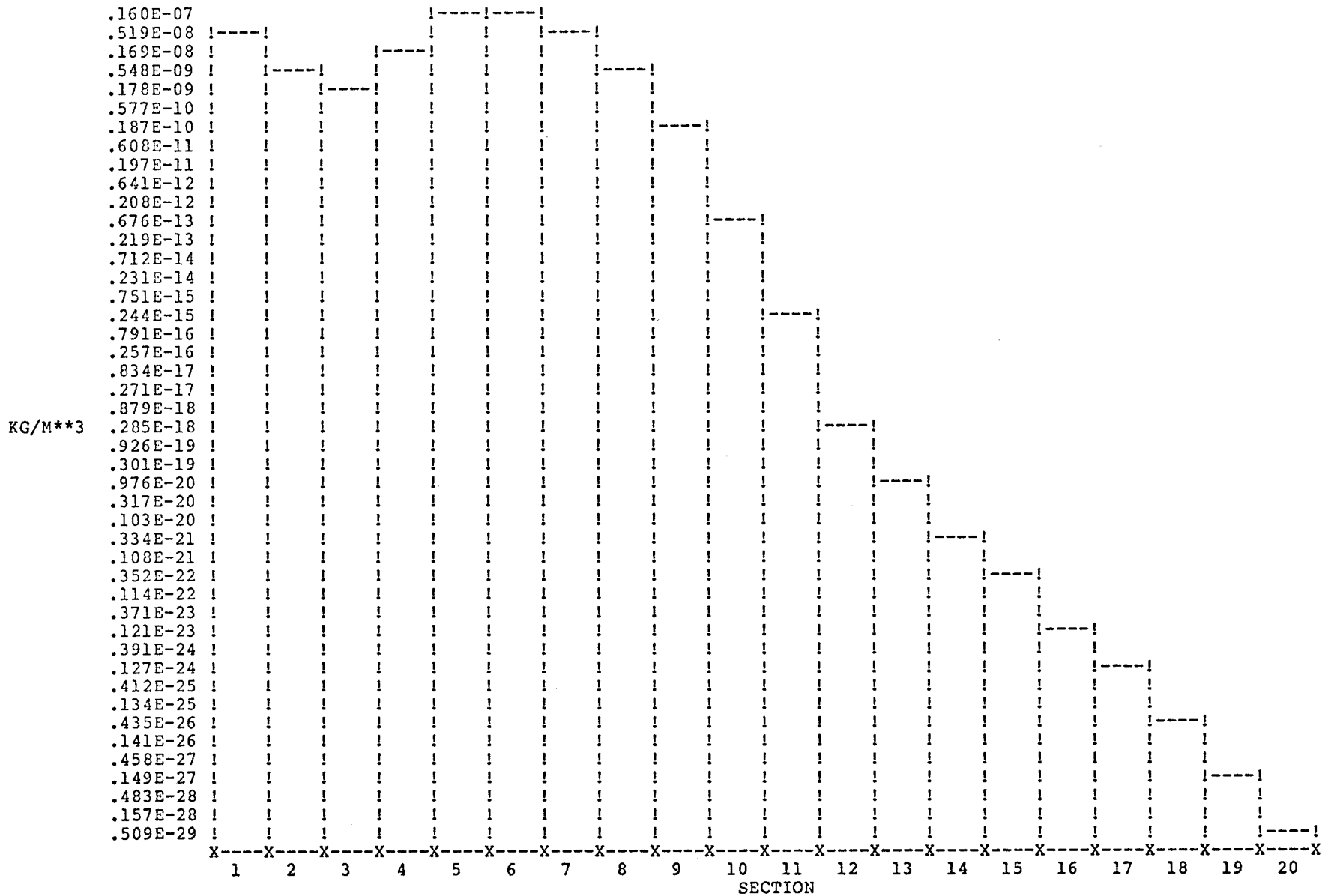
TIME = .200E+03 SECONDS
TOTAL MASS CONCENTRATION
LOGARITHMICALLY SCALED Y AXIS



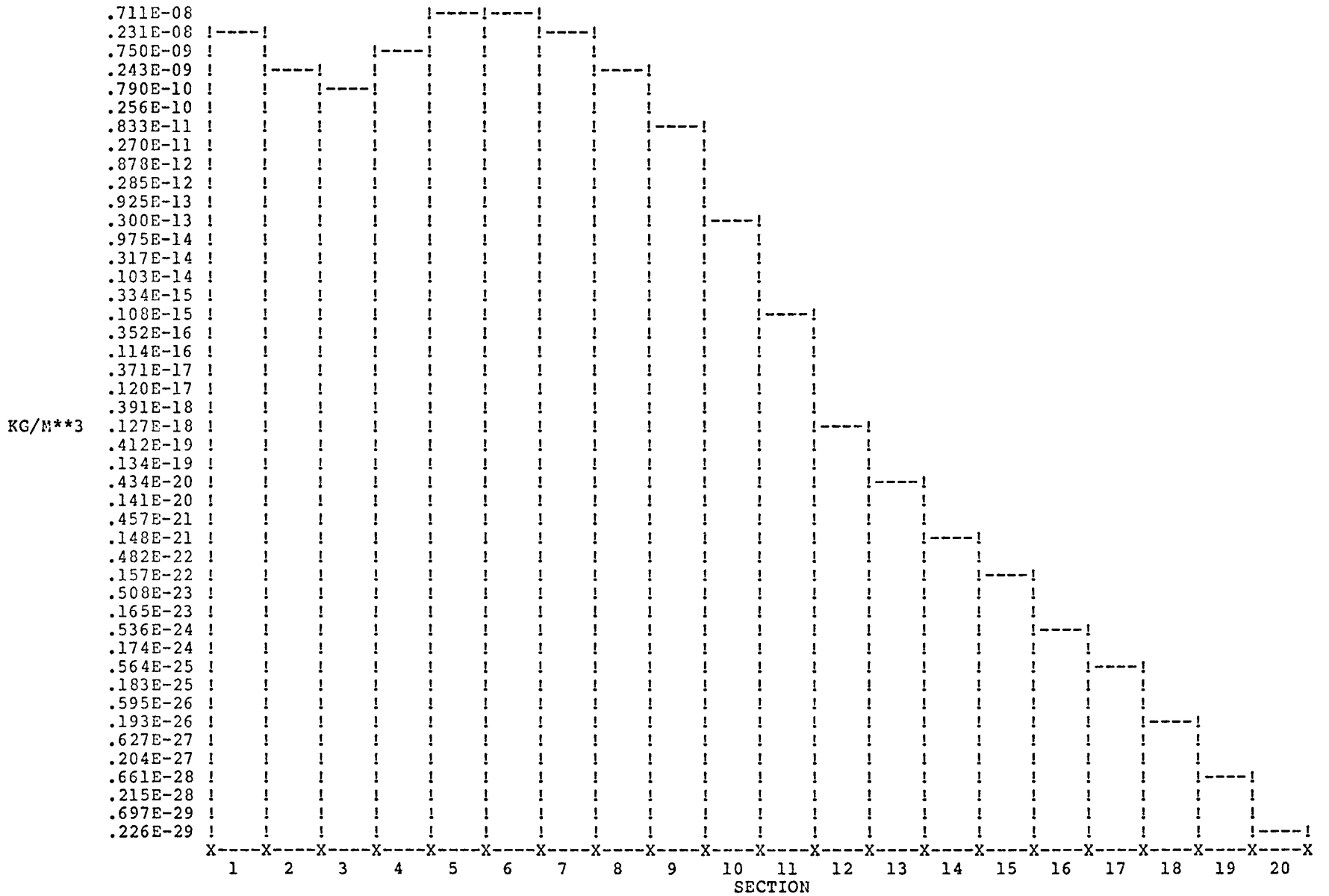
TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 1
LINEARLY SCALED Y AXIS



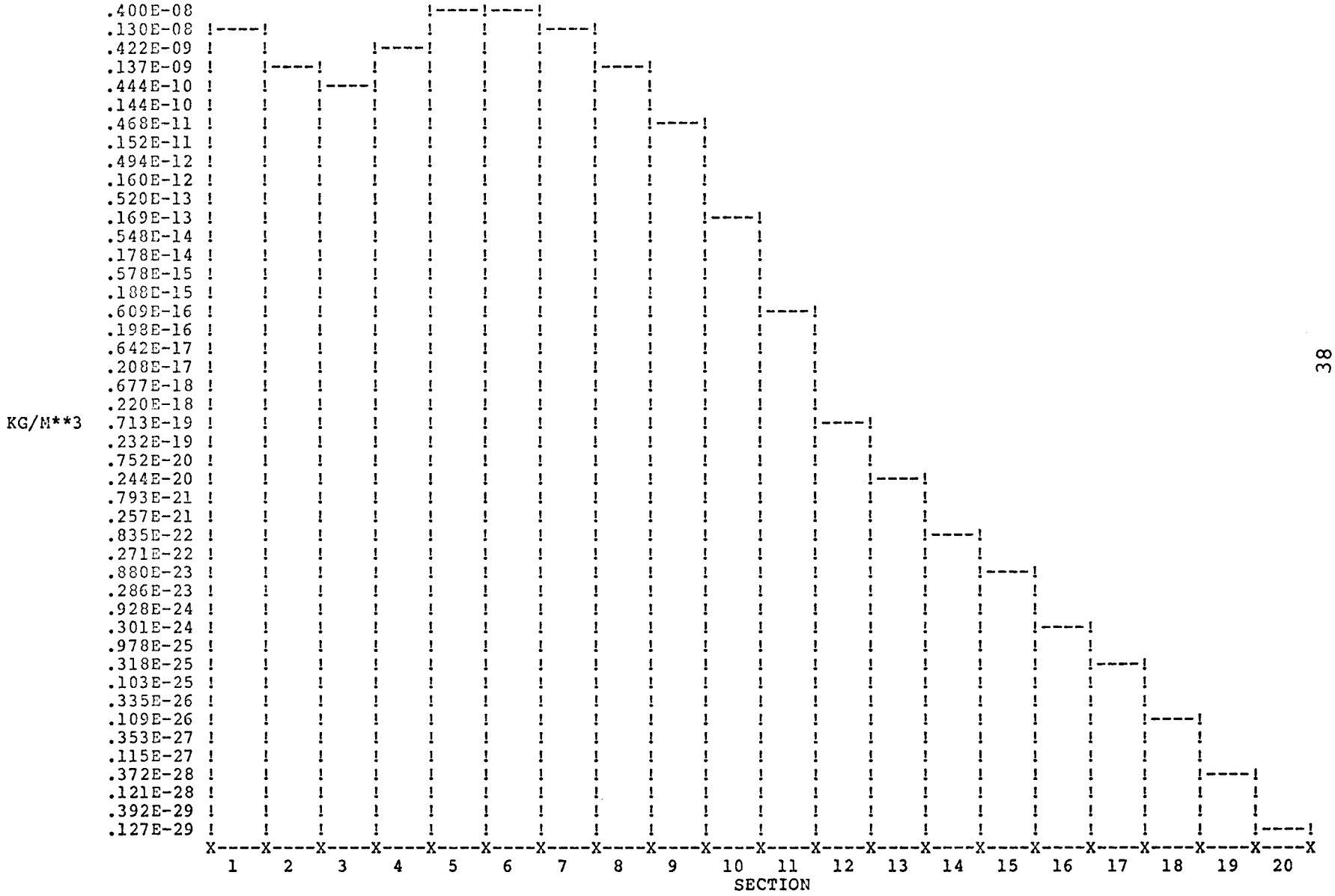
TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 2
LOGARITHMICALLY SCALED Y AXIS



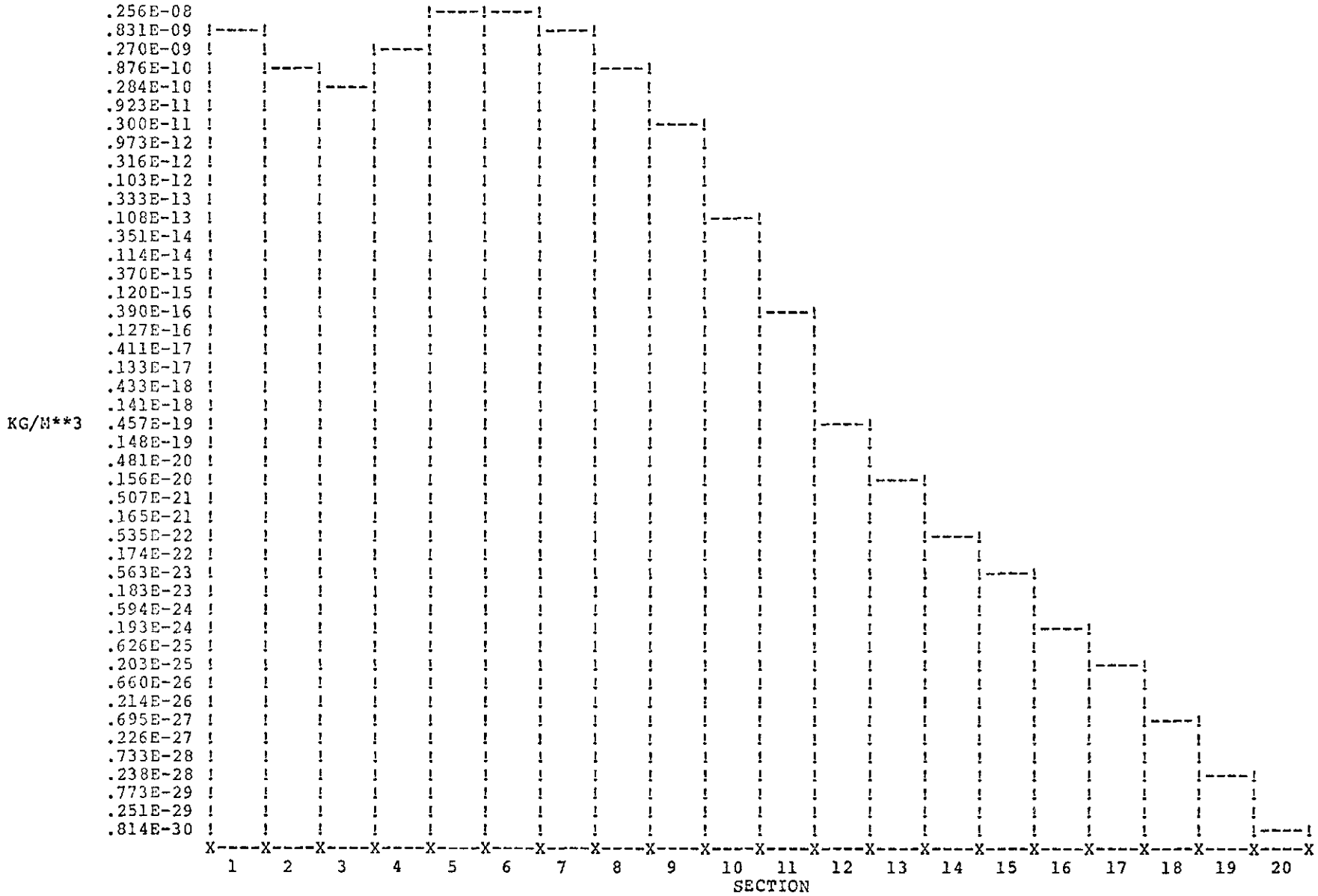
TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 3
LOGARITHMICALLY SCALED Y AXIS



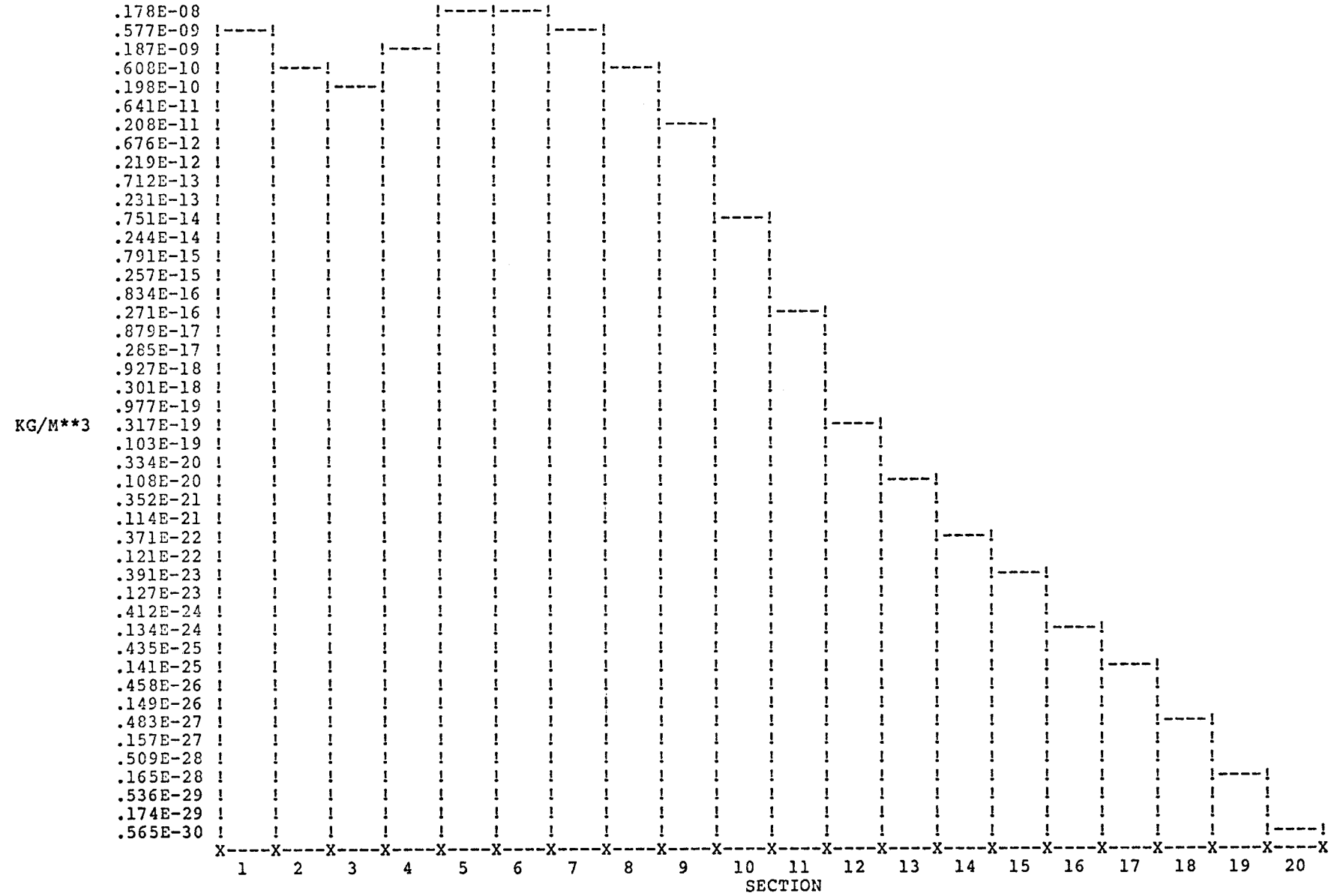
TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 4
LOGARITHMICALLY SCALED Y AXIS



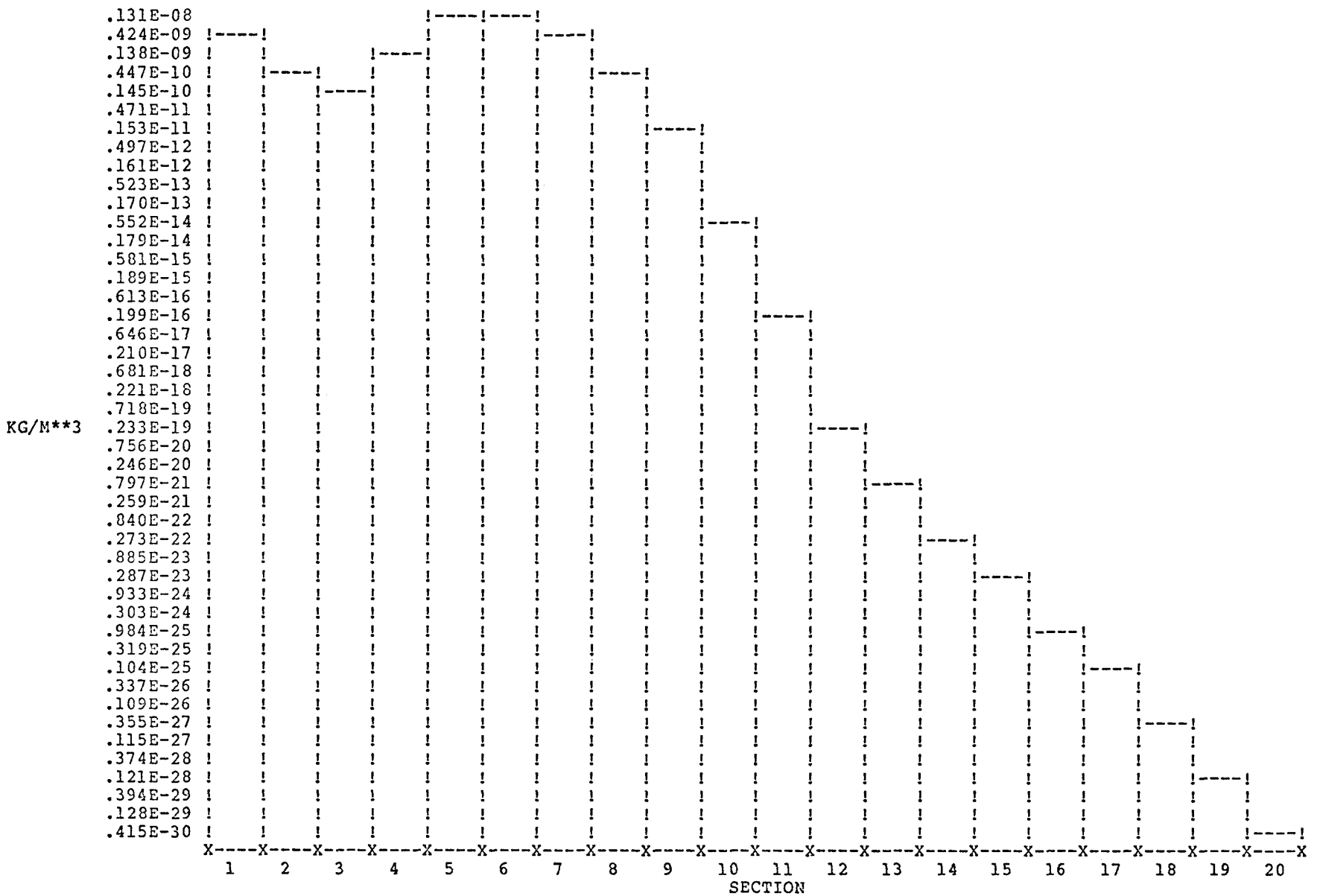
TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 5
LOGARITHMICALLY SCALED Y AXIS



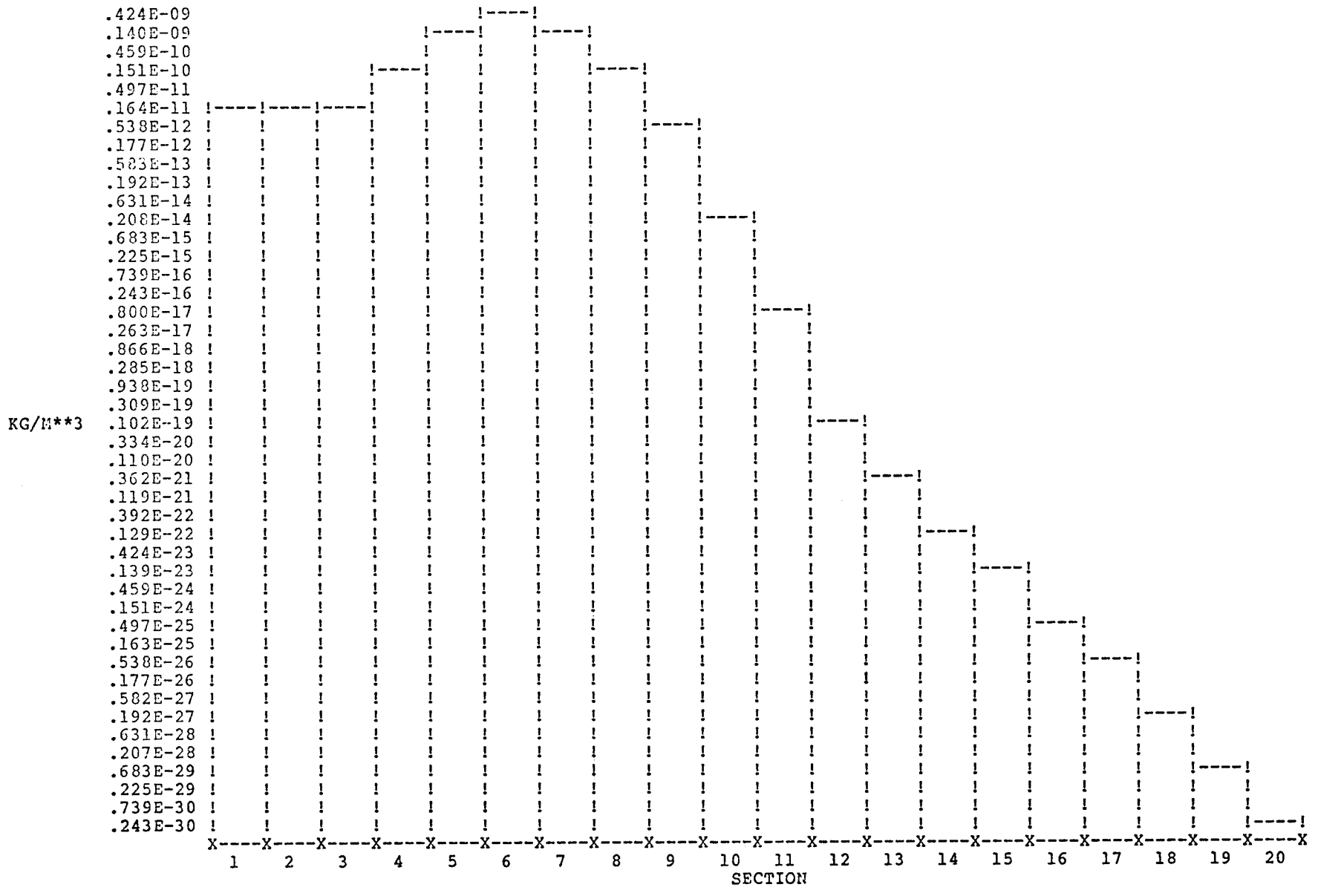
TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 6
LOGARITHMICALLY SCALED Y AXIS



TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 7
LOGARITHMICALLY SCALED Y AXIS



TIME = .200E+03 SECONDS
MASS CONCENTRATION OF COMPONENT 8
LOGARITHMICALLY SCALED Y AXIS



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APPENDIX A

TABLE A.I

COAGULATION COEFFICIENT

Mechanisms	β (m^3/s)
Brownian (4, 6, 8)	$\beta = 2\pi(\mathcal{D}_i+\mathcal{D}_j)(\gamma_i D_i+\gamma_j D_j)/F$

$$\mathcal{D}_i = \frac{kT}{3\pi D_i \eta \chi_i}\left[1+Kn_i\left(1.37+0.4\exp(-1.1/Kn_i)\right)\right]$$

$$F = \frac{D_i+D_j}{D_i+D_j+2g_{i,j}} + \frac{8(\mathcal{D}_i+\mathcal{D}_j)}{\overline{V}_{i,j}(D_i+D_j)}$$

$$g_{i,j} = \sqrt{g_i^2+g_j^2}$$

$$\overline{V}_{i,j} = \sqrt{V_i^2+V_j^2}$$

$$g_i = \frac{1}{3D_i\ell_i}\left\{(D_i+\ell_i)^3 - \left(D_i^2+\ell_i^2\right)^{3/2}\right\} - D_i$$

$$\ell_i = \frac{8\mathcal{D}_i}{\pi V_i}$$

$$V_i = \sqrt{\frac{8kT}{\pi m_i}}$$

$$Kn_i = 2\lambda/D_i$$

TABLE A.I (Continued)

Mechanism	β (m^3/s)
Gravitational (4)	$\beta = \varepsilon\frac{\pi}{4}(\gamma_i D_i+\gamma_j D_j)^2 \lvert V_{Ti}-V_{Tj}\rvert$
	$V_{Ti} = \frac{\rho_{pi} g D_i^2 C_i}{18\eta\chi_i}$
	$C_i = 1+Kn_i\left[1.37 + 0.4\exp(-1.1/Kn_i)\right]$
	$Kn_i = 2\lambda/D_i$
	$\varepsilon = \frac{D_i^2}{(D_i+D_j)^2} \qquad D_i<D_j$
Turbulent (4, 9)	$\beta = \sqrt{\beta_{T1}^2+\beta_{T2}^2}$
	$\beta_{T1} = \sqrt{\frac{\pi\varepsilon_T}{120\nu}}\,(\gamma_i D_i+\gamma_j D_j)^3$
	$\beta_{T2} = \frac{0.04029\rho_g^{1/4}\varepsilon_T^{3/4}}{\eta^{5/4}}(\gamma_i D_i+\gamma_j D_j) \times$
	$\left\lvert \frac{\rho_{p1} C_1 D_1^2}{\chi_1} - \frac{\rho_{p2} C_2 D_2^2}{\chi_2} \right\rvert$
	$C_i = 1+Kn_i\left[1.37 + 0.4\exp(-1.1/Kn_i)\right]$
	$Kn_i = 2\lambda/D_i$

TABLE A.1 (continued)

Notation

D = particle diameter (m)

g = gravitational constant ($m\ s^{-2}$)

k = Boltzmann's constant ($J\ {}^{o}K^{-1}$)

m = particle mass (kg)

T = absolute temperature (${}^{o}K$)

γ = agglomeration shape factor

ε_T = turbulent energy dissipation rate ($m^2\ s^{-3}$)

η = gas viscosity ($kg\ m^{-1}\ s^{-1}$)

λ = mean free path (m)

ν = kinematic viscosity ($m^2\ s^{-1}$)

ρ_g = gas density ($kg\ m^{-3}$)

ρ_p = particle density ($kg\ m^{-3}$)

χ = dynamic shape factor

TABLE A.II

DEPOSITION MECHANISMS (4, 10, 11, 12)

Mechanism	S (s^{-1})
Thermophoresis	$S = -\frac{A_{wall}U}{V_{chamber}}$
	$U = \frac{3\eta C(c_t Kn + k_f/k_s)\nabla T}{2\chi\rho_g T(1+3c_m Kn)(1+2c_t Kn+2k_f/k_s)}$
	$C = 1+Kn[1.37 + 0.4\exp(-1.1/Kn)]$
	$Kn = 2\lambda/D$
Gravity	$S = -\frac{A_{floor}V_T}{V_{chamber}}$
	$V_T = \frac{\rho_p g D^2 C}{18\eta\chi}$
Diffusion	$S = -\frac{\mathcal{D}A_{wall}}{V_{chamber}\Delta}$

TABLE A.II (continued)

Notation

A = surface area (m^2)

c_m = first order slip correction factor

c_t = a constant associated with the thermal accommodation coefficient

D = particle diameter (m)

$\mathcal{D}$ = particle diffusivity ($m^2\ s^{-1}$)

g = gravitational constant ($m\ s^{-2}$)

k_f/k_s = thermal conductivity of gas over that for particle

T = absolute temperature (^oK)

∇T = wall temperature gradient ($^oK\ m^{-1}$)

V = volume (m^3)

Δ = diffusion boundary layer thickness (m)

η = gas viscosity ($kg\ m^{-1}\ s^{-1}$)

λ = mean free path (m)

ρ_g = gas density ($kg\ m^{-3}$)

ρ_p = particle density ($kg\ m^{-3}$)

χ = dynamic shape factor

TABLE A.III

GROWTH RATE

Mechanism	G (s^{-1})
Diffusion (7)	$\frac{2\pi \mathcal{D} D (P-P_{sat} M}{kTm} \left(\frac{1+Kn}{1+1.71Kn+1.33Kn^2} \right)$

$Kn = 2\lambda/D$

APPENDIX B

Array Dimensions

Array dimensions can be determined from the number of sections M, and the number of components KCOMP, as given below. The array dimensions must be at least as large as given below. Array dimensions not given below should not be altered. Note that if M or KCOMP are increased from 20 and 8 respectively, lines 7, 10, 12, 15, 17 and 20, in the subroutine CHECK must be changed to check for the new maximum values of M and KCOMP.

Routine	Dimensions
MAIN	Q(M*KCOMP),SRATE(M*KCOMP),DEPSIT(3,KCOMP),DIAM(M+1)
PRAERO	QT(M),CUMDEP(KCOMP),QTN(M),V(M+1)
PPLOT	NX(M+1),NY(M)
MAEROS	Q(M*KCOMP),SRATE(M*KCOMP), WORK(3+6*M*KCOMP),QTSTRT(KCOMP), QTFNSH(KCOMP),DIAM(M+1),V(M+1)
COEF	V(M+1),X(M+1),DEL(M)
DIFFUN	QT(M)
CHECK	Q(M*KCOMP),SRATE(M*KCOMP),DEPSIT(3,KCOMP),DIAM(M+1),V(M+1)

Common Block	Dimensions
AVGCOF	COEFAV(2*M*M+4*M),SRATE(M*KCOMP)
DBLK	CT1P1,CT1P2,CT2P1 and CT2P2 are to be dimensioned 2*M*M+4*M.

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