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POLLUTION EPISODIC MODEL  
USER'S GUIDE

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OFFICE OF RESEARCH AND DEVELOPMENT  
U.S. ENVIRONMENTAL PROTECTION AGENCY  
RESEARCH TRIANGLE PARK, NORTH CAROLINA 27711

POLLUTION EPISODIC MODEL

USER'S GUIDE

by

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## ABSTRACT

The Pollution Episodic Model (PEM) is an urban-scale model designed to predict short-term average ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants at multiple receptors. The two pollutants may be non-reactive, or chemically-coupled through a first-order chemical transformation. Up to 300 isolated point sources and 50 distributed area sources may be considered in the calculations. Concentration and deposition flux estimates are made using the mean meteorological data for an hour. Up to a maximum of 24 hourly scenarios of meteorology may be included in an averaging period.

The concentration algorithms used in PEM are specially developed to account for the effects of dry deposition, sedimentation, and first-order chemical transformation. The Gaussian plume-type algorithms for point sources are derived from analytical solutions of a gradient-transfer model. In the limit, when deposition and settling velocities of the pollutants and the chemical transformation rate are zero, these expressions reduce to the familiar Gaussian plume diffusion algorithms. The concentration algorithms for area sources in PEM are derived from an innovative approach based on mass balance considerations. These algorithms are simple, efficient, and accurate. The computer program of the Texas Episodic Model is used as a framework for the development of the PEM program.

When the chemical transformation option is considered, PEM calculates the average surface concentrations and deposition fluxes of both the primary (reactant) and the secondary (reaction product) pollutants. The model also permits a possible direct emission of the secondary pollutant. The deposition and settling velocities of the two species may be different. Either of the species may be a gaseous or particulate pollutant.

PEM is intended for studies of the atmospheric transport, transformation, and deposition of acidic, toxic, and other pollutants in urban areas, and to assess the impact of new sources or source modifications on air quality for regulatory purposes and urban planning. The information in this report is directed to the model user and the programmer.

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## SECTION 1

### MODEL OVERVIEW

#### 1.1 INTRODUCTION

The Pollution Episodic Model (PEM) is an urban-scale model designed to predict short-term ground-level concentrations and deposition fluxes of one or two gaseous or particulate reactive atmospheric pollutants in an urban area with multiple point and area sources. PEM uses point and area-source concentration algorithms developed by Rao (1982) which explicitly account for the effects of dry deposition, gravitational settling, and a first-order chemical transformation. These algorithms, derived analytically from a gradient-transfer model, are based on Gaussian plume modeling assumptions. The surface concentrations and deposition fluxes of both the primary (reactant) and the secondary (reaction product) pollutants are calculated.

The PEM is based on the Texas Episodic Model (TEM) developed by the Texas Air Control Board (1979) for the atmospheric dispersion of non-reactive pollutants over a perfectly reflecting surface. In the limit, when the deposition and settling velocities and the chemical transformation rate are zero, the point-source concentration algorithms used in PEM reduce to

the familiar Gaussian plume dispersion algorithms used in TEM. As this limit is approached, the new area source algorithms used in PEM give essentially the same values as TEM for ground-level concentrations of pollutants. The two models share the same framework for calculations. Some of the key assumptions of TEM, also retained in PEM, are as follows:

1. All area source emissions are assumed to occur at the ground-level. The variation of the vertical dispersion coefficient  $\sigma_z(x)$  was expressed by a power law given by Gifford and Hanna (1970). The enhanced near-surface diffusion over urban areas was simulated by decreasing the stability class index by one for all classes except Class A. The horizontal diffusion was ignored for the narrow plumes resulting from distributed area sources.
2. Values for the horizontal and vertical dispersion coefficients,  $\sigma_x(x)$  and  $\sigma_z(x)$ , for point sources were derived from power laws fitted to the empirically-derived Pasquill-Gifford curves given by Turner (1970). Their values were identical to those used in EPA's Climatological Dispersion Model (Busse and Zimmerman, 1973).
3. The wind speed at the anemometer height was adjusted to the stack height using a power law with the exponents given by DeMarrais (1959). The penetration of an inversion layer aloft by a buoyant plume was considered by defining an inversion penetration factor capable of simulating inversions of various strengths.

Some of the important differences between PEM and TEM are listed in Section 3 of this report.

## 1.2 CAPABILITIES AND APPLICATIONS

The capabilities of PEM are as follows:

1. PEM is an urban-scale model applicable to downwind distances of up to 60 km.
2. Up to a maximum of 300 point sources and 50 area sources can be included in the model inputs to estimate concentrations at a maximum of 2500 receptors located on a 50 x 50 square receptor grid.

3. PEM calculates short-term (1 to 24 hr) average ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants.
4. The two pollutants may be non-reactive, or chemically-coupled through a first-order chemical transformation. Either or both of the two pollutants may be gaseous or particulate species.
5. If only one pollutant is calculated, the effects of a first-order chemical decay can be considered.
6. There is no restriction on the size of the particles. The chemical transformation or decay rate may vary from 0.1 to 100 percent per hour.
7. The deposition (and settling) velocities of the two species may be equal or different. Direct emission of the secondary (reaction product) pollutant may be zero or non-zero for point and area sources.

Some areas of potential application of PEM are the following:

1. Urban particulate modeling.
2. Studies of the transport, diffusion, transformation, and deposition of acidic, toxic, and other pollutants in urban areas. An important example is the atmospheric transport and transformation of  $\text{SO}_2$  to  $\text{SO}_4^{2-}$ .
3. Impact analyses of new sources or source modifications for regulatory purposes.
4. Stack parameter design studies.
5. Fuel conversion/switching studies. Evaluation of pollution control technology and strategies.
6. Prevention of significant deterioration.
7. Urban planning.

### 1.3 ASSUMPTIONS AND LIMITATIONS

PEM is based on steady state Gaussian plume modeling assumptions.

Some of the important assumptions of PEM are as follows:

1. The sources are stationary and the emission rates are constant over the concentration-averaging period.

2. Concentration estimates may be made for each hour using the mean meteorological conditions for that hour. Concentrations for a period longer than an hour can be determined by averaging the hourly concentrations of that period. This can be done externally with minimal programming to calculate, for example, 24-hour average concentrations with diurnally varying emission rates.
3. Total concentration at a receptor is the sum of the concentrations calculated at the receptor from each source; i.e., concentrations are additive.
4. Pollutants released from a stack are transported downwind at a rate equal to the mean wind speed at the physical stack height. The wind direction is constant for each hour. The horizontal wind field is homogeneous and the effects of directional wind shear are neglected.
5. Diffusion of continuous plumes gives time-averaged Gaussian distributions for concentrations in the crosswind and vertical directions. The diffusion in the downwind direction is negligible compared to advection.
6. The reactant and the product species are coupled through a first-order chemical transformation. The deposition and settling velocities of the species, and the chemical transformation rate are constant over the concentration-averaging period. The diurnal variation of these parameters can be considered, if necessary, by averaging the hourly concentrations as discussed above.
7. Particulate pollutants consist of particles of a known size (or size distribution) with a representative settling velocity.
8. Pollutant concentration at a receptor due to the distributed area sources depends only on sources located in a narrow upwind sector. Therefore, horizontal diffusion can be ignored for area sources.
9. The crosswind variations of urban area source-strength patterns can be ignored. The contributions of more remote upwind area sources to the concentration at a receptor are quite small. For this reason, it is generally adequate to consider only four area source grid squares immediately upwind of each receptor grid square.
10. The enhanced near-surface diffusion over urban areas is simulated by decreasing the stability class index by one for all classes except Class A. This correction is applied only to distributed urban area sources, assumed to be at ground-level, and not to the isolated point sources, which are generally located at higher elevations.

Every air pollution model is limited by the assumptions used to predict the pollutant concentrations in the atmosphere. PEM is subject to the same basic limitations as any Gaussian plume-type model. The limiting assumptions of the state-of-the-art algorithms developed for PEM are discussed in detail by Rao (1982). Other general limitations of the model can be summarized as follows:

1. Receptors farther than 60 km downwind of a source are ignored. Thus the maximum downwind distance is limited to 60 km.
2. The number of point sources is limited to 300, and the number of area sources is limited to 50. A user can easily expand the maximum number of point and/or area sources, if necessary. All sources are stationary.
3. The maximum number of scenarios (sets of hourly meteorological data) in an averaging period is limited to 24. PEM is designed to calculate only short-term (1 to 24 hr) average surface concentrations and deposition fluxes of one or two pollutants.
4. PEM does not make any adjustment for differences in terrain elevation between sources and/or receptors. The model assumes level terrain.
5. Only a first-order chemical transformation/decay is considered. The transformation rate, and the deposition and settling velocities of the species, should be specified by the user. If area sources are included, the deposition velocities should be non-zero to avoid singularities in the computations.

#### 1.4 SUMMARY OF INPUT DATA

Input to PEM is divided into four main sections:

1) Control parameters

Control parameters remain constant throughout the model run. They specify:

1. An alphanumeric title
2. Time-averaging option
3. Options for types of input and output

4. Number of scenarios (sets of hourly meteorological data)
5. Stack-tip downwash option for point sources
6. Receptor grid coordinates and spacing
7. Automatic receptor grid option
8. Potential temperature gradient  $d\theta/dz$  for calculation of plume rise with E and F atmospheric stability classes
9. Parameters for one or two pollutants
  - a. Deposition velocity
  - b. Gravitational settling velocity
10. Option to calculate chemical transformation or decay for first pollutant
  - a. Chemical transformation or decay rate
  - b. Ratio of molecular weights of product to reactant
11. Scaling factors for area source emission rates
12. Calibration coefficients to be applied to the calculated concentrations
13. Alphanumeric labels for pollutants
14. Alphanumeric labels for the calibrated concentrations

## 2) Scenario Parameters

A scenario is a set of mean meteorological data for one hour. From one to twenty-four scenarios may be included in each run. Each scenario uses the same receptor grid and the same point and area source inventories. Meteorological parameters for each scenario are

1. Atmospheric stability class
2. Wind speed class or specific wind speed
3. Wind direction sector or specific wind direction
4. Ambient temperature
5. Inversion penetration factor
6. Mixing height

3) Area Source Inventory

From zero to fifty area sources may be included in each run. Each area source square is described by:

1. Location in receptor grid coordinates
2. Length of a side
3. Emission rates for pollutants

4) Point Source Inventory

From zero to three hundred point sources may be included in each run.

Each point source is described by:

1. Location in receptor grid coordinates
2. Emission rates for pollutants
3. Stack height
4. Inside exit diameter of the stack
5. Exit velocity of the plume
6. Exit temperature of the plume
7. Alphanumeric identification

Details of the input data to PEM are given in Section 4 of this report.

## 1.5 SUMMARY OF MODEL OUTPUT

For ease of reference, PEM output lists and briefly explains all input control parameters used in a run. Input data for meteorological conditions, area sources, and point sources are also listed.

Calculated values of surface concentrations, deposition fluxes, and other useful information may be displayed in the following optional forms:

1. List Option --- For each receptor in the grid, the calculated values of concentrations and deposition fluxes are listed for each scenario.
2. Spatial Array Option --- The calculated values of concentrations and deposition fluxes at each receptor are displayed in map form for each scenario.
3. Tape Option --- The calculated values of concentrations and deposition fluxes at each receptor are written on a magnetic tape (designated for output) for each scenario. This option may be used to generate inputs to a contour-plotting routine.
4. Culpability List Option --- The five point sources which contributed most to the total concentration at each receptor are identified by point-source sequence number. A list of these source numbers and their percent contributions are printed for each receptor in the grid for each scenario. This option may be used only when the model calculates concentrations of a single pollutant.
5. Maximum Concentration Option --- The maximum calculated values of surface concentration and deposition flux for each scenario, and the receptor where these values occur, are printed for each pollutant at the end of the run.
6. Point Source List Option --- The input stack parameters, the wind speed at physical stack height, the maximum effective source height and the dominant plume rise influence are listed for each point source.

These output options are selected by the user by specifying appropriate values for the control parameters in the inputs to the model. It may not be possible to elect some of these options in combination with the others. The details are discussed in Section 4.

## SECTION 2

### TECHNICAL DISCUSSION

#### 2.1 THEORETICAL BASIS

The concentration algorithms used in PEM are derived from analytical solutions of a steady state gradient-transfer (K-theory) model, which describes the atmospheric transport, diffusion, deposition, and first-order chemical transformation of gaseous or particulate pollutants from an elevated continuous point source. The eddy diffusivity coefficients in these analytical solutions are expressed in terms of the empirical Gaussian plume dispersion parameters, so that the latter can be conveniently specified as functions of the downwind distance and the atmospheric stability class within the framework of the standard turbulence-typing schemes. The point-source concentration algorithms for the primary (reactant) and the secondary (product) pollutants are presented for various stability and mixing conditions of the atmosphere. In the limit when deposition and settling velocities and the chemical transformation rate are zero, these algorithms reduce to the well-known Gaussian plume dispersion algorithms presently used in EPA air quality models. Details of the gradient-transfer model formulations, analytical solutions, parameterizations, and development of the point-source concentration algorithms can be found in the reports by Rao (1982, 1981).

The PEM algorithms for ground-level concentrations of the primary and secondary pollutants resulting from urban area source emissions are derived from an innovative mathematical approach based on mass budgets of the species. These expressions for area sources involve only the point-source algorithms for the well-mixed region; this permits the use of the same subroutines for both point and area sources in the PEM computer program. Thus, the area-source concentration algorithms used in PEM are simple, efficient, and accurate. Details of their mathematical derivation, physical interpretation, and application to multiple urban area sources and receptors can be found in the report by Rao (1982).

PEM uses Briggs' (1969, 1975) plume rise formulations for point sources, empirically-derived Pasquill-Gifford dispersion parameters (Gifford, 1968, 1976), and the urban area-source modeling techniques due to Gifford and Hanna (1970).

## 2.2 POINT SOURCES

### 2.2.1 Concentration Algorithms

The ground-level concentrations of the primary and the secondary pollutants (denoted by subscripts 1 and 2, respectively) from an elevated continuous point source are calculated in PEM from one or both of the following sets of algorithms, depending on the atmospheric stability and mixing conditions:

Near-source region ( $0 < x \leq x_m$ ),

$$c_1 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{21}}{L_z} \quad (1a)$$

$$c_2 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{22}}{L_z} \quad (1b)$$

Well-mixed region ( $x \geq 2x_m$ ),

$$c_1 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{41}}{L} \quad (2a)$$

$$c_2 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{42}}{L} \quad (2b)$$

$$L_y = \sqrt{2\pi} \sigma_y, \quad L_z = \sqrt{2\pi} \sigma_z \quad (3)$$

In the above,  $Q_1$  is emission rate (source strength) of the primary pollutant,  $U$  is mean wind speed at physical stack height,  $L$  is mixing depth (height of inversion lid),  $x_m$  is the downwind distance (from source) at which  $\sigma_z(x_m) = 0.47 L$ , and  $L_y$  and  $L_z$  are length scales characteristic of diffusion in the horizontal crosswind and vertical directions, respectively. The nondimensional functions  $g_1(\hat{x}, \hat{y})$ ,  $g'_{21}(\hat{x}, 0)$ ,  $g'_{22}(\hat{x}, 0)$ ,  $g'_{41}(\hat{x})$ , and  $g'_{42}(\hat{x})$ , defined in terms of dimensionless parameterized variables, are given in Appendix A.

In Eqs. (1) and (2), it should be noted that the concentrations for both primary and secondary pollutants are expressed in terms of  $Q_1$ . This does not preclude consideration of a non-zero value for  $Q_2$ , the direct emission rate of the secondary pollutant. The algorithms  $g'_{22}$  and  $g'_{42}$  provide for this possibility.

The well-mixed region algorithms, Eq. (2), are generally used under convective or neutral stability conditions. The ground-level plume centerline concentrations of the species in the plume-trapping region ( $x_m < x < 2x_m$ ) can be obtained by calculating the concentrations at  $x_m$  and  $2x_m$  from Eqs. (1) and (2), and interpolating between these values on a log-log plot of concentrations versus downwind distance (Turner, 1970). PEM uses this interpolation approach in the plume-trapping region.

### 2.2.2 Plume Rise

Plume rise is calculated from equations given by Briggs (1969, 1975). The stack-exit conditions of the plume and the ambient temperature determine whether the upward motion of the plume is dominated by momentum or buoyancy. For atmospheric stability classes A to D, the unstable/neutral plume rise equations are used. For stability classes E and F, the stable plume rise equations are used. Thus, there are four different situations for plume rise: (1) unstable/neutral atmosphere with buoyancy-dominated plume, (2) stable atmosphere with buoyancy-dominated plume, (3) unstable/neutral atmosphere with momentum-dominated plume, and (4) stable atmosphere with

momentum-dominated plume. In each situation except the last one, the plume rise is calculated as a function of downwind distance from the source until the final plume rise is attained. The equations for these four cases are given in Appendix B.

For a given atmospheric stability class for each scenario, PEM calculates both momentum and buoyancy-dominated maximum plume rises for each stack. Based on the higher of these two values, the appropriate plume-rise equation is selected and used to calculate the plume rise,  $\Delta h(x)$ , for each stack. The effective source height,  $H$ , is then obtained from  $H = h_s + \Delta h$ , where  $h_s$  is the physical stack height.

Following Briggs (1973), PEM provides an option to account for stack-tip downwash effects on the effective stack height. When the stack-exit velocity ( $V$ ) of the plume is less than 1.5 times the mean wind speed ( $U$ ) at the physical stack height, the stack-tip downwash correction term,  $H_c$ , is calculated as

$$H_c = 2 \left(1.5 - \frac{V}{U}\right) d \quad (4)$$

where  $d$  is the inside diameter of the stack-tip. This value of  $H_c$  is subtracted from the effective stack height  $H$ . When this option is used, care should be taken to see that  $H_c$  has the same units as  $H$ .

### 2.2.3 Dispersion Parameters

The Gaussian dispersion parameters,  $\sigma_y$  and  $\sigma_z$ , used in PEM for each hourly scenario, are identical to those used in EPA's Climatological Dispersion Model (Busse and Zimmerman, 1973) to represent a 1-hour average dispersion, and in the Texas Episodic Model (TACB, 1979) to represent a 10-minute average dispersion from point sources. The values of these parameters are calculated from power laws fitted to the Pasquill-Gifford empirical data curves (Turner, 1970; Gifford, 1976), as follows:

$$\sigma_z(x) = a x^b \quad (5a)$$

$$\sigma_y(x) = c x^d \quad (5b)$$

The values of a and b used in PEM for point sources are shown in Table 1 as functions of the atmospheric stability class and the downwind distance. The values of c and d are shown in Table 2. Unlike the TEM, the  $\sigma_y$  values in PEM are not adjusted for horizontal meander of the plume since they are assumed to represent 1-hour average dispersion.

It should be noted that the Pasquill-Gifford curves were derived from measurements taken in open, level to gently rolling terrain, and may not be the best estimate of dispersion coefficients for urban areas or rough terrain. The diffusion over cities is enhanced, compared to that over rural areas, due to increased mechanical and thermal turbulence resulting from the larger surface roughness and heat capacity of the cities. This is reflected in the urban dispersion parameter curves based on interpolation formulas given by Briggs (see Gifford, 1976, Figure 7).

TABLE 1  
 Values of a and b in  $\sigma_z = a x^b$   
 for Point Sources

Atmospheric Stability Class	Downwind Distance (meters)					
	100 < x $\leq$ 500		500 < x $\leq$ 5000		5000 < x	
	a	b	a	b	a	b
A=1	.0383	1.281	.0002539	2.089	.0002539	2.089
B=2	.1393	.9467	.04936	1.114	.04936	1.114
C=3	.1120	.9100	.1014	.926	.1154	.9109
DD=4	.0856	.8650	.2591	.6869	.7368	.5642
DN=5	.0818	.8155	.2527	.6341	1.2970	.4421
E=6	.1094	.7657	.2452	.6358	.9204	.4805
F=7	.05645	.8050	.1930	.6072	1.5050	.3662

TABLE 2  
 Values of c and d in  $\sigma_y = c x^d$   
 for Point Sources

Atmospheric Stability Class	Downwind Distance (meters)			
	x < 10,000		x $\geq$ 10,000	
	c	d	c	d
A=1	.495	.873	.606	.851
B=2	.310	.897	.523	.840
C=3	.197	.908	.285	.867
DD=4	.122	.916	.193	.865
DN=5	.122	.916	.193	.865
E=6	.0934	.912	.141	.868
F=7	.0625	.911	.080	.884

#### 2.2.4      Restrictions on Receptors for Calculations

Pollutants from each point source may not contribute to all of the receptors in a grid. The receptors excluded from calculations are those located upwind of the source, too far from the plume centerline, or more than 60 km downwind of the source. For each source and each scenario, PEM selects a rectangular area of the receptor grid downwind of the source, and calculations for that set of conditions are restricted to the receptors located within that area. The source contribution is considered to be zero at receptors located outside the area. Model inputs used for determining this area are the source coordinates, grid boundaries, wind direction, and the crosswind angle ( $\Delta$ ) between wind direction azimuth and the azimuth from the source to the receptor. If  $\Delta$  exceeds the maximum crosswind angle of the plume ( $\Delta_{\max}$ ), then the receptor is excluded from calculations. The values of the maximum crosswind angle used in PEM for 1-hour averaging of the plume are shown in Table 3 as a function of the atmospheric stability class.

TABLE 3  
Maximum Crosswind Angle Values  
for Point Source Plumes

Atmospheric Stability Class	$\Delta_{\max}$ (degrees)
A	35
B	28
C	21
DD and DN	14
E	10.5
F	7

## 2.3 AREA SOURCES

### 2.3.1 Emission Grid

PEM defines a "calculation grid" by shifting the receptor grid to the South and to the West by one-half the side of a grid square ( $\Delta x/2$ ). Thus each square in the calculation grid has one receptor at its center, since the calculation grid squares are of the same size ( $\Delta x$ ) as the receptor grid squares.

Each area source used in PEM should be sized so that it covers an integral number of calculation grid squares. The size  $\Delta x$  should be defined such that the smallest area source is at least as large as one calculation grid square.

The relationship between area sources and calculation grid squares can be divided into three cases. In the first case, the area source is the size of a calculation grid square. Emissions ( $Q_0$ ) are assumed to be located at the center of the square; contributions of this area source are determined at the receptor ( $R_0$ ) located at the center of the emission grid square, and at the receptors ( $R_1$  to  $R_4$ ) located at the center of each of the four calculation grid squares immediately downwind of the source. This is schematically illustrated in Fig. 1.

The location of the four downwind squares is not apparent in cases when the wind direction is not parallel to one of the calculation grid

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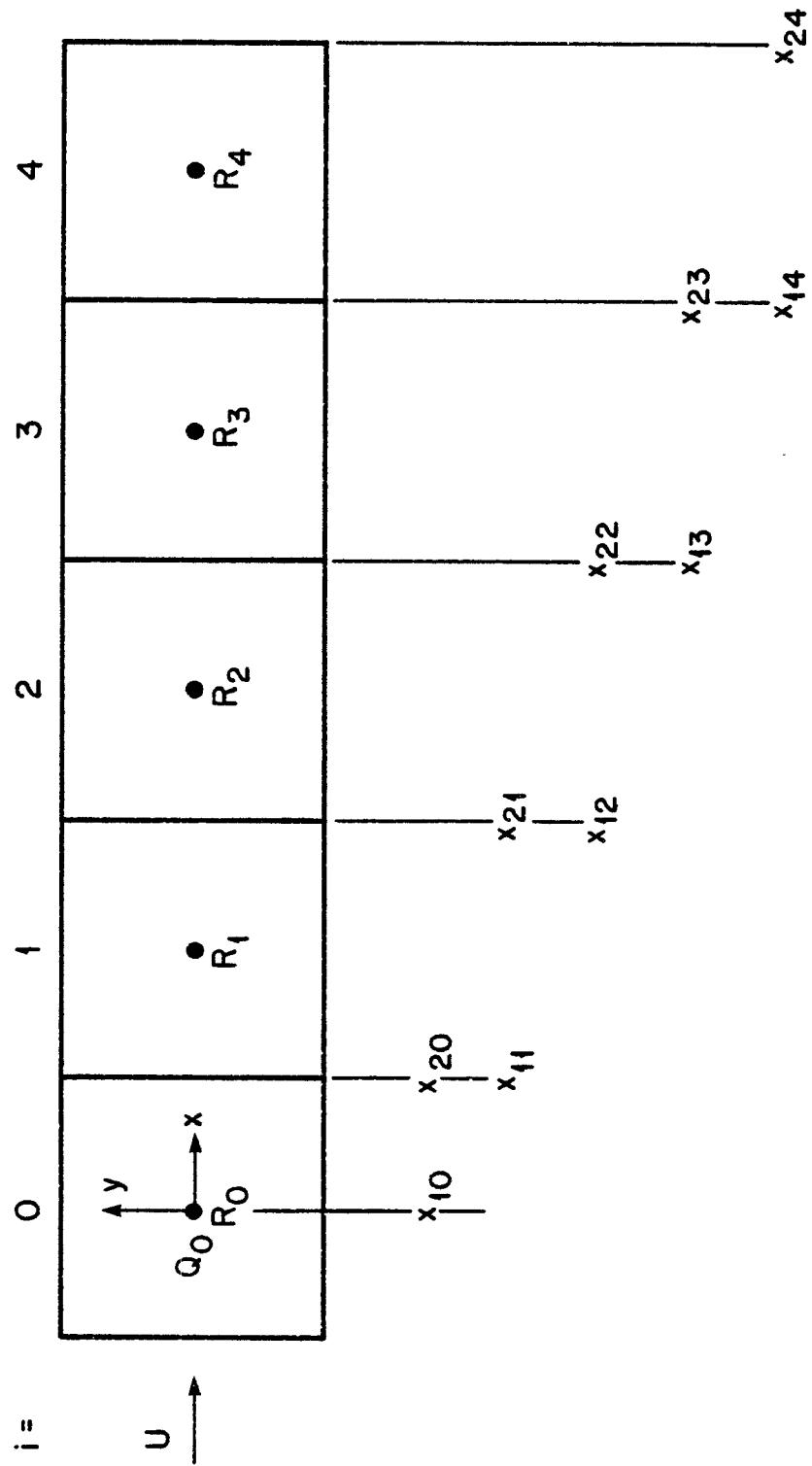


Figure 1. Schematic diagram showing a single grid square with emissions and four downwind calculation grid squares with receptors, and the distances used in area-source algorithms. These distances are measured downwind from the source  $Q_0$ .

coordinate axes as shown in Fig. 2. The angle between the wind azimuth and the nearest calculation grid coordinate axis is defined as  $\xi$ , so  $0^\circ \leq \xi \leq 45^\circ$ . PEM considers ten ranges of values for  $\xi$  as shown in Table 4. For each range of  $\xi$ , the location of the four downwind squares is shown in Fig. 2. For each

TABLE 4

Values of i and j for Each Spatial Pattern  
of Affected Squares Downwind  
of an Area Source

$\xi$ range, degrees	Values for j**				
	i=0*	i=1	i=2	i=3	i=4
0 - 7.12	0	0	0	0	0
7.12 - 9.46	0	0	0	0	1
9.46 - 14.04	0	0	0	1	1
14.04 - 20.56	0	0	1	1	1
20.56 - 26.57	0	0	1	1	2
26.57 - 32.01	0	1	1	2	2
32.01 - 36.87	0	1	1	2	3
36.87 - 39.81	0	1	2	2	3
39.81 - 41.19	0	1	2	3	3
41.19 - 45.00	0	1	2	3	4

\*i is the number of calculation grid squares downwind from the area source

\*\*j is the number of calculation grid squares from the axis used to define  $\xi$

For each value of  $\xi$ , a diagram of the downwind squares is shown in Figure 2.

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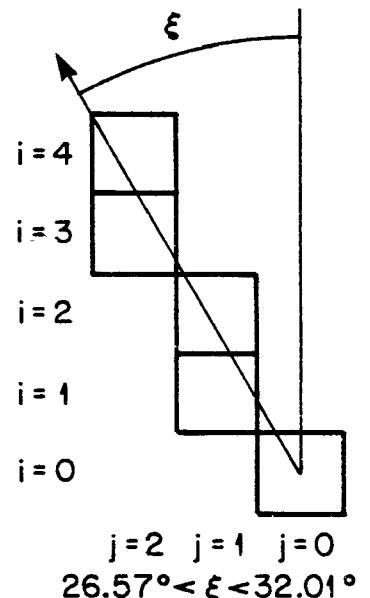
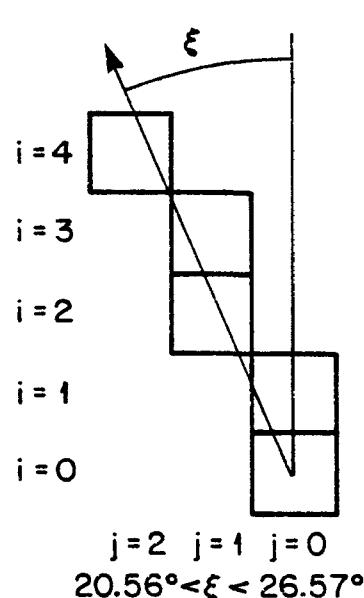
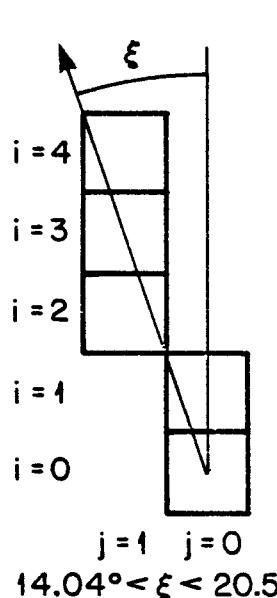
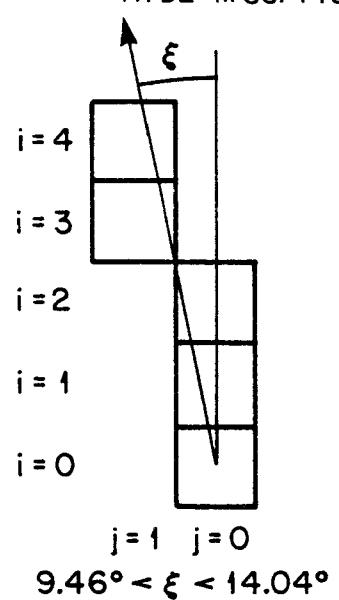
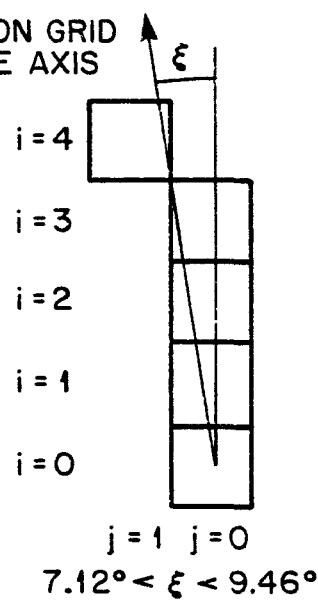
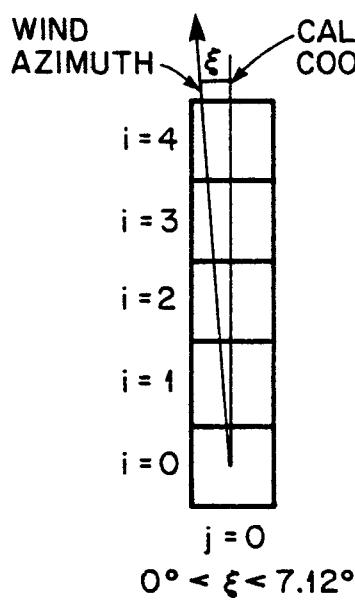


Figure 2. Spatial patterns of affected calculation grid squares downwind of an area source.

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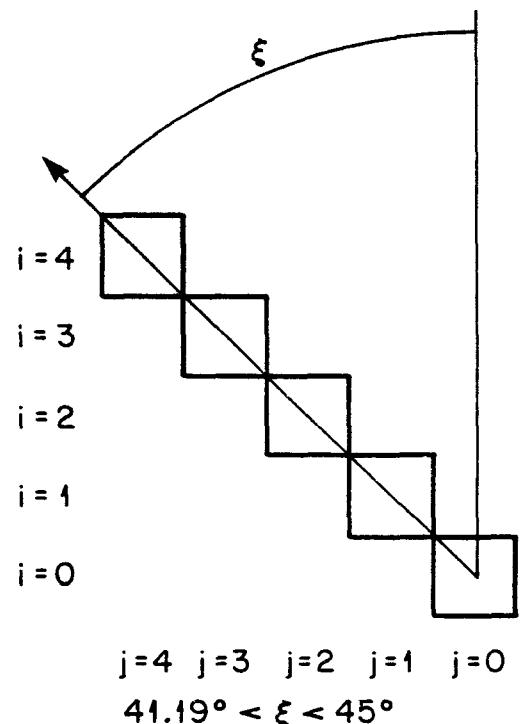
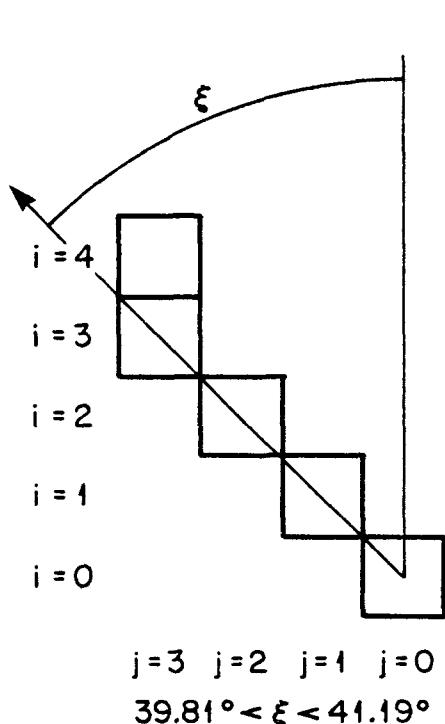
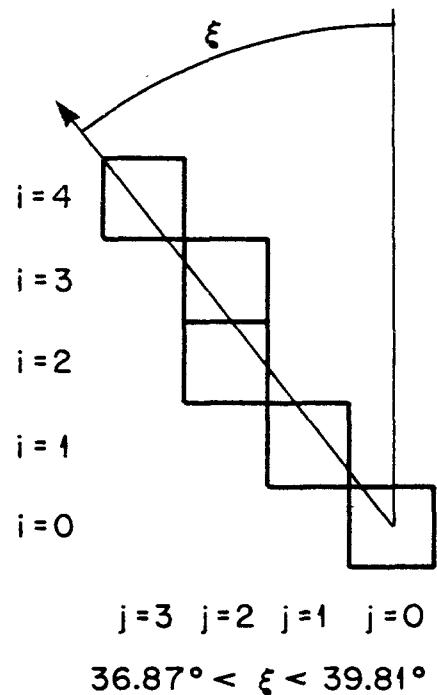
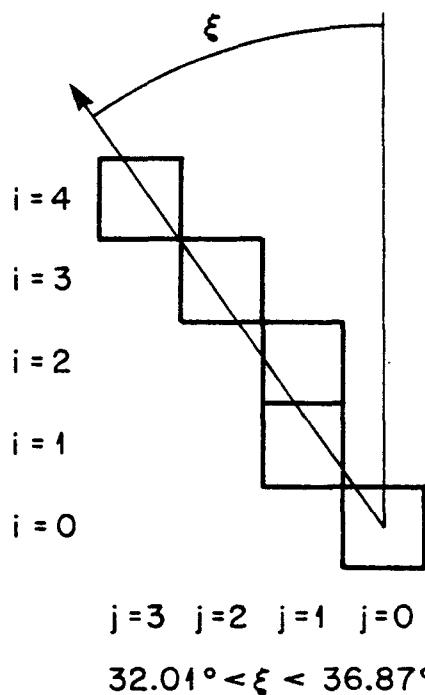


Figure 2. Continued

value of  $\xi$ , the location of each downwind square is denoted by  $i$  (the number of calculation grid squares downwind from the area source) and  $j$  (the number of calculation grid squares from the axis used to define  $\xi$ ). In all cases, the square covered by the area source has  $i=0$  and  $j=0$ . For each value of  $i$ , values for  $j$  depend upon the value for  $\xi$ , as illustrated in Fig. 2 and summarized in Table 4. These patterns of squares are stored in PEM data tables that list values of  $i$  and  $j$  as shown in Table 4. For a given scenario, each area source will have the same spatial pattern of affected squares downwind.

In the second case, the area source is larger than one calculation grid square. Let  $m$  be the number of calculation grid squares covered by the source of area  $A$ . Then the emissions,  $Q$ , from the source are divided into  $m$  component emission rates defined by

$$Q_j = Q A_j / A , \quad j = 1, 2, \dots, m$$

where  $A_j$  is the area of the source contained in the  $j$ th square,

$$A = \sum_{j=1}^m A_j \quad \text{and} \quad Q = \sum_{j=1}^m Q_j .$$

Then the contributions from each of the  $m$  squares are determined as was done from a single square.

In the third case, a small area source may be imbedded in a large area source. For each source the emission rate is divided into components for each covered square as described above. Then each square is considered as an area source with an emission rate equal to the sum of the component emission rates from the original area sources.

### 2.3.2 Concentration Algorithms

The area-source concentration algorithms used in PEM are derived by Rao (1982) from the governing equations, using a new mathematical approach based on mass balance considerations. These algorithms are listed and briefly explained below. For details of their derivation, physical interpretation, extension to multiple sources and receptors, and other related discussion, the user should refer to Rao (1982).

We consider five calculation grid sources (denoted by  $i=0, 1, 2, 3, 4$ ), each with a receptor located at its center, as shown in Fig. 1. The source emissions ( $Q_o$ ) are assumed to be located at the center of the first square ( $i=0$ ) upwind of the receptors. The emission rate of the primary pollutant from this single area source is  $Q_1$ . Then the ground-level concentrations of the primary and secondary pollutants,  $C_{A1i}$  and  $C_{A2i}$  respectively, at the receptor  $R_i$  in the  $i$ th calculation grid square are given by

$$C_{A1i} = \frac{Q_1}{2(1-b)V_{dl}} \left[ g'_{41}(\hat{x}_{li}) - g'_{41}(\hat{x}_{2i}) - \frac{1}{\hat{\tau}_c} \int_{\hat{x}_{li}}^{\hat{x}_{2i}} g'_{41}(\hat{x}) d\hat{x} \right] \quad (6a)$$

$$C_{A2i} = \frac{Q_1}{2(1-b)V_{d2}} \left[ g'_{42}(\hat{x}_{li}) - g'_{42}(\hat{x}_{2i}) + \frac{Y}{\hat{\tau}_c} \int_{\hat{x}_{li}}^{\hat{x}_{2i}} g'_{41}(\hat{x}) d\hat{x} \right] \quad (6b)$$

Here,  $g'_{41}(\hat{x})$  and  $g'_{42}(\hat{x})$  are point-source concentration algorithms for the well-mixed region. These nondimensional functions, and other dimensionless parameters (capped quantities) in this equation, are defined in Appendix A;  $x_{li}$  and  $x_{2i}$  are distances measured from  $Q_0$  to the upwind and downwind edges, respectively, of the calculation grid square with the  $i$ th receptor (see Fig. 1);  $\hat{x}_{li}$  and  $\hat{x}_{2i}$  are the corresponding dimensionless values;  $\tau_c$  is characteristic time scale of the first-order chemical transformation, and  $\hat{\tau}_c$  is its dimensionless value as defined in Appendix A;  $\gamma$  is the ratio of molecular weights of the product species to the reactant species;  $V_{d1}$  and  $V_{d2}$  are deposition velocities of the primary and secondary pollutants, respectively;  $b$  is the value of the exponent in the power-law,

$$\sigma_z(x) = a x^b \quad (7)$$

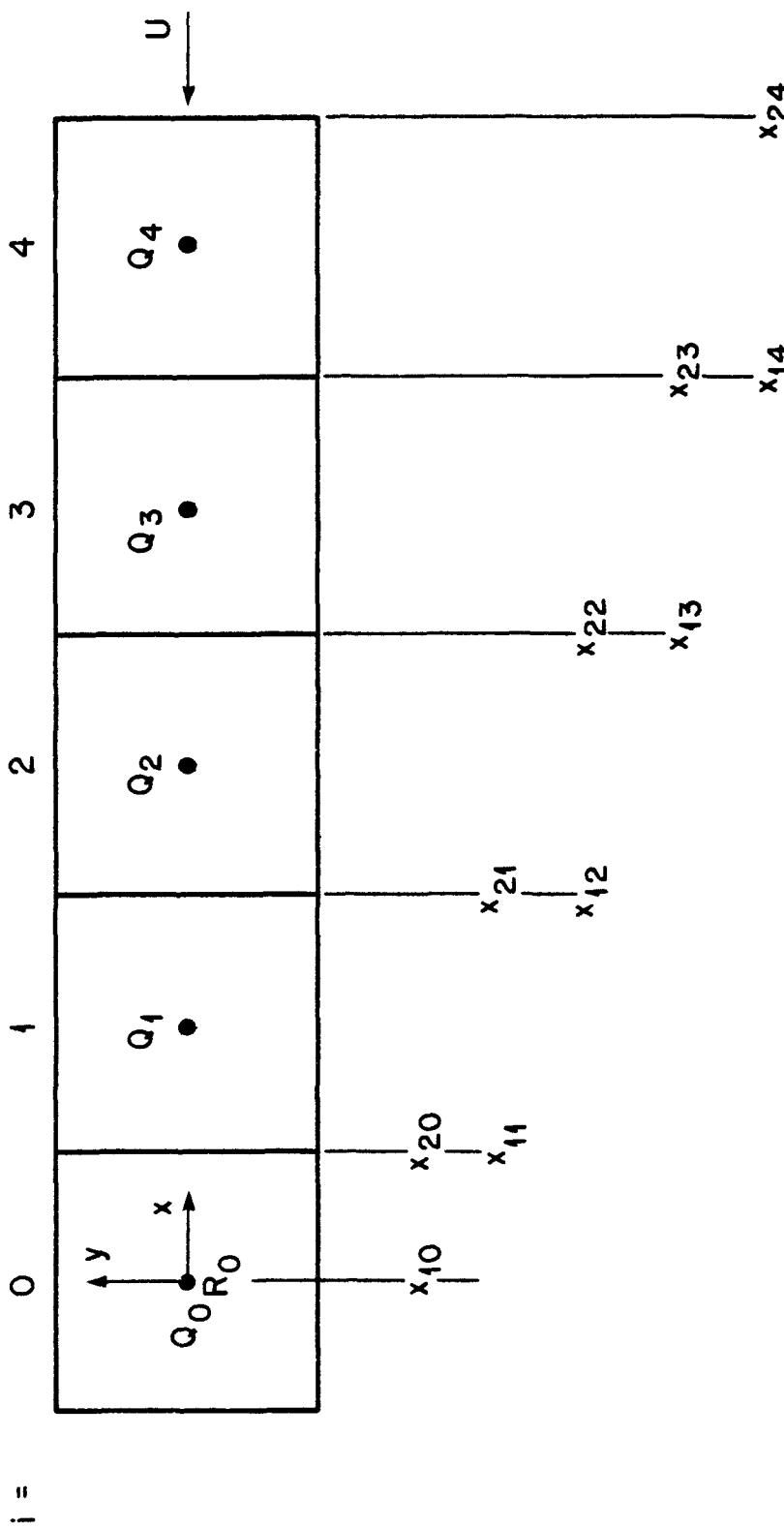
for area sources.

Now let us consider five area sources, located upwind of a single receptor  $R_0$  in  $i=0$ th grid square, as shown in Fig. 3. The total surface concentrations at the receptor in this case can be obtained by summing up the individual contributions of all five area sources, as follows:

$$C_{A1} = \frac{1}{2(1-b)V_{d1}} \sum_{i=0}^4 Q_{li} \left[ g'_{41}(\hat{x}_{li}) - g'_{41}(\hat{x}_{2i}) - \frac{1}{\hat{\tau}_c} \int_{\hat{x}_{li}}^{\hat{x}_{2i}} g'_{41}(\hat{x}) d\hat{x} \right] \quad (8a)$$

$$C_{A2} = \frac{1}{2(1-b)V_{d2}} \sum_{i=0}^4 Q_{li} \left[ g'_{42}(\hat{x}_{li}) - g'_{42}(\hat{x}_{2i}) + \frac{\gamma}{\hat{\tau}_c} \int_{\hat{x}_{li}}^{\hat{x}_{2i}} g'_{41}(\hat{x}) d\hat{x} \right] \quad (8b)$$

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**Figure 3.** Schematic diagram showing a single grid square with receptor and four upwind grid squares with emissions, and the distances used in area-source algorithms. These distances are measured upwind from the receptor  $R_0$ .

Here  $x_{1i}$  and  $x_{2i}$  are the distances measured from the receptor  $R_o$  to the downwind and upwind edges, respectively, of the  $i$ th emission grid square, as shown in Fig. 3. Note that these distances are identical to those used in Eq. (6), since all grid squares are equal in size. The multiple-source algorithms, Eq. (8), can be easily adapted to calculate concentrations at multiple receptors. For details, the user is referred to Rao (1982).

### 2.3.3 Dispersion Parameters

It should be noted that the area source concentration algorithms, given above, ignore horizontal diffusion. Gifford (1959) postulated that concentration at a receptor due to the distributed area sources depends only on sources located in a rather narrow upwind sector. The horizontal width of this sector is generally much less than the usual  $22.5^\circ$  resolution of observed wind directions. Consequently, horizontal diffusion can be ignored. This assumption is also referred to as the "narrow plume hypothesis."

The vertical dispersion parameter is given by Eq. (7). The coefficients  $a$  and  $b$  are functions only of atmospheric stability. Their values, based on extensive observational data, can be found in various texts, handbooks and other references. These values, given by Gifford and Hanna (1970), are listed in Table 5.

TABLE 5

Values of a and b in  $\sigma_z = a x^b$   
for Area Sources

## Atmospheric Stability

Class	a	b
A = 1	0.4	0.91
B = 2	0.4	0.91
C = 3	0.33	0.86
DD = 4	0.22	0.80
DN = 5	0.15	0.75
E = 6	0.06	0.71
F = 7	0.06	0.71

The diffusion over cities is enhanced, compared with that over open country, due to the increased mechanical and thermal turbulence resulting from the larger surface roughness and great heat capacity of the cities. To simulate the increased surface turbulence over urban areas, PEM uses a so-called "decreased stability class index." The latter is obtained by decreasing the atmospheric stability class index by one, for all classes except Class A.

## 2.4 RECEPTORS

2.4.1 Receptor Grid

PEM calculates pollutant concentrations at each receptor in a rectilinear receptor array. A maximum of 2500 receptors may be used, with 50 columns and 50 rows. The spacing between each column and row is uniform, and is specified by the user. Receptors are located at the intersections of grid columns and rows. The grid spacing, number of columns, number of rows, and coordinates of the receptor at the southwest corner of the grid are used to define the grid.

Point and area sources need not necessarily be located within the grid boundaries. If area sources are included in the source inventory, the grid spacing should be selected so that the smallest area source is of the same size as a grid square. An area source is positioned on the grid by specifying the coordinates of its southwest corner. This corner should be located in the center of a receptor grid square, and not at a grid intersection, so that each square covered by the area source is centered on a receptor. For computations involving area sources, a calculation grid is defined with grid squares the same size as receptor grid squares, but with a receptor located in the center of each calculation grid square. For details, see Section 2.3.1.

#### 2.4.2 Automatic Grid Selection

PEM has an optional subroutine which will automatically select a receptor grid for each scenario. The size and location of grids for different scenarios may differ since the selection of the receptor grid is based upon wind speed, wind direction, and atmospheric stability class.

Each source is examined sequentially. Two orthogonal axes are used with the origin located at the origin of the coordinate system for the point sources. The y axis is oriented in the north-south direction with positive values in the northerly direction. The x axis is oriented in the east-west direction with positive values in the easterly direction. Angle E is defined by

$$E = 90^\circ - W$$

where  $W$  is the angle (measured relative to north) of the direction of the flow (see Fig. 4). The axes are then rotated through angle  $E$  such that the wind blows down the  $x$  axis. Negative values of  $E$  correspond to a clockwise rotation of coordinate axes; positive values correspond to a counter-clockwise rotation.

Parameters will be chosen for each scenario to define the automatic grid so as to provide good coverage by receptors near the point of maximum concentration. This point is determined using the Gaussian plume algorithms without pollutant removal or transformation mechanisms. For a point source, the downwind distance to the point of maximum concentration,  $x_{m2}$ , is thus calculated from

$$x_{\max} = \left[ \frac{b H^2}{a^2(b+d)} \right]^{1/2b} \quad (9)$$

where  $H$  is the effective source height, and  $a$ ,  $b$ ,  $d$  are coefficients defined in Tables 1 and 2. This expression is obtained by using the power laws, Eq. (5), for  $\sigma_y$  and  $\sigma_z$  in the equation for ground-level centerline concentration from an elevated point source, differentiating with respect to  $x$ , equating to zero, and solving for  $x$ .

Equation (9) is also used to determine  $x_{m1}$ , the point of maximum concentration using the physical stack height  $h_s$  instead of  $H$ . Then let

$$XTM(1) = XT + x_{m1}$$

$$XTM(2) = XT + x_{m2}$$

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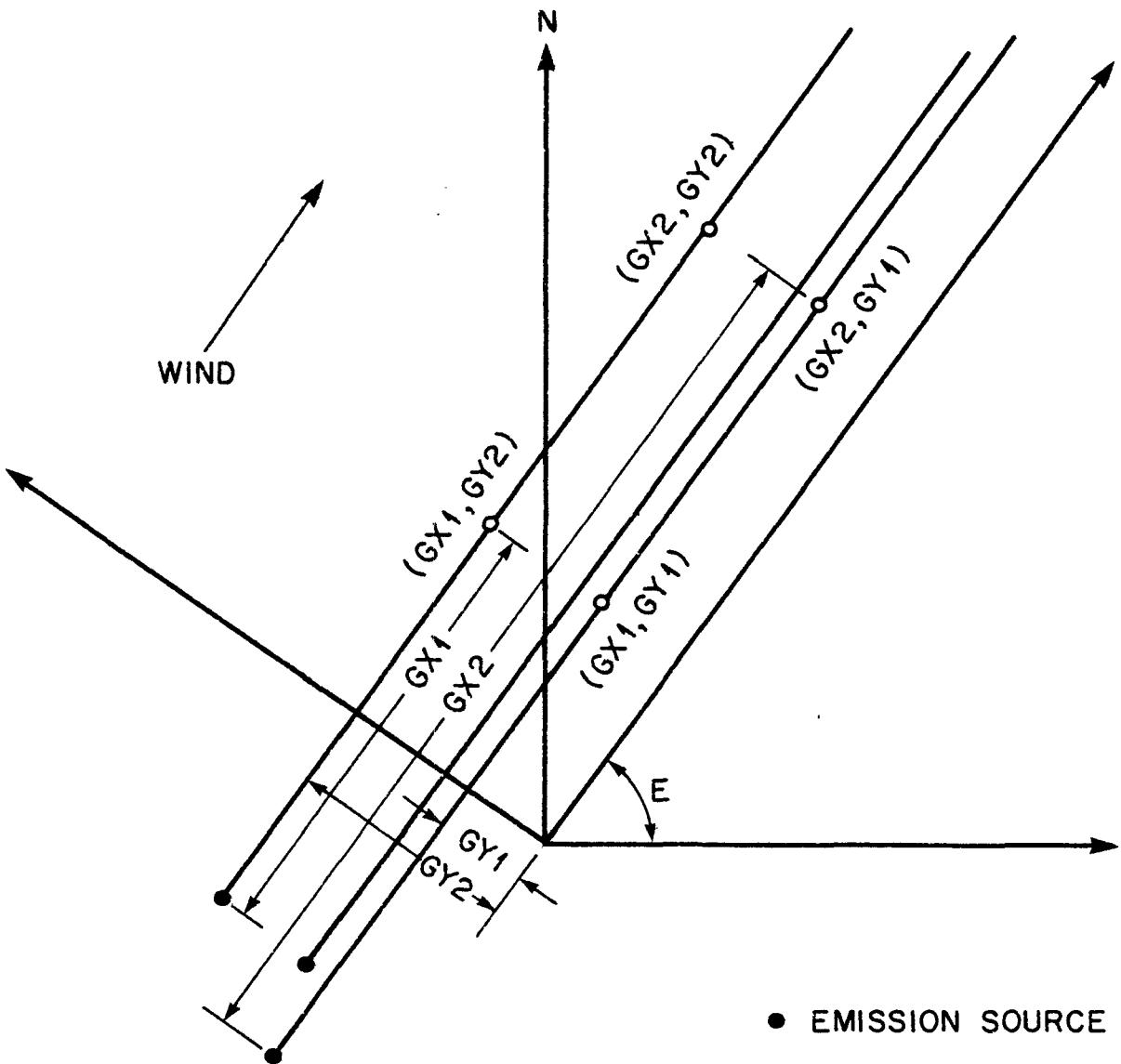


Figure 4. Points used for automatic selection of receptor grid by AUTGRD subroutine.

where XT is the x coordinate of the point source in the rotated coordinate system.

The largest value of XTM(2) for all point sources is GX2 and the smallest value of XTM(1) for all point sources is GX1. Let YT be the y coordinate of the point source in the rotated coordinate system. Then GY2 is the largest value of YT for all point sources and GY1 is the smallest value of YT for all point sources. These points are illustrated in Fig. 4.

Next, the points (GX1, GY1), (GX2, GY1), (GX2, GY2) and (GX1, GY2) are rotated back to the original coordinate system. The largest of the four x values and the largest of the four y values are chosen for the coordinates of the northeast corner of the grid. The smallest of the four x values and the smallest of the four y values are chosen for the coordinates of the southwest corner of the grid.

Then XT is defined as the distance between the x coordinates of the grid corners and YT is the distance between the y coordinates of the grid corners. Let  $D_{max}$  be the larger of XT and YT. Then  $D_{max}$  is used to determine the number of columns and rows in the receptor grid and the grid spacing. If  $D_{max}$  is larger than 10 km, then the number of rows (or columns) is 50 and the grid spacing is  $XT/50$  (or  $YT/50$ ) km. If  $5 < D_{max} < 10$  km, then a grid spacing of 0.2 km is used and the number of rows (or columns) is  $XT/0.2$  (or  $YT/0.2$ ). If  $0.25 < D_{max} < 5$  km, then the number of rows (or columns) is 25, and the grid spacing is  $D_{max}/25$ . If  $D_{max} < 0.25$  km, the grid spacing is 0.01 km, the smallest possible, and the number of rows (or

columns) is  $XT/0.01$  (or  $YT/0.01$ ). A typical example of the receptor grid selected by the automatic grid option is illustrated in Fig. 5.

If the culpability list option is elected in PEM, the receptor grid is limited to 25 rows and 25 columns. In this case, the grid spacing is increased so that the number of rows (or columns) does not exceed 25.

The automatic grid selection procedure, outlined above, considers only point sources. However, the chosen receptor grid may not be suitable if area sources are included in the inventory. Furthermore, the point of maximum concentration determined from Eq. (9) may be significantly in error for problems which include deposition, sedimentation, and chemical decay/transformation. The optimum receptor grid in this case should be determined by trial and error, using the receptor grid defined by this automatic grid option as the first approximation.

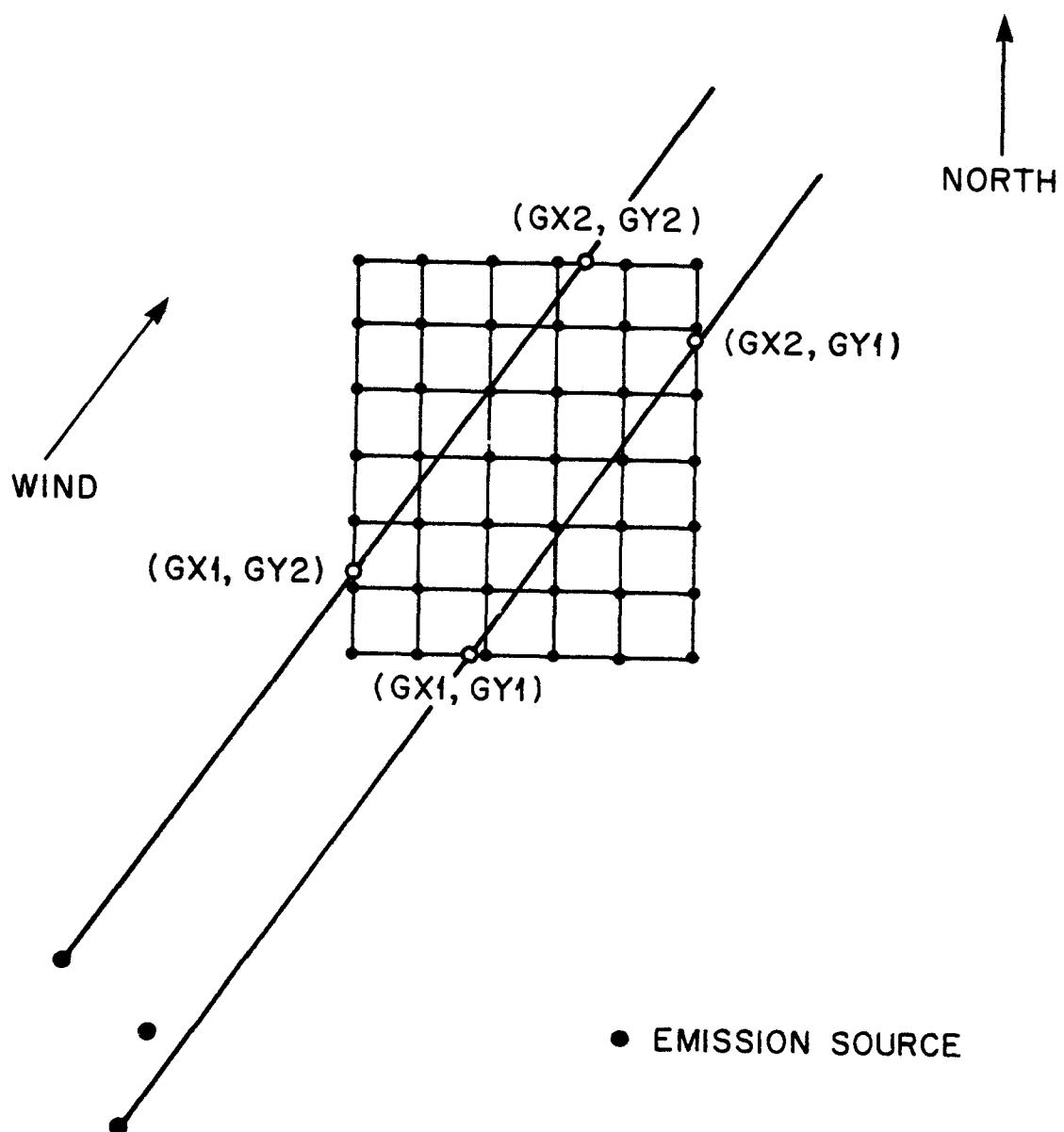


Figure 5. Example of a receptor grid selected by AUTGRD subroutine.

## 2.5 METEOROLOGY

The meteorological data used as input to PEM consist of the atmospheric stability class index, wind speed, wind direction, ambient temperature, mixing depth, and inversion penetration factor. This data set, which represents the mean atmospheric conditions over an hour, is called a scenario. The maximum number of scenarios in an averaging period in PEM is limited to 24, i.e., PEM is designed to predict only short-term (1 to 24 hr) average concentrations.

### 2.5.1 Atmospheric Stability

The Pasquill-Gifford atmospheric stability classes used in PEM are defined in Table 6.

TABLE 6  
Atmospheric Stability Classes

NSC	Atmospheric Stability Class	Description
1	A	Extremely unstable
2	B	Moderately unstable
3	C	Slightly unstable
4	DD	Neutral day
5	DN	Neutral night
6	E	Slightly stable
7	F	Stable (rural only)

The relationship between the atmospheric stability classes and wind speed, incoming solar radiation, and cloud cover is given by Turner (1970) and shown below in Table 7. Class A is the most unstable, while Class F is

the most stable class considered in PEM. Night refers to the period from one hour before sunset to one hour after sunrise. Note that the neutral class, D, should be assumed for overcast conditions during day or night, regardless of wind speed.

TABLE 7

**Atmospheric Conditions Defining  
Stability Classes (Turner, 1970)**

Surface Wind Speed (at 10 meters), m/s	Day			Night	
	Incoming Solar Radiation	Strong	Moderate	Slight	Thinly overcast or $\geq 4/8$ low clouds $\leq 3/8$ cloud
<2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

#### 2.5.2 Wind Speed

PEM gives the user the option of specifying either an hourly mean wind speed or the wind speed class number. The latter is based on National Weather Service (NWS) classification. Any wind speed which lies in a given range is assigned that class number; PEM uses a representative wind speed for each class as shown in Table 8.

TABLE 8

## Wind Speed Classification

NWS Wind Speed Class	Wind Speed Range (knots)	Representative Wind Speed (m/s)
1	0 - 3	1.50
2	4 - 6	2.46
3	7 - 10	4.47
4	11 - 16	6.93
5	17 - 21	9.61
6	> 21	12.52

Wind speed near the surface generally increases with height. Most NWS wind speed measurements are taken at a height ( $h_o$ ) of 10 m above the surface and are listed as "ground-level" wind speeds ( $U_o$ ) in knots. Then the wind speed ( $U$ ) at the physical stack height ( $h_s$ ) is determined as follows:

$$U = U_o (h_s/h_o)^p \quad (10)$$

The wind speed  $U$  is used in the plume rise calculations and the concentration algorithms of PEM. Equation (10) is applied when the stack height is greater than 10 m. The exponent  $p$  is a function of atmospheric stability as shown in Table 9.

TABLE 9

Values of Exponent  $p$  in Wind Speed Power Law  
(DeMarrais, 1959)

Atmospheric Stability Class	$p$
A = 1	0.10
B = 2	0.15
C = 3	0.20
DD = 4	0.25
DN = 5	0.25
E = 6	0.30
F = 7	0.30

### 2.5.3 Wind Direction

By convention, wind direction is defined as the direction from which the wind is blowing. PEM gives the user the option of specifying either an hourly mean wind direction, or the wind direction sector number based on the standard 16-point compass. Wind blowing from any angle in a 22.5° sector is assigned the number of that wind direction sector, and the wind direction is represented in the calculations by the median of that sector, as shown in Table 10.

TABLE 10  
Wind Direction Sectors

Sector Number	Compass Point	Representative Wind Direction (deg)
1	N	0.0
2	NNE	22.5
3	NE	45.0
4	ENE	67.5
5	E	90.0
6	ESE	112.5
7	SE	135.0
8	SSE	157.5
9	S	180.0
10	SSW	202.5
11	SW	225.0
12	WSW	247.5
13	W	270.0
14	WNW	292.5
15	NW	315.0
16	NNW	337.5

PEM also includes an option in which the user specifies the wind direction in degrees for the first of four sub-scenarios; for each

succeeding sub-scenario, the wind direction is automatically shifted clockwise by 90, 45, 30, 15, 10, or 5 degrees, depending on the option number specified in the input. Details of these I/O control parameters are discussed in Section 4.2.1.

#### 2.5.4 Mixing Depth

The turbulent mixing layer near the ground is frequently bounded by a layer of stable air aloft. The latter effectively limits vertical dispersion to the mixing layer. The height of the base of the inversion above the ground is called the mixing depth, L. The hourly mixing depths are specified in the input to PEM.

If vertical mixing is limited, pollutants emitted from a point source into the mixing layer will be trapped and, beyond some point downwind, will become uniformly mixed in the vertical. PEM uses different sets of concentration algorithms for the (near-source) mixing region and the well-mixed region. The concentrations in the intermediate plume-trapping region are then obtained by interpolation as described in Section 2.2.1. The determination of the mixing regime and the algorithms to be used in the model depend on the atmospheric stability class, mixing depth, effective height of the source, and the downwind distance.

If the physical stack height exceeds the mixing depth, pollutants are emitted into the stable layer aloft; these pollutants will not be brought to the ground level and the source is neglected.

If the physical stack height is less than the mixing depth, but the effective source height ( $H$ ) exceeds  $L$ , then the plume may or may not escape the mixing layer, depending on the value of  $H - L$  and the strength of the inversion. A strong inversion layer can retard the plume rise, causing the plume to be trapped in the mixing layer. PEM simulates inversions of various strengths by defining an inversion penetration factor,  $I$ . This is an optional user-specified input parameter with a default value of 2.0. The weakest inversion uses  $I = 1$ . If  $H > I \cdot L$ , then it is assumed that the plume escapes the mixing layer and the source is neglected. If  $L < H \leq I \cdot L$ , then it is assumed that the plume is trapped within the mixing layer and  $H$  is set equal to  $L$ . Though somewhat crude, this procedure allows the user to account for the strength of the inversion and to obtain conservative estimates of concentrations.

## SECTION 3

### COMPUTER PROGRAM OVERVIEW

#### 3.1 BASIS FOR PEM PROGRAM

The PEM (Version 82360) computer program, listed in Appendix F, is based on the FORTRAN program of the Texas Episodic Model Version 8 (TEM-8) and its Users' Guide published by the Texas Air Control Board (1979). The latter model uses the Gaussian plume concentration algorithms developed for non-reactive pollutants and a perfectly reflecting lower boundary. Chemical and physical depletion processes are therefore ignored, except for an option which allows a simple exponential decay of pollutant with travel time. This method requires an accurate estimate of the pollutant's half-life.

In contrast, PEM explicitly accounts for the dry deposition, gravitational settling, and a first-order transformation of two chemically-coupled gaseous or particulate (any size) pollutants in the concentration algorithms. The latter were developed especially for PEM by Rao (1982). The surface concentrations and deposition fluxes of both the primary pollutant (species-1 or reactant) as well as the secondary pollutant (species-2 or reaction product) are calculated. Thus, the concentration algorithms used in PEM and TEM-8 are different, though both models share essentially the same framework for calculations. Figures 2, 4, 5 and several tables shown in this report are

There are several other important differences between PEM and TEM-8.

These are briefly listed below:

1. PEM uses standard EPA values for 1-hour average dispersion parameters for point sources. These correspond to the values of the 10-minute average dispersion parameters used in TEM.
2. For averaging periods longer than 10 minutes, TEM-8 uses a power law to adjust the values of  $\sigma_y$  to account for the greater horizontal plume meander due to fluctuations in wind direction. This is not done in PEM, since its  $\sigma_y$  values are assumed to represent 1-hour average dispersion of the plume.
3. TEM has eight averaging time options (NTOPT), whereas PEM has only three, namely, 1-hour, 24-hour, and N-hour ( $1 < N < 24$ ) averaging options.
4. TEM uses the area-source algorithms given by Gifford and Hanna (1970) to calculate ground-level concentrations. The area-source algorithms used in PEM are derived by Rao (1982) from an innovative alternate approach based on mass balance considerations. These efficient new algorithms do not require additional subroutines in the program.
5. TEM uses the fast numerical technique of Christiansen and Porter (1975) in which the horizontal and vertical diffusion functions in the equation for relative concentration from a point source are precalculated for selected values of model parameters, and stored in large arrays. For multiple sources and receptors, this technique considerably reduces the computation times required by the model, at the expense of some accuracy. Because of the large number of model parameters, PEM does not use this tabular data technique in calculations.
6. In TEM, input data can be specified in metric or British units. PEM uses only metric units.

### 3.2 STRUCTURE OF THE PROGRAM

Figure 6 shows the structure of PEM computer program, its subroutines and functions. All input data to the model is read through subroutine

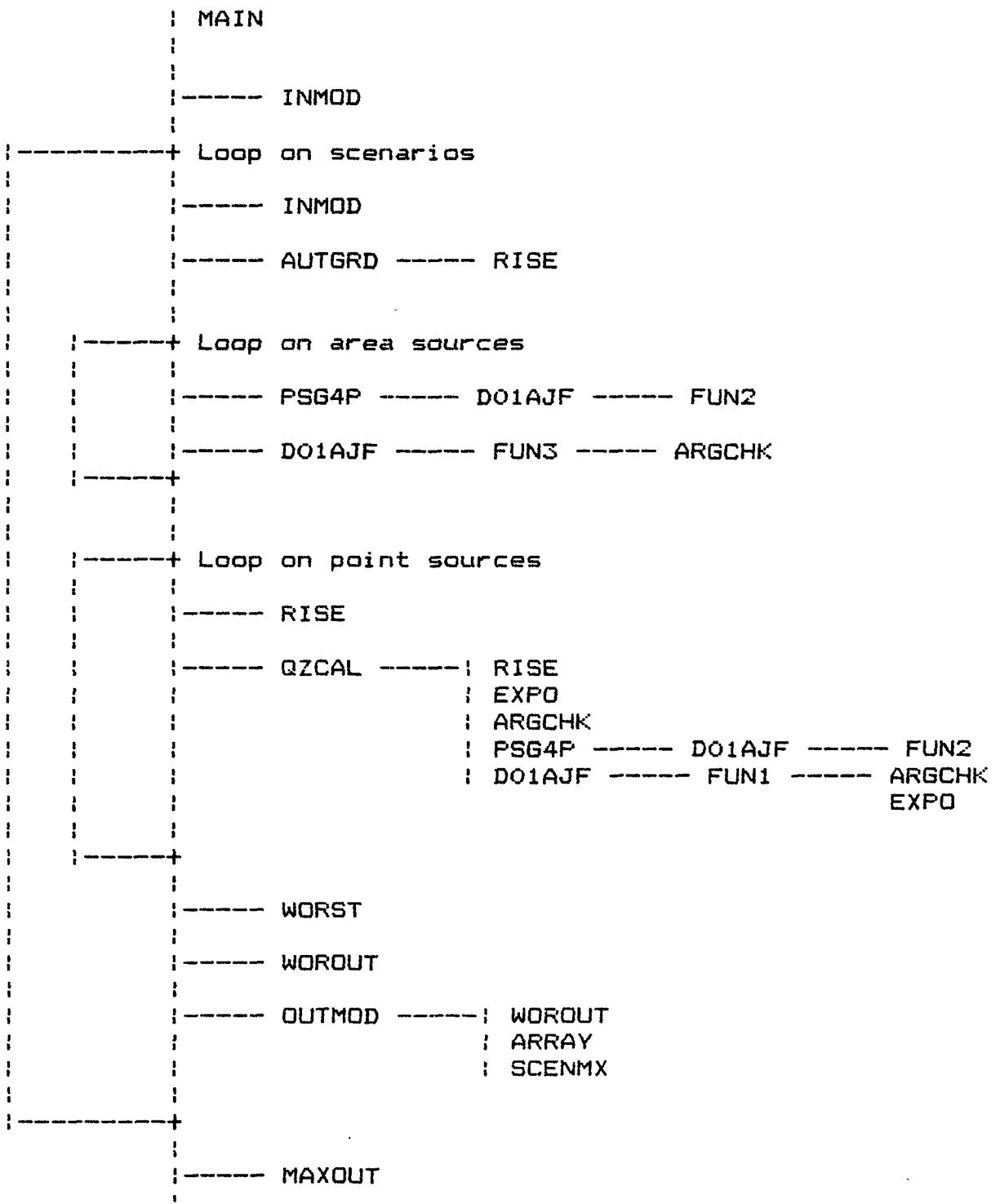


Figure 6. Structure of PEM computer program.

INMOD. For area source concentrations, the main program calls subroutines PSG4P (to calculate  $g'_{41}$  and  $g'_{42}$ ) and D01AJF. The latter is a general purpose integration routine which calculates the integral of a function over a finite interval. After area source calculations are completed, the program starts point source calculations by calling subroutines RISE and QZCAL. The latter calculates the probability densities of vertical distributions of concentrations of the two pollutants using the appropriate algorithms. All output is printed in subroutine OUTMOD, which calls and uses other optional output routines. This procedure is repeated for all scenarios.

### 3.3 GENERAL FLOW OF THE PROGRAM

At the beginning of the run, PEM reads in all input data, screens them, prints warning messages, and sets default values as necessary. All control parameters are listed and explained. Input data for meteorological conditions, area sources, and point sources are also listed. Some errors in input data may be serious enough to cause cancellation of the run; however, in general, PEM attempts to recover from input errors and complete the run using default values.

Inventories of area and point sources must include the locations of the sources on a receptor grid, their emission rates, the size for area sources, and stack parameters for point sources.

The inventories are used with sets of hourly meteorological data called scenarios. For each scenario, the concentration and surface deposition flux are calculated at each impacted receptor in the grid.

Output options are many and varied. Concentration and surface deposition flux may be presented in the form of lists, array maps, and records on tape. Other options include a culpability list of point sources, a list of receptors with the highest concentration for each pollutant for each scenario, and information on plume rise and effective stack height for point sources. The calculation of the surface deposition fluxes of the species is discussed in Appendix C.

## SECTION 4

### PROGRAM USER'S GUIDE

#### 4.1 SUMMARY OF PROGRAM INPUT

##### Control Parameters (6 cards)

Control parameters remain constant throughout the run. They specify 1) a title; 2) options for time averaging, types of input and output, and use of the stack-tip downwash algorithm; 3) receptor grid coordinates and spacing; 4) pollutant parameters and an option to calculate chemical transformation or decay; 5) scaling factors for area source emissions and calibration coefficients to be applied to the calculated concentration; and 6) labels for the pollutants and calibration coefficients.

##### Scenario Parameters (1-24 cards)

Each card contains information for one scenario, that is, the meteorological data for one hour. It includes atmospheric stability class, wind speed, wind direction, temperature, the inversion penetration factor, and mixing height.

##### Area Source Parameters (0-50 cards)

Each card contains information for one area source. It includes the location of the area source on the receptor grid, the size of the area source, and its emission rates.

A blank card must follow the last area source card to signal the end of the area source data.

##### Point Source Parameters (0-300 cards)

Each card contains information for one point source. It includes the location of the point source on the receptor grid; its emission rates; the stack parameters of height, diameter, exit velocity, and exit temperature; and a label which identifies the point source.

A blank card must follow the last point source card to signal the end of the point source data.

## 4.2 DETAILS OF PROGRAM INPUT

### 4.2.1 Control Parameters (6 cards)

Card 1 : Title    FORMAT(20A4)

Alphanumeric information which identifies the run. The information is printed at the top of each page of output.

Card 2 : Input and output options    FORMAT(13I5)

NTOPT    Averaging time option

In PEM, a scenario is a set of meteorological data for one hour.

=1    One hour: Concentrations are calculated for each scenario. No averaging is done.

=2    Twenty-four hours: Concentrations are calculated for exactly 24 scenarios and averaged.

=3    Variable: Concentrations are calculated for a given number of scenarios (2 to 24) and averaged.

The default value is NTOPT=1 .

NWDOPT    Wind direction input option

=0    The user will specify wind direction in degrees for each scenario.

=1    The user will specify a wind direction sector number for each scenario.

=2-7    The user will specify wind direction in degrees for the first of four sub-scenarios. For each succeeding sub-scenario, the wind direction is automatically shifted clockwise by 90, 45, 30, 15, 10, or 5 degrees, depending on the option number selected.

NWDOPT= 2-7 is not allowed with time averaging (NTOPT=2 or 3).

The default value is NWDOPT=0 .

NWSOPT    Wind speed input option

Surface wind speed is measured at 10 meters.

=0    The user will specify surface wind speed in meters/second for each scenario.

=1    The user will specify a wind speed class number for each scenario.

The default value is NWSOPT=0 .

NSCEN    Number of scenarios

=1-24    The number of sets of one-hour meteorological data to be read and processed by the program. When the time-averaging option NTOPT=2, NSCEN must equal 24 . If NSCEN is not specified properly, the input data file will be misread.

The default value is NSCEN=1 .

**NLIST**      Output option for lists of calculated concentration and surface deposition flux at each receptor in the grid.  
 =0      The lists are not printed.  
 =1      Lists of concentration and surface deposition flux are printed, one column of the grid per page.  
 The default value is NLIST=0 .  
 NLIST=1 may not be used with the automatic windshift option (NWDOPT>1) .

**NARRAY**      Output option for array maps of calculated concentration and surface deposition flux at each receptor in the grid.  
 =0      No array maps are printed.  
 =1      Separate maps of uncalibrated and calibrated concentration and surface deposition flux are printed--a total of four maps for each pollutant.  
 =2      Maps of uncalibrated values only are printed --two maps for each pollutant.  
 =3      Maps of calibrated values only are printed --two maps for each pollutant.  
 The default value is NARRAY=0 .

**NTAPE**      Output option for a list on tape of concentration and surface deposition flux at each receptor in the grid.  
 =0      The list is not written to tape.  
 =1      A list of concentration and surface deposition flux is written on a separate output tape, one receptor per record. Control parameter INTER may be set to limit the number of receptors written onto tape. The program checks the total number of records to be written; if the number is greater than 10,000 a message is printed and NTAPE is set to zero.  
 The default value is NTAPE=0 .  
 NTAPE=1 may not be used with the automatic windshift option (NWDOPT>1) .

**NCSOPT**      Output option for a culpability list of the five point sources which contribute most to the total concentration calculated at each receptor.  
 =0      The culpability list is not printed.  
 =1      For each receptor in the grid, the program lists up to five point sources and the percent of the total concentration contributed by each source. The total concentration and surface deposition flux at each receptor are also listed. The information is printed one column of the grid per page.  
 The default value is NCSOPT=0 .

NCSOPT=1 may not be used when two pollutants are specified (NPOL=2) , or when the number of columns in the grid (LX) or the number of rows in the grid (LY) is greater than 25 .

NMAX Output option for lists of the maximum concentration and surface deposition flux calculated for each pollutant for each scenario.  
=0 The lists are not printed.  
=1 At the end of the run, lists are printed to show the receptor in each scenario which received the highest concentration and surface deposition flux for each pollutant.  
The default value is NMAX=0 .

NSTDWN Option for point source stack-tip downwash algorithm  
=0 The stack-tip downwash algorithm is used to determine stack-tip downwash effects for point sources.  
=1 The algorithm is not used.  
Note that the default value NSTDWN=0 means the algorithm is used.

INTER Interval option for receptors written to tape  
=N When the output option NTAPE=1 is selected, the value of INTER determines which receptors are written on the tape. When INTER is specified as integer N, every Nth receptor in each column and row is listed. Thus, if INTER = 2, one fourth of the receptors will be listed ; if INTER is 5, one twenty-fifth will be listed. Effectively, an output grid is set up with spacing equal to the value of INTER, and only those receptors on the "new" grid are written onto the tape.  
The default value is INTER=1 ; that is, every receptor in the grid will be listed on the tape.  
INTER is used only when output option NTAPE=1 is selected.

NPRINT Output option for point source information  
= 0 Input point source data is printed only at the beginning of the run.  
= 1 A list of input point source parameters and calculated plume rise information is printed at the beginning of each scenario.  
The default value is NPRINT=0 .

INPTSC Input option for point source data  
= 1 Point source data is read from the normal input stream (on cards, for example).  
= 2 Point source data is read from a disk file specified by the user in his job control set.  
The default value is INPTSC=1 .

Card 3 : Grid information FORMAT (2F10.0,2I10,3F10.0)

XRSWC The x, or east-west coordinate of the receptor at the southwest corner of the grid, in kilometers.

The default value is XRSWC=0.0 km.

YRSWC The y, or north-south coordinate of the receptor at the southwest corner of the grid, in kilometers.

The default value is YRSWC=0.0 km.

LX The number of columns of receptors in the receptor grid.  
Allowable values are 1 to 50 .  
The default value is LX=1 .

LY The number of rows of receptors in the receptor grid.  
Allowable values are 1 to 50 .  
The default value is LY=1 .

GRID Automatic grid option or grid spacing  
=0.0 The program chooses the size and placement of the receptor grid to insure that the point of maximum concentration calculated from point sources will fall within the grid. Note that area sources are not taken into consideration in this selection.  
#0.0 The size of the spacing between columns and rows of receptors in the grid, in kilometers.  
The default value is GRID=0.0 km., the automatic grid selection.

DTDZ(1), DTDZ(2) The potential temperature gradient,  $d\theta/dz$ , for Class E and Class F atmospheric stability, in units of degrees Celsius/meter.  
The potential temperature gradient is used in the stable/buoyant and stable/momentun plume rise equations.  
The default values are DTDZ(1)=0.02 deg C/meter and DTDZ(2)=0.035 deg C/meter.

Card 4 : Pollutant information and calculation option  
FORMAT(2I5,6F10.0)

NPOL      The number of pollutants  
Allowable values are 1 or 2 .  
The default value is NPOL=1 .

ICT      Option to calculate chemical transformation or decay  
=0      Chemical transformation loss of pollutant(s) is not considered.  
=1      When NPOL=1, the first-order chemical decay of the pollutant is considered.  
When NPOL=2, the first-order chemical transformation of pollutant-1 to pollutant-2 is considered.  
The default value is ICT=0 .

VD1      Deposition velocity for pollutant-1, in cm/second  
When area source calculations are included, VD1 should not be zero.

W1      Settling velocity for pollutant-1, in cm/second

VD2      Deposition velocity for pollutant-2, in cm/second. When NPOL=2 and area source calculations are included, VD2 should not be zero.

W2      Settling velocity for pollutant-2, in cm/second  
  
In general, for deposition to occur, the settling velocity (W) should be less than or equal to the deposition velocity (VD). For gases and very small particles, W should be zero. For small particles, W should be less than VD. For medium and large particles, W should equal VD.

XKT      Chemical transformation or decay rate of pollutant-1, in percent/hour. Allowable values are 0.1 to 100.0 percent/hour; input values outside that range are set to the nearer limit. For example, if XKT=0.0 is specified, the program prints a message and sets XKT=0.1 percent/hr.  
XKT is used only when option ICT=1 is selected.

GAMMA      The ratio of the molecular weights of pollutant-2 (product) to pollutant-1 (reactant) in the chemical transformation.  
GAMMA is used only when option ICT=1 is selected.  
The default value is GAMMA=0.0 .

Card 5 : Scaling and calibration FORMAT(6F10.0)

ASCALE(1), ASCALE(2) Area source scaling factors for pollutants 1 and 2 .  
All area source emission rates are multiplied by ASCALE(1) for pollutant-1 and by ASCALE(2) for pollutant-2 .

The default values are ASCALE(1)=1.0 and ASCALE(2)=1.0 .

The entire area source inventory can be scaled to reflect higher traffic volume, etc. in future years, without having to generate an entire new set of area sources.

A(1), B(1) Coefficients used to calibrate the calculated concentration of pollutant-1.  
The calibrated value Xcal is computed by applying A and B to the concentration X by the formula

$$X_{\text{cal}} = A + BX$$

The default values are A(1)=0.0 and B(1)=0.0 .

A(2), B(2) Coefficients used to calibrate the calculated concentration of pollutant-2.  
The default values are A(2)=0.0 and B(2)=0.0 .

The normal output units for calculated concentration are micrograms per cubic meter. The calibration coefficients can be used to convert to percent allowable , parts per million, or any other convenient units.

Card 6 : Labels FORMAT (3A4,7A4,3A4,7A4)

POLNAM(1) Name for pollutant-1  
Up to 12 alphanumeric characters are allowed.

CALNAM(1) Label for calibrated values of concentration of pollutant-1, computed from calibration coefficients A(1) and B(1) on Card 5.  
Up to 28 alphanumeric characters are allowed.

POLNAM(2) Name for pollutant-2  
Up to 12 alphanumeric characters are allowed.

CALNAM(2) Label for calibrated values of concentration of pollutant-2, computed from calibration coefficients A(2) and B(2) on Card 5.  
Up to 28 alphanumeric characters are allowed.

Defaults for all labels are blanks.

#### 4.2.2 Scenario Parameters      FORMAT(3I5,5F10.0)

One to 24 cards, each containing a set of meteorological data for one hour.

NSC	Atmospheric stability class number Allowable values are 1 through 7; an input value outside that range will be set to the nearer limit. See List of Tables for atmospheric stability classes used in PEM.
NWS	Wind speed class Allowable values are 1 through 6; an input value outside that range will be set to the nearer limit. See List of Tables for wind speed classes used in PEM.  Note that NWS is used only when the windspeed input option NWSOPT on Card 2 is specified as NWSOPT=1 .
NWD	Wind direction sector Allowable values are 1 through 16; any input value outside that range will be set to the nearer limit. See List of Tables for wind direction sectors used in PEM.  Note that NWD is used only when the wind direction option NWDOPT on Card 2 is specified as NWDOPT=1 .
WS	Wind speed Surface wind speed in meters/second measured at a height of ten meters. If WS=0.0 is specified, a message is printed and WS is set to 1.0 m/sec.  Note that WS is used only when the wind speed input option NWSOPT on Card 2 is specified as NWSOPT=0 .
WD	Wind direction The azimuthal angle in degrees from which the wind is blowing. Allowable values are 0.0 through 360.0 degrees. The default value is WD=0.0 , wind from the north. Note that WD is used only when the wind direction input option NWDOPT on Card 2 is specified as NWDOPT=0 or 2 through 7 .
TA	Ambient temperature in degrees Celsius. The default value is TA=0.0 deg C.

PEN      Inversion penetration factor  
When the top of a stack is below the mixing height, but the calculated effective stack height is greater than the mixing height, the inversion penetration factor is used to determine whether the plume can penetrate the upper level inversion boundary.  
Values for PEN can range from 1.0 for a weak inversion to 2.0 or more for a strong inversion.

The default value is PEN=2.0 .

HMX      Mixing height  
The distance in meters from the ground to the bottom of a layer of stable air.  
The default value is HMX=9999.99 m.

#### 4.2.3 Area Source Parameters      FORMAT(5F10.0)

Zero to 50 cards, each containing parameters for one area source. A blank card must follow the last area source data card.

XA      The x, or east-west, coordinate of the south-west corner of the area source, in kilometers.  
The default value is XA=0.0 km.

YA      The y, or north-south, coordinate of the south-west corner of the area source, in kilometers.  
The default value is YA=0.0 km.

SIZE      The length of a side of the area source, in meters.  
The default value is SIZE=GRID\*1000.0, the size of one grid square in meters. If GRID is specified as zero, then SIZE is set to 1.0E-4 meters.

EA(1), EA(2)      Emission rates for pollutants 1 and 2 in grams/second.

Note that this is not an emission rate per unit area; this is the emission rate of an equivalent point source located at the center of the area source.

The default values are EA(1)=0.0 g/sec and EA(2)=0.0 g/sec.

Note: The area source inventory is followed by a blank card to signal the end of area source data.

#### 4.2.4 Point Source Parameters      FORMAT(8F9.0,2A4)

Zero to 300 cards, each containing parameters for one point source. A blank card must follow the last point source data card.

XP        The x, or east-west, coordinate of the point source, in kilometers.

The default value is XP=0.0 km.

YP        The y, or north-south, coordinate of the point source, in kilometers.

The default value is YP=0.0 km.

EP(1), EP(2) Emission rates for pollutants 1 and 2 in grams/second.

The default values are EP(1)=0.0 g/sec and EP(2)=0.0 g/sec.

HP        The physical height of the stack, in meters.

The default value is HP=0.0 m.

DP        The inside exit diameter of the stack, in meters. If DP=0.0 is specified, a message is printed and DP is set to 1.0E-4 meters.

VP        The stack-exit velocity of the plume, in meters/second.

The default value is VP=0.0 meters/sec, which will yield zero plume rise.

TP        The stack-exit temperature of the plume, in degrees Celsius.

The default value is TP=0.0 deg C, which usually results in a momentum-dominated plume rise.

NAME      Label which identifies the point source. Up to eight alphanumeric characters may be used. The default is blanks.

Note: The point source inventory is followed by a blank card to signal the end of the point source data.

#### 4.2.5 Discussion of Input Parameters

The PEM, designed to predict short-term (1 to 24 hr) average ground-level concentrations, assumes that emission rates are constant over the averaging period for NTOPT > 1. This may not be a good assumption for cases where the emissions are strongly time-dependent. For these cases, concentration estimates may be made for each hour using the appropriate emissions and the mean meteorological conditions for that hour. Then concentrations for a period longer than an hour can be determined by averaging the hourly concentrations of that period. This can be done externally with minimal programming.

The deposition and sedimentation velocities of the species and the chemical transformation rate are also assumed to be constant over the concentration-averaging period. If it is important to consider the hourly variations of these parameters, a procedure similar to that described above for emissions, can be used in the concentration calculations.

The meteorological data input to PEM consist of atmospheric stability class, wind speed, wind direction, temperature, the inversion penetration factor, and mixing height. Each of these hourly data sets is called a scenario. For a given set-up of the receptor grid, the pattern of the impacted receptors downwind of a source depends primarily on the wind direction. For urban-planning or regulatory purposes, it may be necessary to investigate the effects of different wind directions on the calculated concentration patterns in the receptor grid. The PEM has an option which divides each scenario into four sub-scenarios, each consisting of the same

hourly meteorological data except for the wind direction. When the user selects this automatic windshift option (i.e., NWDOPT > 1), the wind direction for only the first of the four sub-scenarios is specified by the user. For each succeeding sub-scenario, the wind direction is automatically shifted clockwise by a fixed number of degrees and the concentration calculations are repeated. The magnitude of this shift may be as large as 90° (for NWDOPT = 2), or as small as 5° (for NWDOPT = 7).

The calculated concentrations,  $C_i$ , of the species in the PEM are given in  $\mu\text{g}/\text{m}^3$ ; these are referred to as uncalibrated values, and represent only the contributions of the sources to the concentrations at the receptors. The user may add the background concentrations, or express the calculated concentrations in parts per million or percent allowable, by the formula

$$C_i^* = A_i + B_i \cdot C_i, \quad i = 1 \text{ or } 2,$$

where  $A_i$  and  $B_i$  are the user-specified calibration coefficients (with default values of zero), and  $C_i^*$  are the calibrated concentrations of the species. Depending on the value specified for NARRAY, the PEM output may consist of array maps of either uncalibrated values or calibrated values, or both, of concentrations and surface deposition fluxes.

The culpability list output option, NCSOPT, is used for evaluation of control strategies. When this option is in effect, the five point sources which contributed most to the total concentration at each receptor are identified and their percent contributions are printed for each scenario. This option may be used only when the model calculates concentrations of a single pollutant (NPOL = 1).

Based on the number of pollutants (NPOL = 1 or 2) and the chemical transformation/decay option parameter (ICT = 0 or 1) specified in the input to the model, PEM program does one of the following:

- (1) If NPOL = 1 and ICT = 0 or 1, surface concentrations and deposition fluxes of one gaseous or particulate pollutant, with the given deposition and settling velocities, VD1 and W1 respectively, are calculated. If ICT = 1, then chemical decay of the pollutant is also considered if the decay rate XKT > 0. is given.
- (2) If NPOL = 2 and ICT = 0, surface concentrations and deposition fluxes of two different and uncoupled gaseous or particulate pollutant species with the given deposition and settling velocities, VD1 and W1 (for species-1) and VD2 and W2 (for species-2) respectively, are calculated. Emission rates for both species may be different. Chemical decay is not considered for either species even if XKT > 0.
- (3) If NPOL = 2 and ICT = 1, the two gaseous or particulate pollutant species are coupled through a first-order chemical transformation. The surface concentrations and deposition fluxes of both the primary pollutant (species-1 or reactant) as well as the secondary pollutant (species-2 or reaction product) are calculated. The chemical transformation rate (XKT > 0.) should be given. Non-zero direct emissions of the secondary pollutant from the point and/or area sources may also be specified as input for this case.

In the expressions for concentrations from area sources, Eq. (8), the parameter  $V_{d1}$  and  $V_{d2}$  should be non-zero to avoid singularities in the computations. If either one of these parameters is input as zero, PEM uses a default value of 0.01 cm/s when area sources are included in the emission inventory. The specification of the deposition and gravitational settling velocities in the model is discussed in Appendix C.

#### 4.3 GUIDE TO PROGRAM OUTPUT

At the beginning of each scenario or sub-scenario\*:

NPRINT---Point source parameter list

For each point source, the output lists its coordinates on receptor grid, emission rates, stack parameters, dominant influence of plume rise, wind speed at physical stack height, and maximum effective source height.

At the end of each scenario or sub-scenario:

NCSOPT---Point source culpability list

For each receptor in the grid, the five point sources which contributed most to the total concentration at the receptor are identified. For each receptor, the output includes the five point source sequence numbers, the percent of the total concentration each of the five produced, and the total concentration and surface deposition flux at the receptor. The information is printed one column of the grid per page. To reduce the amount of output produced, only columns containing non-zero concentrations are printed.

NLIST---Concentration and surface deposition flux list

For each receptor in the grid, the calculated concentration and surface deposition flux are listed, one column of the grid per page. To reduce the amount of output produced, only columns containing non-zero concentrations are printed.

NTAPE---Concentration and surface deposition flux tape

The calculated concentration and surface deposition flux at each receptor on the grid are written onto a separate output tape. All records on the tape contain eighty alphanumeric characters. A separate record is written for every receptor in the grid, unless the interval parameter INTER has been specified as greater than one.

The first record on the tape contains the title information given on Card 1 of the Control Parameter cards, written by FORMAT(20A4). Succeeding records contain the x,y coordinates of the receptor; values for concentration,

\*When the automatic windshift option is selected (NWDOPT>1), a scenario is divided into four sub-scenarios, each with a different wind direction.

surface deposition flux, calibrated concentration, and calibrated surface deposition flux for pollutant-1; and values for concentration, surface deposition flux, calibrated concentration, and calibrated surface deposition flux for pollutant-2. These values are written by FORMAT(10F8.2).

NARRAY---Array maps of concentration and surface deposition flux

Separate maps are printed for concentration and surface deposition flux for each pollutant. The concentration or surface deposition flux at each receptor is printed at its relative location on the grid to aid in visualization of the distribution of the pollutant.

The value specified for NARRAY determines which maps are printed. If output for both uncalibrated and calibrated values is chosen, four maps will be produced for each pollutant. If output is chosen for only uncalibrated, or only calibrated, values, two maps will result for each pollutant. Each map can require one, two, or four pages of output to display the entire grid, since each page can display values for up to 25 grid columns and 25 grid rows.

At the end of the run:

NMAX---Maximum concentration and surface deposition flux

For each scenario, the receptor which receives the highest concentration of pollutant-1 and the receptor which receives the highest concentration of pollutant-2, and the concentration at each, are listed. A second list gives the surface deposition flux at these receptors.

When time averaging is selected (NTOPT=2 or 3), NC5OPT output is printed after each scenario, but output for NLIST, NTAPE, and NARRAY is printed only after all scenarios have been processed, and only for the averaged time.

#### 4.4 EXAMPLE PROBLEMS

Three example runs are described here and their results shown in Appendix E to demonstrate the use of the PEM program.

##### Example 1

Pollutant-1 is a gas, and pollutant-2 is made of small particles which deposit on the ground without significant settling ( $V_d > 0$  and  $W = 0$ ). This example uses an area source and two point sources on a finely-spaced receptor grid. Chemical transformation is selected with a transformation rate of one percent/hour; however, the relatively high emission rates chosen for pollutant-2 probably contribute most to its concentration. The example is a simple one, with no time averaging and only one scenario. Wind speed class number and wind direction sector number are specified. The output options selected print point source plume rise information, concentration and surface deposition flux array maps, and the receptor with the highest concentration.

##### Example 2

This example demonstrates the chemical transformation of a gaseous pollutant to a small-particulate pollutant whose deposition is due primarily to non-gravitational effects ( $V_d > W > 0$ ). A fast transformation rate of twenty percent/hour is specified. Concentrations contributed by multiple point and area sources are calculated and averaged over three hours with the meteorological data held constant. Array maps of concentration and surface deposition flux and the receptor with the highest concentration are printed.

##### Example 3

A gaseous pollutant and a large-particulate pollutant are modeled, using one large area source and three point sources on a widely-spaced receptor grid. In this example, point source emission rates for pollutant-2 are specified as zero. Under this condition, the chemical transformation of pollutant-1, at a rate of ten percent/hour, accounts for all of the pollutant-2 concentration produced by the point sources. Concentrations are averaged over six hours of slightly varying meteorological data. The general atmospheric conditions are slightly stable, with relatively cool temperatures and low mixing heights; low wind speeds and constant wind direction are specified in meters/second and degrees, respectively. The output includes point source plume rise information for each scenario, array maps of concentration and surface deposition flux, and the receptor with the highest concentration in each of the six scenarios.

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## APPENDIX A

### POINT SOURCE ALGORITHMS

The algorithms used in PEM to calculate ground-level concentrations of gaseous or particulate pollutants released from an elevated continuous point source are derived by Rao (1982). These algorithms are based on a gradient-transfer model which describes the atmospheric transport, diffusion, dry deposition, sedimentation, and a first-order chemical transformation of pollutants. The analytical solutions of the model are expressed in terms of the empirical Gaussian plume dispersion parameters and extended to various atmospheric stability and mixing conditions. Details of the model and the solutions can be found in that reference. Here we only list the parameterized point source algorithms for the primary (reactant) and the secondary (reaction product) pollutants, denoted by subscripts 1 and 2, respectively.

For convenience, we adopt the following nondimensionalization scheme: All velocities are nondimensionalized by  $U$ , the constant mean wind speed. The horizontal downwind distance  $x$  and all vertical height quantities are nondimensionalized by  $\sqrt{2} \sigma_z$ ; the chemical transformation time scale  $\tau_c$  is nondimensionalized by  $\sqrt{2} \sigma_z/U$ . The horizontal crosswind distance  $y$  is nondimensionalized by  $\sqrt{2} \sigma_y$ . Thus, we define

$$\begin{aligned}
\hat{v}_{d1} &= v_{d1}/U & , \quad \hat{v}_{d2} &= v_{d2}/U \\
\hat{w}_1 &= w_1/U & , \quad \hat{w}_2 &= w_2/U \\
\hat{v}_{11} &= \hat{v}_{d1} - \hat{w}_1/2 & , \quad \hat{v}_{12} &= \hat{v}_{d2} - \hat{w}_2/2 \\
\hat{v}_{13} &= \hat{v}_{11} - (\hat{w}_1 - \hat{w}_2)/2 & & (A-1) \\
\hat{v}_{21} &= \hat{v}_{d1} - \hat{w}_1 & , \quad \hat{v}_{22} &= \hat{v}_{d2} - \hat{w}_2 \\
\hat{x} &= x/\sqrt{2} \sigma_z & , \quad \hat{z} &= z/\sqrt{2} \sigma_z \\
\hat{H} &= H/\sqrt{2} \sigma_z & , \quad \hat{L} &= L/\sqrt{2} \sigma_z \\
\hat{\tau}_c &= \tau_c U/\sqrt{2} \sigma_z & , \quad \hat{y} &= y/\sqrt{2} \sigma_y
\end{aligned}$$

where

- $H$  = effective height of source
- $L$  = height of the inversion lid or mixing depth
- $v_{d1}, v_{d2}$  = dry deposition velocities of primary and secondary pollutants
- $w_1, w_2$  = gravitational settling velocities of primary and secondary pollutant particles
- $x, y, z$  = horizontal downwind, horizontal crosswind, and vertical coordinates
- $\sigma_y, \sigma_z$  = Gaussian dispersion parameters in y and z directions
- $\tau_c$  = characteristic time scale of first-order chemical transformation.

The nondimensional functions  $g'_{21}$  and  $g'_{22}$  used in Eq. (1) of Section 2.2.1 are now defined as follows:

$$g_1(\hat{x}, \hat{y}) = \exp(-\hat{y}^2) \quad (A-2)$$

$$g'_{21}(\hat{x}, 0) = \exp(-\beta_1^2 - \hat{H}^2 - \hat{x}/\hat{\tau}_c) \cdot (2 - \alpha_1) \quad (A-3)$$

where

$$\beta_1^2 = -2 \hat{w}_1 \hat{x} \hat{H} + \hat{w}_1^2 \hat{x}^2$$

$$\alpha_1 = 4\sqrt{\pi} \hat{v}_{11} \hat{x} e^{\frac{\xi_1^2}{4}} \operatorname{erfc} \xi_1 \quad (A-4)$$

$$\xi_1 = \hat{H} + 2 \hat{v}_{11} \hat{x}$$

$$g'_{22}(\hat{x}, 0) = e^{-\beta_2^2} \left[ (Q_2/Q_1 + \gamma) e^{-\hat{H}^2} \cdot (2 - \alpha_2) - \gamma \exp(-\hat{H}^2 - \hat{x}/\hat{\tau}_c) \cdot (2 - \alpha_3) - \gamma 4\sqrt{\pi} (\hat{v}_{21} - \hat{v}_{22}) \hat{x} \cdot F_1(\hat{x}, 0) \right] \quad (A-5)$$

where

$$\beta_2^2 = -2 \hat{w}_2 \hat{x} \hat{H} + \hat{w}_2^2 \hat{x}^2$$

$$\alpha_2 = 4\sqrt{\pi} \hat{v}_{12} \hat{x} e^{\frac{\xi_2^2}{4}} \operatorname{erfc} \xi_2$$

$$\alpha_3 = 4\sqrt{\pi} \hat{v}_{13} \hat{x} e^{\frac{\xi_3^2}{3}} \operatorname{erfc} \xi_3$$

$$\xi_2 = \hat{H} + 2 \hat{v}_{12} \hat{x}, \quad \xi_3 = \hat{H} + 2 \hat{v}_{13} \hat{x} \quad (A-6)$$

and

$$F_1(\hat{x}, 0) = \frac{1}{\pi} \int_0^1 \frac{1}{\sqrt{t(1-t)}} \exp\left(-\frac{\hat{H}^2}{t} - \frac{\hat{x}t}{\hat{t}_c}\right) dt$$

$$\left[ 1 - \sqrt{\pi} (\xi_4 - \hat{H}/\sqrt{t}) e^{\frac{\xi_4^2}{4}} \operatorname{erfc} \xi_4 \right]$$

$$\left[ 1 - \sqrt{\pi} \xi_5 e^{\frac{\xi_5^2}{4}} \operatorname{erfc} \xi_5 \right] dt \quad (A-7)$$

where

$$\xi_4 = \hat{H}/\sqrt{t} + 2 \hat{v}_{13} \hat{x} \sqrt{t}$$

$$\xi_5 = 2 \hat{v}_{12} \hat{x} \sqrt{1-t} \quad (A-8)$$

In Eq. (A-5),  $\gamma$  is the ratio of molecular weight of the secondary pollutant to molecular weight of the primary pollutant, and  $Q_2/Q_1$  is the corresponding ratio of emission rates of species. In Eq. (A-7),  $t$  is a dimensionless dummy variable of integration with limits of 0 and 1.

The nondimensional functions  $g'_{41}$  and  $g'_{42}$  used in Eq. (2) of Section 2.2.1 are defined as follows:

For  $\hat{v}_{d1} \neq \hat{w}_1$  or  $\hat{v}_{21} \neq 0$ ,

$$g'_{41}(\hat{x}) = \exp(-\beta_1^2 - \hat{x}/\hat{\tau}_c) \left[ (\hat{v}_{11}/\hat{v}_{21}) e^{\frac{\xi_1^2}{2}} \operatorname{erfc} \xi_1 - (\hat{w}_1/2\hat{v}_{21}) e^{\frac{\beta_1^2}{2}} \operatorname{erfc} \beta_1 \right] \quad (A-9)$$

where  $\xi_1 = 2 \hat{v}_{11} \hat{x}$  and  $\beta_1 = \hat{w}_1 \hat{x}$ .

For  $\hat{v}_{d1} = \hat{w}_1$  or  $\hat{v}_{21} = 0$ ,

$$g'_{41}(\hat{x}) = \exp(-\xi_1^2 - \hat{x}/\hat{\tau}_c) \left[ (1 + 2 \xi_1^2) e^{\frac{\xi_1^2}{2}} \operatorname{erfc} \xi_1 - 2 \xi_1/\sqrt{\pi} \right] \quad (A-10)$$

where  $\xi_1 = 2 \hat{v}_{11} \hat{x} = \hat{v}_{d1} \hat{x} = \hat{w}_1 \hat{x}$ .

For  $\hat{v}_{21} \neq 0$  and  $\hat{v}_{22} \neq 0$ ,

$$\begin{aligned} g'_{42}(\hat{x}) = & e^{-\beta_2^2} \left[ (Q_2/Q_1 + \gamma) \left\{ (\hat{v}_{12}/\hat{v}_{22}) e^{\frac{\xi_2^2}{2}} \operatorname{erfc} \xi_2 - (\hat{w}_2/2\hat{v}_{22}) e^{\frac{\beta_2^2}{2}} \operatorname{erfc} \beta_2 \right\} \right. \\ & - \gamma e^{-\hat{x}/\hat{\tau}_c} \left\{ (\hat{v}_{13}/\hat{v}_{21}) e^{\frac{\xi_3^2}{2}} \operatorname{erfc} \xi_3 - (\hat{w}_2/2\hat{v}_{21}) e^{\frac{\beta_2^2}{2}} \operatorname{erfc} \beta_2 \right\} \\ & \left. - \gamma 4\sqrt{\pi} (\hat{v}_{21} - \hat{v}_{22}) \hat{x} \cdot F_2(\hat{x}) \right] \end{aligned} \quad (A-11)$$

where  $\xi_2 = 2 \hat{v}_{12} \hat{x}$ ,  $\beta_2 = \hat{w}_2 \hat{x}$

$$\xi_3 = 2 \hat{v}_{13} \hat{x}, \quad \hat{v}_{13} = \hat{v}_{11} - (\hat{w}_1 - \hat{w}_2)/2 \quad (A-12)$$

$$F_2(\hat{x}) = \frac{1}{2\pi} \int_0^1 \frac{1}{\sqrt{t}} \exp(-\hat{x}t/\hat{\tau}_c) \left[ 1 - \sqrt{\pi} \xi_4 e^{\xi_4^2} \operatorname{erfc} \xi_4 \right].$$

$$\left[ (\hat{v}_{12}/\hat{v}_{22}) e^{\xi_5^2} \operatorname{erfc} \xi_5 - (\hat{w}_2/2\hat{v}_{22}) e^{\xi_6^2} \operatorname{erfc} \xi_6 \right] dt, \quad (A-13)$$

where  $\xi_4 = \xi_3 \sqrt{t}$ ,  $\xi_5 = \xi_2 \sqrt{1-t}$ ,  $\xi_6 = \beta_2 \sqrt{1-t}$  (A-14)

For  $\hat{v}_{21} \neq 0$  and  $\hat{v}_{22} = 0$ ,

$$\begin{aligned} g'_{42}(\hat{x}) = & e^{-\xi_2^2} \left[ (Q_2/Q_1 + \gamma) \left\{ (1 + 2 \xi_2^2) e^{\xi_2^2} \operatorname{erfc} \xi_2 - 2 \xi_2 / \sqrt{\pi} \right\} \right. \\ & - \gamma e^{-\hat{x}/\hat{\tau}_c} \left\{ (\hat{v}_{13}/\hat{v}_{21}) e^{\xi_3^2} \operatorname{erfc} \xi_3 - (\hat{w}_2/2\hat{v}_{21}) e^{\xi_2^2} \operatorname{erfc} \xi_2 \right\} \\ & \left. - \gamma 4\sqrt{\pi} \hat{v}_{21} \hat{x} \cdot F_2(\hat{x}) \right] \end{aligned} \quad (A-15)$$

where  $\xi_2 = 2 \hat{v}_{12} \hat{x} = \hat{v}_{d2} \hat{x} = \hat{w}_2 \hat{x} = \beta_2$

$$\xi_3 = 2 \hat{v}_{13} \hat{x}$$

$$F_2(\hat{x}) = \frac{1}{2\pi} \int_0^1 \frac{1}{\sqrt{t}} \exp(-\hat{x}t/\hat{\tau}_c) \cdot \left[ 1 - \sqrt{\pi} \xi_4 e^{\xi_4^2} \operatorname{erfc} \xi_4 \right] \cdot$$

$$\left[ (1 + 2 \xi_5^2) e^{\xi_5^2} \operatorname{erfc} \xi_5 - 2 \xi_5 / \sqrt{\pi} \right] dt, \quad (A-16)$$

with  $\xi_4 = \xi_3 \sqrt{t}$ ,  $\xi_5 = \xi_2 \sqrt{1-t}$ .

For  $\hat{v}_{21} = 0$  and  $\hat{v}_{22} \neq 0$ ,

$$g'_{42}(\hat{x}) = e^{-\xi_3^2} \left[ (Q_2/Q_1 + \gamma) \left\{ (\hat{v}_{12}/\hat{v}_{22}) e^{\xi_2^2} \operatorname{erfc} \xi_2 - (\hat{w}_2/2\hat{v}_{22}) e^{\xi_3^2} \operatorname{erfc} \xi_3 \right\} \right.$$

$$- \gamma e^{-\hat{x}/\hat{\tau}_c} \left\{ (1 + 2 \xi_3^2) e^{\xi_3^2} \operatorname{erfc} \xi_3 - 2 \xi_3/\sqrt{\pi} \right\}$$

$$\left. + \gamma 4\sqrt{\pi} \hat{v}_{22} \hat{x} \cdot F_2(\hat{x}) \right] \quad (A-17)$$

where  $\xi_2 = 2 \hat{v}_{12} \hat{x}$ ,  $\xi_3 = 2 \hat{v}_{13} \hat{x} = \hat{w}_2 \hat{x} = \beta_2$ ,

and  $F_2(\hat{x})$  is given by Eq. (A-13).

For  $\hat{v}_{21} = 0$  and  $\hat{v}_{22} = 0$ ,

$$g'_{42}(\hat{x}) = [ Q_2/Q_1 + \gamma (1 - e^{-\hat{x}/\hat{\tau}_c}) ] .$$

$$e^{-\xi_2^2} \left\{ (1 + 2 \xi_2^2) e^{\xi_2^2} \operatorname{erfc} \xi_2 - 2 \xi_2/\sqrt{\pi} \right\} \quad (A-18)$$

where  $\xi_2 = \hat{w}_2 \hat{x} = \beta_2$ .

In Eqs. (A-7), (A-13), and (A-16),  $t$  is a parameterized integration variable. The integrand functions in these equations have singularities at the end-points  $t=0$  and  $t=1$  of the integration domain in  $t$ . Because of their complexity, these integrations cannot be carried out analytically; therefore, they should be evaluated by numerical integration to a sufficiently high degree of accuracy.

A computer-library subroutine named D01AJF, developed by the Numerical Algorithms Group (NAG), is utilized in PEM (Version 82360) for numerical integration. This general purpose integrator routine, which is capable of handling the singularities, has been selected because of its accuracy and applicability. It estimates the value of a definite integral of an externally defined function over a finite range, to a specified absolute or relative accuracy, using Gauss-Kronrod rules in an adaptive strategy with extrapolation. Further details of this subroutine can be found in Appendix D.

In the limit, when  $V_{di} = W_i = 0$  and  $\tau_c = \infty$ , the algorithms for  $g'_{21}$ ,  $g'_{22}$ ,  $g'_{41}$ , and  $g'_{42}$  (defined above) reduce to the familiar Gaussian-plume diffusion algorithms currently used in EPA air quality assessment models. Thus the new algorithms given in this section may be thought of as extensions of the latter to include deposition, sedimentation, and chemical transformation.

It should be noted that the algorithms for  $g'_{41}$  and  $g'_{42}$  are also used in Eqs. (6) and (8) of Section 2.3.2 to calculate ground-level concentrations from area sources. In these equations,  $V_{d1}$  and  $V_{d2}$  should be non-zero to avoid singularities.

REFERENCE

Rao, K. S., 1982: Plume Concentration Algorithms with Deposition, Sedimentation, and Chemical Transformation. EPA-, U.S. Environmental Protection Agency, Research Triangle Park, NC; NOAA Tech. Memo. ERL ARL-; ATDL Contribution File No. 82/27, 87 pp.

## APPENDIX B

### PLUME RISE EQUATIONS

PEM calculates plume rise from equations given by Briggs (1969, 1975). These equations are listed below. For details, the user should consult the references cited.

For unstable/neutral atmosphere, with a buoyancy-dominated plume,

$$\Delta h(x) = 1.6 F^{1/3} x^{2/3} U^{-1}, \text{ for } x < 3.5x^*, \quad (B-1)$$

and

$$\Delta h_{MAX} = 1.6 F^{1/3} (3.5x^*)^{2/3} U^{-1}, \text{ for } x \geq 3.5x^* \quad (B-2)$$

where

$$x^* = 14 F^{5/8} \quad \text{if } F < 55 \text{ m}^4/\text{s}^3, \text{ and} \quad (B-3)$$

$$x^* = 34 F^{2/5} \quad \text{if } F \geq 55 \text{ m}^4/\text{s}^3.$$

For stable atmosphere, with a buoyancy-dominated plume,

$$\Delta h(x) = 1.6 F^{1/3} x^{2/3} U^{-1} \quad (B-4)$$

and

$$\Delta h_{MAX} = 2.6 \left(\frac{F}{U s}\right)^{1/3} \quad (B-5)$$

where  $s = 0.02 g/T_A$  for E-stability,  
(B-6)

and  $s = 0.035 g/T_A$  for F-stability.

For unstable/neutral atmosphere, with a momentum-dominated plume,

$$\Delta h(x) = 3.78 \left[ \frac{V^2}{U(V+3U)} \right]^{2/3} \left( \frac{xR^2}{2} \right)^{1/3} \quad (B-7)$$

and

$$\Delta h_{MAX} = 6RV/U \quad (B-8)$$

For stable atmosphere, with a momentum-dominated plume,

$$\Delta h_{MAX} = 1.5 (VR)^{2/3} U^{-1/3} s^{-1/6} \quad (B-9)$$

where  $s$  is defined in Eq. (B-6).

The variables used in the above equations are defined below:

$$F = gVR^2 (T-T_A) / T \quad (B-10)$$

is the plume buoyancy flux at the stack exit,  $m^4/s^3$

$g$  = acceleration due to gravity,  $9.8 m/s^2$

$\Delta h$  = plume rise,  $m$

$\Delta h_{MAX}$  = maximum plume rise,  $m$

$R$  = inside radius of stack exit,  $m$

$T$  = plume temperature at stack exit,  $^{\circ}K$

$T_A$  = ambient temperature,  $^{\circ}K$

$U$  = mean wind speed at physical stack height,  $m$

$V$  = plume velocity at stack exit,  $m/s$

$x$  = downwind distance,  $m$

## REFERENCES

Briggs, G. A., 1969: Plume Rise. AEC Critical Review Series. Available as TID-25075 from NTIS, Springfield, VA, 81 pp.

Briggs, G. A., 1975: Plume Rise Predictions. Lectures on Air Pollution and Environmental Impact Analyses, D. A. Haugen, Workshop Coordinator, Amer. Meteorol. Soc., Boston, MA, 59-111.

## APPENDIX C

### SURFACE DEPOSITION FLUXES, AND DEPOSITION AND SETTLING VELOCITIES

#### C.1 SURFACE DEPOSITION FLUXES

The surface deposition fluxes of the primary and the secondary pollutants at ground level receptors are calculated directly as

$$D_1(\hat{x}, \hat{y}) = v_{d1} \cdot C_1(\hat{x}, \hat{y}, 0) \quad (C-1)$$

$$D_2(\hat{x}, \hat{y}) = v_{d2} \cdot C_2(\hat{x}, \hat{y}, 0) \quad (C-2)$$

D gives the amount of pollutant deposited per unit time per unit surface area, and is usually calculated as  $\text{kg}/\text{km}^2\text{-hr}$ , while seasonal estimates are expressed as  $\text{kg}/\text{km}^2\text{-month}$ . The estimation of the monthly or yearly surface deposition fluxes at a given downwind distance x from the source in a given wind-directional sector requires the knowledge of the fraction of the time that a mean wind of a given magnitude blows in that direction in a month or a year, respectively. To obtain D in  $\text{kg}/\text{km}^2\text{-hr}$  when  $v_d$  is given in  $\text{cm}/\text{s}$  and C in  $\text{g}/\text{m}^3$ , the right-hand side of the equations should be multiplied by 36000. To obtain D in  $\mu\text{g}/\text{m}^2\text{-hr}$  when  $v_d$  is given in  $\text{cm}/\text{s}$  and C in  $\mu\text{g}/\text{m}^3$ , the corresponding multiplication factor is 36. For D calculations, the ground-level receptor

is generally defined as any receptor which is not higher than 1 meter above the local ground-level elevation.

PEM calculates the surface deposition fluxes of one or two pollutants. These values are printed in a map or list form, as specified by the user, in the same way the program prints the concentrations. The flux units are generally  $\mu\text{g}/\text{m}^2\text{-hr}$ ; however, if these values are too large to be clearly printed in a map format, then the program converts them into  $\text{kg}/\text{km}^2\text{-hr}$  before printing.

## C.2 DEPOSITION AND SETTLING VELOCITIES

The values of the settling and deposition velocities primarily depend on the particle diameter  $d$ . In the trivial case of  $W = V_d = 0$ , settling and deposition effects are negligible. For very small particles ( $d < 0.1 \mu\text{m}$ ), gravitational settling can be neglected, and dry deposition occurs primarily due to nongravitational effects. In this case,  $W = 0$  but  $V_d > 0$ . For small to medium-sized particles ( $d = 0.1\text{--}50 \mu\text{m}$ ),  $0 < W < V_d$ ; deposition is enhanced here beyond that due to gravitational settling, primarily because of increased turbulent transfer resulting from surface roughness. For larger particles ( $d > 50 \mu\text{m}$ ), it is generally assumed that  $V_d = W > 0$ , since gravitational settling is the dominant deposition mechanism. When  $W > V_d > 0$ , re-entrainment of the deposited particles from the surface back into the atmosphere is implied, as in a dust storm, for example. The first four types of model parameters given above are widely used in atmospheric dispersion and deposition of particulate material. The deposition of gases is a special case of the

particulate problem with  $W = 0$ . Thus, one has to carefully select the values of  $W$  and  $V_d$  for use in the models. A more complete discussion of these model parameters is given by Rao (1982).

#### REFERENCE

Rao, K. S., 1982: Plume Concentration Algorithms with Deposition, Sedimentation, and Chemical Transformation. EPA-\_\_\_\_\_, U.S. Environmental Protection Agency, Research Triangle Park, NC; NOAA Tech. Memo. ERL ARL-\_\_\_\_\_; ATDL Contribution File No. 82/27, 87 pp.

## D01AJF – NAG FORTRAN Library Routine Document

NOTE: before using this routine, please read the appropriate implementation document to check the interpretation of bold *italicised* terms and other implementation-dependent details. The routine name may be precision-dependent.

### 1. Purpose

D01AJF is a general-purpose integrator which calculates an approximation to the integral of a function  $F(x)$  over a finite interval  $(A, B)$ :

$$I = \int_A^B F(x) dx.$$

### 2. Specification

```
SUBROUTINE D01AJF (F, A, B, EPSABS, EPSREL, RESULT, ABSERR,
1   W, LW, IW, LIW, IFAIL)
C   INTEGER LW, IW(LIW), LIW, IFAIL
C   real F, A, B, EPSABS, EPSREL, RESULT, ABSERR, W(LW)
C   EXTERNAL F
```

---

### 3. Description

D01AJF is based upon the QUADPACK [3] routine DQAGS. It is an adaptive routine, using the Gauss 10-point and Kronrod 21-point rules. The algorithm, described in [1], incorporates a global acceptance criterion (as defined by Malcolm and Simpson [2]) together with the  $\epsilon$ -algorithm [4] to perform extrapolation. The local error estimation is described in [3].

The routine is suitable as a general purpose integrator, and can be used when the integrand has singularities, especially when these are of algebraic or logarithmic type.

### 4. References

- [1] DE DONCKER, E.  
An Adaptive Extrapolation Algorithm for Automatic Integration.  
Signum Newsletter 13, No. 2, pp. 12–18, 1978.
- [2] MALCOLM, M.A. and SIMPSON, R.B.  
Local versus Global Strategies for Adaptive Quadrature.  
A.C.M. Trans. Math. Software 1, pp. 129–146, 1976.
- [3] PIJSESENS, R., DE DONCKER, E., UBERHUBER, C. and KAHANER, D.  
'QUADPACK', A Quadrature Subroutine Package.  
To be published, 1980.
- [4] WYNN, P.  
On a Device for Computing the  $e_m(S_n)$  Transformation.

M.T.A.C, 10, pp. 91–96, 1956.

### 5. Parameters

**F – *real* FUNCTION, supplied by the user.**

F must return the value of the integrand at a given point.

Its specification is:

*real* FUNCTION F(X)  
*real* X

**X – *real*.**

On entry, X specifies the point at which the integrand value is required by D01AJF. X must not be reset by F.

F must be declared as EXTERNAL in the (sub)program from which D01AJF is called.

**A – *real*.**

On entry, A must specify the lower limit of integration.

Unchanged on exit.

**B – *real*.**

On entry, B must specify the upper limit of integration.

Unchanged on exit.

**EPSABS – *real*.**

On entry, EPSABS must specify the absolute accuracy required. If EPSABS is negative, the absolute value is used. See Section 10.

Unchanged on exit.

**EPSREL - real.**

On entry, EPSREL must specify the relative accuracy required. If EPSREL is negative, the absolute value is used. See Section 10.

Unchanged on exit.

**RESULT - real.**

On exit, RESULT contains the approximation to the integral  $I$ .

**ABSERR - real.**

On exit, ABSERR contains an estimate of the modulus of the absolute error, which should be an upper bound for  $|I - \text{RESULT}|$ .

**W - real array of DIMENSION (LW).**

Used as workspace.

**LW - INTEGER.**

On entry, LW must specify the dimension of W as declared in the calling (sub)program. LW/4 is an upper bound for the number of subintervals into which the interval of integration is divided. A value in the range 800 to 2000 is adequate for most problems. The more difficult the integrand, the larger LW should be. Trivially LW  $\geq 4$ . See IW below.

LW is unchanged on exit.

**IW - INTEGER array of DIMENSION (LIW).**

Used as workspace.

On exit, IW(1) contains the amount of *real* workspace actually used (the smallest possible value of LW).

**LIW - INTEGER.**

On entry, LIW must specify the dimension of IW, as declared in the calling (sub)program. LIW  $\geq \text{LW}/8 + 2$ .

Unchanged on exit.

**IFAIL - INTEGER.**

Before entry, IFAIL must be assigned a value. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

Unless the routine detects an error (see next section), IFAIL contains 0 on exit.

**6. Error Indicators and Warnings****Errors detected by the routine:-****IFAIL = 1**

The maximum number of subdivisions allowed with the given workspace has been reached without the accuracy requirements being achieved. Look at the integrand in order to determine the integration difficulties. If the position of a local difficulty within the interval can be determined (e.g. a singularity of the integrand or its derivative, a peak, a discontinuity...) one will probably gain from splitting up the interval at this point and calling the integrator on the subranges. If necessary, another integrator which is designed for handling the type of difficulty involved, must be used. Alternatively consider relaxing the accuracy requirements specified by EPSABS and EPSREL, or increasing the amount of workspace.

**IFAIL = 2**

Roundoff error prevents the requested tolerance from being achieved. The error may be under-estimated. Consider requesting less accuracy.

**IFAIL = 3**

Extremely bad local integrand behaviour causes a very strong subdivision around one (or more) points of the interval. The same advice applies as in the case of IFAIL = 1.

**IFAIL = 4**

The requested tolerance cannot be achieved, because the extrapolation does not increase the accuracy satisfactorily; the returned result is the best which can be obtained. The same advice applies as in the case of IFAIL = 1.

**IFAIL = 5**

The integral is probably divergent, or slowly convergent. It must be noted that divergence can also occur with any non-zero value of IFAIL.

**IFAIL = 6**

On entry, LW  $< 4$ , or LIW  $< \text{LW}/8 + 2$ .

**7. Auxiliary Routines**

This routine calls NAG Library routines D01AJV, D01AJX, D01AJY, D01AJZ, P01AAF, X02AAF, X02ABF and X02ACF.

**8. Timing**

This depends on the integrand and the accuracy required.

## 9. Storage

The storage required by internally declared arrays is 107 *real* elements.

## 10. Accuracy

The routine cannot guarantee, but in practice usually achieves, the following accuracy:

$$|I-RESULT| \leq tol$$

where

$$tol = \max\{|\text{EPSABS}|, |\text{EPSREL}| \times |I|\}$$

and EPSABS and EPSREL are user-specified absolute and relative error tolerance. Moreover it

returns the quantity ABSERR which, in normal circumstances, satisfies  $|I-RESULT| \leq ABSERR \leq tol$ .

## 11. Further Comments

Labelled COMMON block AD01AJ is used by this routine and must therefore be avoided by the user.

## 12. Keywords

Quadrature, Extrapolation, Globally Adaptive, Singularities.

## 13. Example

To compute

$$\int_0^{2\pi} \frac{x \cdot \sin(30x)}{\sqrt{(1 - (\frac{x}{2\pi})^2)}} dx$$

**WARNING:** This single precision example program may require amendment for certain implementations. The results produced may not be the same. If in doubt, please seek further advice (see *Essential Introduction to the Library Manual*).

### 13.1. Program Text

```
C  D01AJF EXAMPLE PROGRAM TEXT
C  MARK 8 RELEASE. NAG COPYRIGHT 1979.
C  .. SCALARS IN COMMON ..
REAL PI
INTEGER KOUNT
C  ..
C  .. LOCAL SCALARS ..
REAL A, ABSERR, B, EPSABS, EPSREL, EX, EXACT, RESULT
INTEGER IFAIL, NOUT
C  ..
C  .. LOCAL ARRAYS ..
REAL W(800)
INTEGER IW(102)
C  ..
C  .. FUNCTION REFERENCES ..
REAL X01AAF
C  ..
C  .. SUBROUTINE REFERENCES ..
C  D01AJF
C  ..
C  EXTERNAL FST
COMMON /TELNUM/ PI, KOUNT
DATA EXACT /-0.2543259618893530E+01/
DATA NOUT /6/
WRITE (NOUT,99999)
PI = X01AAF(PI)
EPSABS = 0.E0
EPSREL = 1.E-04
A = 0.E0
B = 2.E0*PI
KOUNT = 0
IFAIL = 1
CALL D01AJF(FST, A, B, EPSABS, EPSREL, RESULT, ABSERR, W,
* 800, IW, 102, IFAIL)
WRITE (NOUT,99998) A, B, EPSABS, EPSREL
WRITE (NOUT,99997) RESULT, ABSERR, KOUNT, IW(1), IFAIL
EX = ABS(EXACT-RESULT)
WRITE (NOUT,99996) EX
STOP
99999 FORMAT (4(1X/), 31H D01AJF EXAMPLE PROGRAM RESULTS/1X)
99998 FORMAT (1H , 2X, 1H A, 6X, 31H- LOWER LIMIT OF INTEGRATION = ,
```

```

    • F10.4/1H , 2X, 1HB, 6X, 31H- UPPER LIMIT OF INTEGRATION = .
    • F10.4/1H , 2X, 39HEPSABS - ABSOLUTE ACCURACY REQUESTED = .
    • E9.2/1H , 2X, 39HEPSREL - RELATIVE ACCURACY REQUESTED = .
    • E9.2/)

99997 FORMAT (1H , 2X, 41HRESULT - APPROXIMATION TO THE INTEGRAL = ,
    • E14.5/1H , 2X, 42HABSER - ESTIMATE OF THE ABSOLUTE ERROR = ,
    • E10.3/1H , 2X, 42HKOUNT - NUMBER OF FUNCTION EVALUATIONS = ,
    • I4/1H , 2X, 43HIW(1) - ELEMENTS OF REAL WORKSPACE USED = ,
    • I4/1H , 2X, 22HIFAIL - ERROR FLAG = . 14/)

99996 FORMAT (1H , 7X, 27H - EXACT ABSOLUTE ERROR = , E10.3)
END
REAL FUNCTION FST(X)
C .. SCALAR ARGUMENTS ..
REAL X
C ..
C .. SCALARS IN COMMON ..
REAL PI
INTEGER KOUNT
C ..
C .. FUNCTION REFERENCES ..
REAL SIN, SQRT
C ..
COMMON /TELNUM/ PI, KOUNT
KOUNT = KOUNT + 1
FST = X*SIN(30.E0*X)/SQRT(1.E0-X**2/(4.E0*PI**2))
RETURN
END
C D01AJF EXAMPLE PROGRAM TEXT
C MARK 8 RELEASE. NAG COPYRIGHT 1979.

```

### 13.2. Program Data

None.

### 13.3. Program Results

#### D01AJF EXAMPLE PROGRAM RESULTS

```

A      - LOWER LIMIT OF INTEGRATION =      0.0000
B      - UPPER LIMIT OF INTEGRATION =      6.2832
EPSABS - ABSOLUTE ACCURACY REQUESTED =  0.00E 00
EPSREL - RELATIVE ACCURACY REQUESTED =  0.10E-03

RESULT - APPROXIMATION TO THE INTEGRAL = -0.25433E 01
ABSER - ESTIMATE OF THE ABSOLUTE ERROR =  0.128E-04
KOUNT - NUMBER OF FUNCTION EVALUATIONS =  777
IW(1) - ELEMENTS OF REAL WORKSPACE USED =  76
IFAIL - ERROR FLAG =      0

- EXACT ABSOLUTE ERROR =  0.893E-08

```

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**APPENDIX E**

**INPUT AND OUTPUT LISTINGS  
OF EXAMPLE PROBLEMS**

TABLE 11

## INPUT DATA FOR EXAMPLE PROBLEM 1

CARD IMAGES									
<b>CONTROL CARDS</b>									
1 TITLE	PEP EXAMPLE 1	1	CHEMICAL TRANSFORMATION GAS TU	SMALL PARTICLE					
2 OPTIONS	1	1	0	0	1	0	1	1	0.
3 GRID	0.	0.	25	25	04	0.	0.	0.	0.
4 POLLUTANTS	2	1	1.0	0.0	0.1	0.0	1.0	1.0	1.0
5 SCALING	1.0	1.0	0.	0.	0.	0.	0.	0.	0.
6 LABELS	GAS 1				GAS 2				
<b>SCENARIO CARDS</b>									
4	3	9			15.0	1.	1000.		
<b>AREA SOURCE CARDS</b>									
	*38		*02	120.	0.5	0.05			
BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY									
<b>POINT SOURCE CARDS</b>									
	.20	0.0	1.0	0.10	15.0	1.0	5.0	32.4	STACK 1
	.68	.04	1.0	0.10	10.0	3.0	0.5	32.4	STACK 2
BLANK CARD TO SIGNAL END OF POINT SOURCE INVENTORY									

TABLE 12

OUTPUT LISTING FOR EXAMPLE PROBLEM 1

PEP (VERSION 82360)

POLLUTION EPISODIC MODEL

INCLUDING  
DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION  
OF POLLUTANTS

POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS: PEN EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

AVERAGING TIME OPTION: NCPT=1

A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR

- 1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO
- 2 24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE AVERAGED
- 3 VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN NUMBER (12 TO 24) OF SCENARIOS ARE AVERAGED

WIND DIRECTION OPTION: NWCDPT=1

- 0 DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO
- 1 SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO
- 2-7 DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOUR SUB-SCENARIOS.
- FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRECTION IS AUTOMATICALLY INCREASED BY 90, 45, 30, 15, 10, OR 5 DEGREES, DEPENDING ON THE OPTION NUMBER SELECTED.

WIND SPEED OPTION: NWSOPT=1

- 0 SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO
- 1 WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO

NUMBER OF SCENARIOS: NSCEN= 1

STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDW=0

- C ALGORITHM IS IN EFFECT
- I ALGORITHM IS NOT USED

RECEPTOR GRID:                    COLUMNS: LX= 25                    ROWS: LY= 25  
    SPACING: GH(0)= 0.040 KM  
    SOUTHWEST CORNER        XRSWC= 0.0    KM W  
    YRSWC= 0.0    KM S

POTENTIAL TEMPERATURE GRADIENT: DTGZ(1)= 0.020 DEGM/H                    STABILITY CLASS E  
DTGZ(2)= 0.035 DEGM/H                    STABILITY CLASS F

POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS: PEP EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

NUMBER OF POLLUTANTS: NPOL=2	POLLUTANT-1: GAS 1	POLLUTANT-2: GAS 2
AREA SOURCE SCALING FACTOR:	ASCALE= 1.000	ASCALE= 1.000
CALIBRATION COEFFICIENTS:	A= 0.0	B= 0.0
CALIBRATION IDENTIFICATION:		
DEPOSITION VELOCITY (CM/S):	VOL= 1.000	VD2= 0.100
SETTLING VELOCITY (CM/S):	W1= 0.0	W2= 0.0

CHEMICAL TRANSFORMATION OPTION: ICT=1

NPOL=2  
 ICT=0 CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED  
 ICT=1 FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO POLLUTANT-2 IS CONSIDERED

CHEMICAL TRANSFORMATION RATE: XK1= 1.00 PERCENT/HR

RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO POLLUTANT-1 (REACTANT): GAMMA= 1.000

OUTPUT OPTIONS SELECTED:

NARRAY=2 MAPS OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR IN THE GRID,  
 UNCALIBRATED ONLY  
 NPRINT=1 LIST OF POINT SOURCE PARAMETERS AND EFFECTIVE STACK HEIGHTS  
 PRINTED AT BEGINNING OF EACH SCENARIO  
 NMAX=1 LIST OF RECEPTORS WITH HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX  
 FOR EACH SCENARIO - PRINTED AT END OF RUN

POLLUTION EPISODIC MODEL

INPUT SCENARIO PARAMETERS: PEN EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

SECTOR NUMBER	DIRECTION (DEG)	SECTOR NUMBER	DIRECTION (DEG)	WIND SPEED CLASSES			STABILITY CLASSES		
				CLASS INDEX	SPEED (M/S)	CLASS INTERVALS	CLASS INDEX	CLASS	
1	N NNE	0.0 22.5	9 10	S SSW	180.0 202.5	1 2	1.50 2.46	0-3 4-6	A
2	NE	45.0	11	SW	225.0				B
3	E	67.5	12	WSW	247.5	3	4.47	7-10	C
4	ENF	90.0	13	W	270.0	4	6.93	11-16	DU (DAY)
5	ESE	112.5	14	WNW	292.5	5	9.61	17-21	DN (NIGHT)
6	SE	135.0	15	NW	315.0	6	12.52	OVER 21	E
7	SSE	157.5	16	NNW	337.5				F

SCENARIO NUMBER	STABILITY CLASS	WIND SPEED CLASS	WIND SPEED (M/S)	WIND SECTOR	WIND DIRECTION (DEG)	AMBIENT TEMPERATURE (DEG C)	INVERSION PENETRATION FACTOR	MIXING HEIGHT (M)
1	EE	3	4.476	9	180.00	15.00	1.000	1000.0

POLLUTION EPISODIC MODEL

INPUT AREA SOURCE PARAMETERS: PEN EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

AREA SOURCE NUMBER	COORDINATES		LENGTH OF SIDE (M)	POLLUTANT-1		POLLUTANT-2	
	X (KM)	Y (KM)		EMISSION RATE INPUT (G/S)	SCALED	EMISSION RATE INPUT (G/S)	SCALED
1	0.38	0.02	120.00	0.500	0.500	0.050	0.050
SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN			0.500	C.500	0.050	0.050	

POLLUTION EPISODIC MODEL

INPUT POINT SOURCE PARAMETERS: PEM EXAMPLE 1 CHEMICAL TRANSFURMATION GAS TO SMALL PARTICLE

POINT SOURCE NUMBER	SOURCE LABEL	COORDINATES X(KM)	COORDINATES Y(KM)	EMISSION RATE POLLUTANT-1 (G/S)	EMISSION RATE POLLUTANT-2 (G/S)	HEIGHT (M)	DIA METER (M)	EXIT VEL (M/S)	EXIT TEMP (DEG C)
1	STACK 1	0.20	0.0	1.000	0.100	15.00	1.000	5.000	32.400
2	STACK 2	0.68	0.04	1.000	0.100	10.00	10.00	0.500	32.400
SUMS OF THE POINT SOURCE EMISSION RATES									
				2.000 G/S	0.200 G/S				

POLLUTION EPISODIC MODEL

OUTPUT: PFM EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

SCENARIO 1 PCINT SOURCE PLUME RISE CALCULATIONS

MIXING HEIGHT: HMIX=1000.00 M  
IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN 1000.0 M, THE SOURCE IS IGNORED

POINT SOURCE	SOURCE COORDINATES X(KM) Y(KM)	EMISSION RATES		HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	EXIT TEMP (DEG K)	DOMINANT INFLUENCE	WIND SPEED AT STACK HEIGHT (M/S)	MAXIMUM EFFECTIVE SOURCE HEIGHT(M)
		POL-1 (G/S)	POL-2 (G/S)							
1	0.20 0.0	0.00	1.00	0.10	15.00	1.000	2.000	305.55 BUGYANCY DOWNWASH	4.947	17.43
2	0.68 C.C4	1.00	0.10	10.00	2.000	0.500	305.55 BUGYANCY DOWNWASH	4.470	10.00	

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 1, PEM EXAMPLE 1, CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE  
 STABILITY=DD, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 1 HR., POLLUTANT-1: GAS 1  
 UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

	0.0	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96
0.96	0	1	5	12	21	25	21	12	5	1	0	0	0
0.92	0	1	4	12	22	27	22	12	4	1	0	0	0
0.88	0	1	4	12	23	29	23	12	4	1	0	0	0
0.84	0	1	4	12	24	31	24	12	4	1	0	0	0
0.80	0	1	3	12	25	33	25	12	3	1	0	0	0
0.76	0	0	3	11	26	35	26	11	3	0	0	0	0
0.72	0	0	2	11	27	37	27	11	2	0	0	0	0
0.68	0	0	2	10	28	40	28	10	2	0	0	0	0
0.64	0	0	1	9	29	43	29	9	1	0	0	0	0
0.60	0	0	1	8	30	47	30	8	1	0	0	0	0
0.56	0	0	1	7	31	51	31	7	1	0	0	0	0
0.52	0	0	0	6	31	55	31	6	0	0	0	0	0
0.48	0	0	0	4	31	60	31	4	0	0	0	0	0
0.44	0	0	0	3	30	65	30	3	0	0	0	0	0
0.40	0	0	0	2	28	70	28	2	0	0	0	0	0
0.36	0	0	0	1	25	75	25	1	0	0	0	0	0
0.32	0	0	0	0	20	78	20	0	0	0	0	0	0
0.28	0	0	0	13	78	13	0	0	9	9	0	0	0
0.24	0	0	0	7	71	7	0	0	21	21	0	0	0
0.20	0	0	0	0	2	56	2	0	0	38	38	0	0
0.16	0	0	0	0	0	30	0	0	0	62	62	0	0
0.12	0	0	0	0	0	7	0	0	0	252	252	252	0
0.08	0	0	0	0	0	0	0	0	0	234	234	234	0
0.04	0	0	0	0	0	0	0	0	0	201	201	201	0
0.00	0	0	0	0	0	0	0	0	0	0	0	0	0
0.00	0.008	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 1, PEM EXAMPLE 1, CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE  
 STABILITY=DC, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 1 HR, POLLUTANT-1: GAS 1  
 UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUARE KILOMETRE PER HOUR

	0.0	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96						
0.96	C	0	0	0	1	1	0	0	0	0	1	1	0	0	0	0	0	0.96	
0.92	C	0	0	0	1	1	0	0	0	0	0	1	1	0	0	0	0	0.92	
0.88	C	0	0	0	1	1	1	0	0	0	0	1	1	1	0	0	0	0.88	
0.84	C	0	0	0	1	1	1	0	0	0	0	0	1	1	1	0	0	0.84	
0.80	C	0	0	0	1	1	1	0	0	0	0	0	1	1	1	0	0	0.80	
0.76	0	0	0	0	1	1	1	0	0	0	0	0	1	2	1	1	0	0.76	
0.72	C	0	0	0	1	1	1	0	0	0	0	0	0	1	2	1	1	0	0.72
0.68	C	0	0	0	1	1	1	0	0	0	0	0	0	1	2	1	1	0	0.68
0.64	C	0	0	0	1	2	1	C	C	C	C	C	C	C	C	C	C	0.64	
0.60	C	0	0	0	1	2	1	0	0	0	0	0	0	1	2	1	1	0	0.60
0.56	C	0	0	0	1	2	1	C	C	C	C	C	C	C	C	C	C	0.56	
0.52	C	0	0	0	1	2	1	C	C	C	C	C	C	C	C	C	C	0.52	
0.48	C	0	0	0	1	2	1	C	C	C	C	C	C	C	C	C	C	0.48	
0.44	C	0	0	0	1	2	1	C	C	C	C	C	C	C	C	C	C	0.44	
0.40	C	0	0	0	1	3	1	C	C	C	C	C	C	C	C	C	C	0.40	
0.36	C	0	0	0	1	3	1	C	C	C	C	C	C	C	C	C	C	0.36	
0.32	C	0	0	0	1	3	1	C	C	C	C	C	C	C	C	C	C	0.32	
0.28	C	0	0	0	0	3	C	C	C	C	C	C	C	C	C	C	C	0.28	
0.24	C	0	0	0	0	3	C	C	C	C	C	C	C	C	C	C	C	0.24	
0.20	C	0	0	0	0	2	0	0	0	0	0	0	0	1	0	0	0	0.20	
0.16	C	0	0	0	0	1	C	C	C	C	C	C	C	C	C	C	C	0.16	
0.12	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.12	
0.08	C	0	0	0	0	0	C	C	C	C	C	C	C	C	C	C	C	0.08	
0.04	C	0	0	0	0	0	C	C	C	C	C	C	C	C	C	C	C	0.04	
0.0	C	0	0	0	0	0	C	C	C	C	C	C	C	C	C	C	C	0.0	
0.0	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96							

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 1, PEM EXAMPLE 1, CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE  
 STABILITY=DD, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 1 HR.  
 UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER  
 POLLUTANT-2: GAS 2

	0.0	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96
0.96	0	0	1	1	2	3	2	1	1	0	0	0	0
0.92	0	0	0	1	2	3	2	1	0	0	0	0	0
0.88	0	0	0	1	3	3	3	1	0	0	0	0	0
0.84	0	0	0	1	3	3	3	1	0	0	0	0	0
0.80	0	0	1	3	4	3	1	0	0	0	0	0	0
0.76	0	0	0	1	3	4	3	1	0	0	0	0	0
0.72	0	0	0	1	3	4	3	1	0	0	0	0	0
0.68	0	0	0	1	3	4	3	1	0	0	0	0	0
0.64	0	0	0	1	3	5	3	1	0	0	0	0	0
0.60	0	0	0	1	3	5	3	1	0	0	0	0	0
0.56	0	0	0	1	3	5	3	1	0	0	0	0	0
0.52	0	0	0	1	3	6	3	1	0	0	0	0	0
0.48	0	0	0	0	3	6	3	0	0	0	0	0	0
0.44	0	0	0	0	3	7	3	0	0	0	0	0	0
0.40	0	0	0	0	3	7	3	0	0	0	0	0	0
0.36	0	0	0	0	3	8	3	0	0	0	0	0	0
0.32	0	0	0	0	2	8	2	0	0	0	0	0	0
0.28	0	0	0	0	1	8	1	0	0	1	1	0	0
0.24	0	0	0	0	1	7	1	0	0	2	2	0	0
0.20	0	0	0	0	0	6	0	0	0	4	4	0	0
0.16	0	0	0	0	0	3	0	0	0	6	6	0	0
0.12	0	0	0	0	0	1	0	0	0	25	25	0	0
0.08	0	0	0	0	0	0	0	0	0	24	24	0	0
0.04	0	0	0	0	0	0	0	0	0	20	20	0	0
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.0	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96

PEM OUTPUT: SECTION 1 OF 1; SCENARIO 1; PEM EXAMPLE 1; CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE  
 STABILITY=0C, WIND SPD= 4.67 M/S, WIND DIR=180, CO DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 1 HR. PULLUTANT-2: GAS 2  
 UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQUARE METER PER HOUR

	0.0	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96
0.96	0	1	2	5	8	10	8	5	2	1	0	0	0
0.92	0	0	2	5	9	11	9	5	2	0	0	0	0
0.88	0	0	2	5	9	11	9	5	2	0	0	0	0
0.84	0	0	1	5	10	12	10	5	1	0	0	0	0
0.80	0	0	1	5	10	13	10	5	1	0	0	0	0
0.76	0	0	1	4	10	14	10	4	1	0	0	0	0
0.72	0	0	1	4	11	15	11	4	1	0	0	0	0
0.68	0	0	1	4	11	16	11	4	1	0	0	0	0
0.64	0	0	1	4	12	17	12	4	1	0	0	0	0
0.60	0	0	0	3	12	18	12	3	0	0	0	0	0
0.56	0	0	0	3	12	20	12	3	0	0	0	0	0
0.52	0	0	0	2	12	21	12	2	0	0	0	0	0
0.48	0	0	0	2	12	23	12	2	0	0	0	0	0
0.44	0	0	0	1	12	25	12	1	0	0	0	0	0
0.40	0	0	0	1	11	27	11	1	0	0	0	0	0
0.36	0	0	0	0	9	29	9	0	6	0	0	0	0
0.32	0	0	0	0	7	30	7	0	0	0	0	0	0
0.28	0	0	0	0	5	29	5	0	0	4	4	0	0
0.24	0	0	0	0	3	27	3	0	0	9	9	0	0
0.20	0	0	0	0	1	21	1	0	0	15	15	0	0
0.16	0	0	0	0	0	11	0	0	0	23	23	0	0
0.12	0	0	0	0	0	2	0	0	0	91	91	0	0
0.08	0	0	0	0	0	0	0	0	0	85	85	85	0
0.04	0	0	0	0	0	0	0	0	0	73	73	73	0
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0	0.08	0.16	0.24	0.32	0.40	0.48	0.56	0.64	0.72	0.80	0.88	0.96	

POLLUTION EPISODIC MODEL

OUTPUT: PFM EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR EACH SCENARIO

UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CUBIC METER - CALIBRATION, POLLUTANT-1;  
CALIBRATION, POLLUTANT-2;

POLLUTANT-1: GAS 1

SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	CONCENTRATION		COORDINATES	
		UNCALIBRATED	CALIBRATED	X(KM)	Y(KM)
1	1	0.68	0.20	268.5979	0.0

POLLUTANT-2: GAS 2					
SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	CONCENTRATION		COORDINATES	
		UNCALIBRATED	CALIBRATED	X(KM)	Y(KM)
1	1	0.68	0.20	28.2320	0.0

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 1    CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLUTANT FOR EACH SCENARIO

UNCALIBRATED VALUES IN MICROGRAMS PER SQUARE METER PER HOUR - CALIBRATION, POLLUTANT-1;  
CALIBRATION, POLLUTANT-2;

SCENARIO NUMBER	WIND DIRECTION SLB-SCENARIO	POLLUTANT-1: GAS 1		POLLUTANT-2: GAS 2	
		COORDINATES X(KM) Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED CALIBRATED	COORDINATES X(KM) Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED CALIBRATED
1	1	0.68	0.20	9669.5234	0.0
					0.68      0.20      101.6351      0.0

IMC0021 STOP C

TABLE 13  
INPUT DATA FOR EXAMPLE PROBLEM 2

CONTROL CARDS		CARD IMAGES									
1	TITLE	PEN	EXAMPLE 2	CHEMICAL TRANSFORMATION GAS TO PARTICLE	3-HR AVG CONCENTRATIONS						
2	OPTIONS	3	1	3	0	2	0	1	0	0	1
3	GRID	0.	0.	0.	25	25	25	0.	0.	0.	0.
4	POLLUTANTS	2	1	2.C	0.0	0.5	0.5	.25	20.0	20.0	1.5
5	SCALING	GAS	1.0	1.C	0.	0.	0.	0.	0.	0.	0.
6	LABELS										
SCENARIO CARDS											
		5	4	11				5.0	1.	1000.	
		5	4	11				5.0	1.	1000.	
		5	4	11				5.0	1.	1000.	
AREA SOURCE CARDS											
		1.	1.	4000.	15.	15.	15.				
		21.	1.	2000.	25.	25.	25.				
		25.	1.	2000.	25.	25.	25.				
		29.	1.	2000.	25.	25.	25.				
BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY											
POINT SOURCE CARDS											
		2.	2.	10.	.10	.10	.10	2.0	2.0	1.0	32.4 STACK 1
		14.	2.	30.	.30	.30	.30	2.0	2.0	1.5	100. STACK 2
		2.	16.	30.	.30	.30	.30	35.	35.	1.0	125. STACK 3
BLANK CARD TO SIGNAL END OF POINT SOURCE INVENTORY											

TABLE 14

OUTPUT LISTING FOR EXAMPLE PROBLEM 2

PEN (VERSION 82360)

POLLUTION EPISODIC MODEL

INCLUDING  
DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION  
OF POLLUTANTS

POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS: PEN EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS

AVERAGING TIME OPTION: NTOPT=3

A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR

- 1 1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO
- 2 24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE AVERAGED
- 3 VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED

WIND DIRECTION OPTION: NWDOPT=1

- 0 DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO
- 1 SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO
- 2-7 DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOUR SUB-SCENARIOS.  
FOR EACH SUCCESSING SUB-SCENARIO, WIND DIRECTION IS AUTOMATICALLY INCREASED  
BY 90,45,30,15,10,OR 5 DEGREES, DEPENDING ON THE OPTION NUMBER SELECTED.

WIND SPEED OPTION: NNSOPT=1

- 0 SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO
- 1 WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO

NUMBER OF SCENARIOS: NSCEN= 3

STACK-TIP DOWNWASH ALGORITHM OPTION: NSTUWN=0

- 0 ALGORITHM IS IN EFFECT
- 1 ALGORITHM IS NOT USED

RECEPTOR GRID: COLUMNS: LX=25 ROWS: LY=25  
SPACING: GRID= 2.000 KM XRSWC= 0.0 KM W  
SOUTHWEST CORNER YRSWC= 0.0 KM S

POTENTIAL TEMPERATURE GRADIENT: DTQZ(1)= 0.020 DEG/M STABILITY CLASS E  
DTQZ(2)= 0.035 DEG/M STABILITY CLASS F

POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS: PFM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS

NUMBER OF POLLUTANTS: NPOL=2	POLLUTANT-1: GAS	POLLUTANT-2: PARTICLE
AREA SOURCE SCALING FACTOR:	A SCALE= 1.000	A SCALE= 1.000
CALIBRATION COEFFICIENTS:	A= 0.0	B= 0.0
CALIBRATION IDENTIFICATION:		
DEPOSITION VELOCITY (CM/S):	V D1= 2.000	V D2= 0.500
SETTLING VELOCITY (CM/S):	W1= 0.0	W2= 0.250

CHEMICAL TRANSFORMATION OPTION: ICT=1

NPOL=2  
ICT=0 CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED  
ICT=1 FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO POLLUTANT-2 IS CONSIDERED

CHEMICAL TRANSFORMATION RATE: XKT= 20.000 PERCENT/HR

RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO POLLUTANT-1 (REACTANT): GAMMA= 1.500

OUTPUT OPTIONS SELECTED:

NARRAY=2 MAPS OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR IN THE GRID,  
UNCALIBRATED ONLY  
NMAX=1 LIST OF RECEPTORS WITH HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX  
FOR EACH SCENARIO - PRINTED AT END OF RUN

POLLUTION EPISODIC MODEL

INPUT SCENARIO PARAMETERS: PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS							
WIND DIRECTIONS				WIND SPEED CLASSES			
SECTOR NUMBER	DIRECTION (DEG)	SECTOR NUMBER	DIRECTION (DEG)	CLASS INDEX	SPEED (M/S)	CLASS INTERVAL (KT)	STABILITY CLASSES
1	N	0.0	9	1	1.50	0-3	A
2	NNE	22.5	10	1	1.50	0-3	A
3	NE	45.0	11	2	2.46	4-6	B
4	ENE	67.5	12	2	2.46	4-6	B
5	E	90.0	13	3	4.47	7-10	C
6	ESE	112.5	14	4	6.93	11-16	DD (DAY)
7	SE	135.0	15	5	9.61	17-21	DN (NIGHT)
8	SSE	157.5	16	6	12.52	OVER 21	E
							F
SCENARIO NUMBER							
STABILITY CLASS		WIND SPEED CLASS	WIND SECTOR	WIND DIRECTION (DEG)	AMBIENT TEMPERATURE (DEG C)	INVERSION PENETRATION FACTOR	MIXING HEIGHT (M)
1	CN	4	6.930	11	225.00	5.00	1000.0
2	DN	4	6.930	11	225.00	5.00	1000.0
3	DN	4	6.930	11	225.00	5.00	1000.0

POLLUTION EPISODIC MODEL

INPUT AREA SOURCE PARAMETERS: PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS

AREA SOURCE NUMBER	COORDINATES		LENGTH OF SIDE (M)	POLLUTANT-1		POLLUTANT-2	
	X (KM)	Y (KM)		EMISSION RATE INPUT (G/S)	SCALED	EMISSION RATE INPUT (G/S)	SCALED
1	1.00	1.00	4000.00	15.00	15.00	0.15	0.15
2	21.00	1.00	2000.00	25.00	25.00	0.25	0.25
3	25.00	1.00	2000.00	25.00	25.00	0.25	0.25
4	29.00	1.00	2000.00	25.00	25.00	0.25	0.25
SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN				90.00	90.00	0.90	0.90

POLLUTION EPISODIC MODEL

INPUT POINT SOURCE PARAMETERS: PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS

POINT SOURCE NUMBER	SOURCE LABEL	COORDINATES X(KM)	COORDINATES Y(KM)	EMISSION RATE POLLUTANT-1 (G/S)	EMISSION RATE POLLUTANT-2 (G/S)	HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	EXIT TEMP (DEG C)
1	STACK 1	2.00	2.00	10.00	0.10	20.00	2.00	10.000	32.400
2	STACK 2	14.00	2.00	30.00	0.30	10.00	2.00	15.000	100.000
3	STACK 3	2.00	16.00	30.00	0.30	35.00	1.000	12.000	125.000
SUMS OF THE POINT SOURCE EMISSION RATES									0.70 G/S
									70.00 G/S

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 3 PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS  
 STABILITY=ON, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 3 HR.  
 UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00
48.00	0	0	0	0	0	0	0	0	0	0	1	1	0
46.00	0	0	0	0	0	0	0	0	0	0	0	0	0
44.00	0	0	0	0	0	0	0	0	0	0	0	0	0
42.00	0	0	0	0	0	0	0	0	0	0	0	0	0
40.00	0	0	0	0	0	0	0	0	0	0	0	0	0
38.00	0	0	0	0	0	0	0	0	0	0	0	0	0
36.00	0	0	0	0	0	0	0	0	0	0	0	0	0
34.00	0	0	0	0	0	0	0	0	0	0	0	0	0
32.00	0	0	0	0	0	0	0	0	0	0	0	0	0
30.00	0	0	0	0	0	0	0	0	0	0	0	0	0
28.00	0	0	0	0	0	0	0	0	0	0	0	0	0
26.00	0	0	0	0	1	7	1	0	0	0	0	1	0
24.00	0	0	0	1	10	1	0	0	0	0	0	1	0
22.00	0	0	0	16	1	0	0	0	0	0	1	2	1
20.00	0	0	28	0	0	0	0	0	0	0	2	3	1
18.00	0	0	60	0	0	0	0	1	1	0	0	0	0
16.00	0	0	0	0	0	0	1	1	0	0	2	5	2
14.00	0	0	0	0	0	2	1	0	0	0	0	2	0
12.00	0	0	0	0	1	3	0	0	0	1	8	2	0
10.00	0	0	0	1	5	1	0	0	1	12	1	0	4
8.00	0	0	0	1	8	1	0	0	0	17	1	0	5
6.00	0	0	2	15	1	0	0	0	30	0	0	7	0
4.00	0	10	43	2	0	0	0	55	0	0	14	0	14
2.00	0	10	10	0	0	0	0	0	0	65	0	65	0
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00

PEN OUTPUT: SECTION 1 QF 1, SCENARIO 3, PEN EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS  
 STABILITY=DN, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 3 HR.  
 UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUARE KILOMETER PER HOUR

	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00
48.00	0	0	0	0	0	0	0	0	0	0	0	0	0
46.00	0	0	0	0	0	0	0	0	0	0	0	0	0
44.00	0	0	0	0	0	0	0	0	0	0	0	0	0
42.00	0	0	0	0	0	0	0	0	0	0	0	0	0
40.00	0	0	0	0	0	0	0	0	0	0	0	0	0
38.00	0	0	0	0	0	0	0	0	0	0	0	0	0
36.00	0	0	0	0	0	0	0	0	0	0	0	0	0
34.00	0	0	0	0	0	0	0	0	0	0	0	0	0
32.00	0	0	0	0	0	0	0	0	0	0	0	0	0
30.00	0	0	0	0	0	0	0	0	0	0	0	0	0
28.00	0	0	0	0	0	0	0	0	0	0	0	0	0
26.00	0	0	0	0	0	0	0	0	0	0	0	0	0
24.00	0	0	0	0	0	0	0	0	0	0	0	0	0
22.00	0	0	0	0	0	0	0	0	0	0	0	0	0
20.00	0	0	0	0	0	0	0	0	0	0	0	0	0
18.00	0	0	0	0	0	0	0	0	0	0	0	0	0
16.00	0	0	0	0	0	0	0	0	0	0	0	0	0
14.00	0	0	0	0	0	0	0	0	0	0	0	0	0
12.00	0	0	0	0	0	0	0	0	0	0	0	0	0
10.00	0	0	0	0	0	0	0	0	0	0	0	0	0
8.00	0	0	0	0	0	0	0	0	0	0	0	0	0
6.00	0	0	0	0	0	0	0	0	0	0	0	0	0
4.00	0	1	3	0	0	0	0	4	0	0	1	0	1
2.00	0	1	1	0	0	0	0	0	5	0	5	0	0
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 3, PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS  
 STABILITY=ON, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 3 HR.  
 UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00	
48.00	0	0	0	0	0	0	0	0	0	0	1	1	0	0
46.00	0	0	0	0	0	0	0	0	0	0	1	1	0	0
44.00	0	0	0	0	0	0	0	0	0	0	1	1	0	0
42.00	0	0	0	0	0	0	0	0	0	0	1	1	0	0
40.00	0	0	0	0	0	0	0	0	0	0	1	1	0	0
38.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1
36.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1
34.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1
32.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1
30.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24.00	0	0	0	0	2	0	0	0	0	0	0	1	1	0
22.00	0	0	0	0	2	0	0	0	0	0	0	1	2	1
20.00	0	0	0	0	2	0	0	0	0	0	0	0	1	0
18.00	0	0	2	0	0	0	0	0	0	0	0	1	2	1
16.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6.00	0	0	0	0	1	0	0	0	0	0	0	0	0	0
4.00	0	0	2	0	0	0	0	0	0	0	0	0	0	0
2.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00	

PEN OUTPUT: SECTION 1 OF 1, SCENARIO 3, PEW EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS  
 STABILITY=DN, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 3 HR, POLLUTANT-2: PARTICLE  
 UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQUARE METER PER HOUR

	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00	
48.00	0	0	0	0	0	0	0	0	0	0	1	5	10	5
46.00	0	0	0	0	0	0	0	0	0	1	4	10	13	10
44.00	0	0	0	0	0	0	0	0	0	1	4	10	14	10
42.00	0	0	0	0	0	0	0	0	0	3	10	15	10	4
40.00	0	0	0	0	0	0	0	0	0	3	10	15	10	4
38.00	0	0	0	0	0	0	0	0	0	2	10	16	10	3
36.00	0	0	0	0	0	0	0	0	1	10	17	10	3	0
34.00	0	0	0	0	0	0	0	1	9	18	10	2	0	2
32.00	0	0	0	0	0	0	0	0	8	20	9	1	0	0
30.00	0	0	0	0	0	0	0	0	7	21	8	1	0	0
28.00	0	0	0	0	0	0	5	23	7	0	0	0	1	4
26.00	0	0	0	0	0	3	25	5	0	0	0	1	4	6
24.00	0	0	0	1	28	3	0	0	0	1	4	6	4	1
22.00	0	0	0	31	1	0	0	0	1	4	7	4	1	0
20.00	0	0	0	37	0	0	0	0	0	4	7	4	1	0
18.00	0	0	44	0	0	0	0	0	3	8	4	1	0	1
16.00	0	0	0	0	0	0	0	0	3	9	3	0	0	12
14.00	0	0	0	0	0	0	0	0	0	10	3	0	0	14
12.00	0	0	0	0	0	0	0	0	2	11	2	0	0	12
10.00	0	0	0	0	1	13	2	0	0	0	2	45	5	0
8.00	0	0	0	0	15	1	0	0	0	49	2	0	0	2
6.00	0	0	1	18	0	0	0	0	55	0	0	0	2	0
4.00	0	2	28	1	0	0	0	0	53	0	0	0	3	0
2.00	0	2	2	0	0	0	0	0	0	13	0	13	0	0
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.0	4.00	8.00	12.00	16.00	20.00	24.00	28.00	32.00	36.00	40.00	44.00	48.00	

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS

HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR EACH SCENARIO  
UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CUBIC METER - CALIBRATION, POLLUTANT-1:  
CALIBRATION, POLLUTANT-2:

SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	POLLUTANT-1: GAS		POLLUTANT-2: PARTICLE	
		COORDINATES X(KM)	CONCENTRATION UNCALIBRATED CALIBRATED	COORDINATES X(KM)	CONCENTRATION UNCALIBRATED CALIBRATED
1	1	30.00	2.00	65.0452	0.0

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE 3-HR AVG CONCENTRATIONS

HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLUTANT FOR EACH SCENARIO

UNCALIBRATED VALUES IN MICROGRAMS PER SQUARE METER PER HOUR - CALIBRATION, POLLUTANT-1;  
CALIBRATION, POLLUTANT-2;

SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES		SURFACE DEPOSITION FLUX		SURFACE DEPOSITION FLUX			
		X(KM)	Y(KM)	UNCALIBRATED	CALIBRATED	X(KM)	Y(KM)	UNCALIBRATED	CALIBRATED
1	1	30.00	2.00	4683.2500	0.0	10.00	6.00	55.3507	0.0
!HC002!	STOP	0							

TABLE 15  
INPUT DATA FOR EXAMPLE PROBLEM 3

CARD IMAGES									
<b>CONTROL CARDS</b>									
1 TITLE	PEM EXAMPLE 3	0	6	2	0	1	1	0	0
2 OPTIONS	0.0	0.0	0.0	25	25	4.0	0.0	0.0	0.0
3 GRID	0.0	0.0	0.0	0.0	2.0	1.0	10.0	1.5	0.0
4 POLLUTANTS	2	1	1.0	0.0	0.0	0.0	0.0	0.0	0.0
5 SCALING	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6 LABELS	GAS					PARTICLE			
<b>SCENARIO CARDS</b>									
7	0	0	2.0	270.0	5.0	1.0	200.0		
7	0	0	2.5	270.0	3.0	1.0	200.0		
7	0	0	2.0	270.0	1.0	1.0	175.0		
7	0	0	2.5	270.0	-1.0	1.0	175.0		
7	0	0	2.0	270.0	-3.0	1.0	150.0		
7	0	0	2.5	270.0	-5.0	1.0	150.0		
<b>AREA SOURCE CARDS</b>									
	6.0	18.0	20000.	250.0	2.5				
BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY									
<b>POINT SOURCE CARDS</b>									
	16.0	8.0	10.0	0.0	10.0	0.50	1.0	60.0	STACK AR
	4.0	48.0	12.5	0.0	15.0	0.75	2.0	70.0	STACK AS
	48.0	28.0	20.0	0.0	30.0	1.00	3.0	80.0	STACK AT
BLANK CARD TO SIGNAL END OF POINT SOURCE INVENTORY									

TABLE 16

OUTPUT LISTING FOR EXAMPLE PROBLEM 3

PEM (VERSION 82360)

POLLUTION EPISODIC MODEL

INCLUDING  
DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION  
OF POLLUTANTS

POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS: PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

AVERAGING TIME OPTION: NTOPT=3

A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR

- 1 1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO
- 2 24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE AVERAGED
- 3 VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED

WIND DIRECTION OPTION: NWDOPT=0

- 0 DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO
- 1 SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO
- 2-7 DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOUR SUB-SCENARIOS.  
FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRECTION IS AUTOMATICALLY INCREASED  
BY 90,45,30,15,10,OR 5 DEGREES, DEPENDING ON THE OPTION NUMBER SELECTED.

WIND SPEED OPTION: NWSPDT=0

- 0 SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO
- 1 WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO

NUMBER OF SCENARIOS: NSCEN= 6

STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=1

- 0 ALGORITHM IS IN EFFECT
- 1 ALGORITHM IS NOT USED

RECEPTOR GRID: COLUMNS: LX=25 ROWS: LY=25  
SPACING: GRID= .000 KM  
SOUTHWEST CORNER XRSWC= 0.0 KM W  
YRSWC= 0.0 KM S

POTENTIAL TEMPERATURE GRADIENT: DT0Z(1)= 0.020 DEG/M STABILITY CLASS E  
DT0Z(2)= 0.035 DEG/M STABILITY CLASS F

## POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS: PEW EXAMPLE 3    CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

NUMBER OF POLLUTANTS: NPOL=2

POLLUTANT-1: GAS

POLLUTANT-2: PARTICLE

AREA SOURCE SCALING FACTOR:	A=	ASCALE=	1.000	B=	0.0	A=	ASCALE=	1.000
CALIBRATION COEFFICIENTS:	A=	0.0				B=	0.0	0.0
CALIBRATION IDENTIFICATION:								
DEPOSITION VELOCITY (CM/S):	V01=	1.000		V02=	2.000			
SETTLING VELOCITY (CM/S):	W1=	0.0		W2=	1.000			

CHEMICAL TRANSFORMATION OPTION: ICT=1

NPOL=2  
 ICT=0    CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED  
 ICT=1    FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO POLLUTANT-2 IS CONSIDERED

CHEMICAL TRANSFORMATION RATE: XKT= 10.000 PERCENT/HR

RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO POLLUTANT-1 (REACTANT): GAMMA= 1.500

OUTPUT OPTIONS SELECTED:

NARRAY=2    MAPS OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR IN THE GRID,  
 UNCALIBRATED ONLY  
 NPRINT=1    LIST OF POINT SOURCE PARAMETERS AND EFFECTIVE STACK HEIGHTS  
 PRINTED AT BEGINNING OF EACH SCENARIO  
 NMAX=1    LIST OF RECEPTORS WITH HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX  
 FOR EACH SCENARIO - PRINTED AT END OF RUN

POLLUTION EPISODIC MODEL

INPUT SCENARIO PARAMETERS: PFM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

SECTOR NUMBER	DIRECTION (DEG)	SECTOR NUMBER	DIRECTION (DEG)	WIND SPEED CLASSES			STABILITY CLASSES		
				CLASS INDEX	SPEED (M/S)	CLASS INTERVAL (KT)	CLASS INDEX	CLASS	CLASS
1	N	0.0	9	S	180.0	1	1.50	0-3	A
2	NNE	22.5	10	SSW	202.5	2	2.46	4-6	B
3	NE	45.0	11	SW	225.0	3	4.47	7-10	C
4	ENE	67.5	12	WSW	247.5	4	6.93	11-16	DD (DAY)
5	E	90.0	13	W	270.0	5	9.61	17-21	DN (NIGHT)
6	ESE	112.5	14	WNW	292.5	6	12.52	OVER 21	E
7	SE	135.0	15	NW	315.0				F
8	SSE	157.5	16	NNW	337.5				

SCENARIO NUMBER	STABILITY CLASS	WIND SPEED CLASS	WIND SPEED (M/S)	WIND SECTOR	WIND DIRECTION (DEG)	AMBIENT TEMPERATURE (DEG C)	INVERSION PENETRATION FACTOR	MIXING HEIGHT (M)
1	F	2.000	2.000	270.00	5.00	1.000	200.0	
2	F	2.500	2.500	270.00	3.00	1.000	200.0	
3	F	2.000	2.000	270.00	1.00	1.000	175.0	
4	F	2.500	2.500	270.00	-1.00	1.000	175.0	
5	F	2.000	2.000	270.00	-3.00	1.000	150.0	
6	F	2.500	2.500	270.00	-5.00	1.000	150.0	

POLLUTION EPISODIC MODEL

INPUT AREA SOURCE PARAMETERS: PEN EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

AREA SOURCE NUMBER	COORDINATES		LENGTH OF SIDE (M)	POLLUTANT-1		POLLUTANT-2	
	X(KM)	Y(KM)		EMISSION RATE INPUT (G/S)	EMISSION RATE INPUT (G/S)	SCALED INPUT (G/S)	SCALED INPUT (G/S)
1	6.00	18.00	20000.00	250.000	250.000	2.500	2.500
SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN			250.000	250.000	2.500	2.500	

## POLLUTION EPISODIC MODEL

## INPUT POINT SOURCE PARAMETERS: PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

POINT NUMBER	SOURCE LABEL	COORDINATES X(KM)	COORDINATES Y(KM)	EMISSION RATE POLLUTANT-1 (G/S)	EMISSION RATE POLLUTANT-2 (G/S)	HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	EXIT TEMP (DEG C)
1	STACK AR	16.00	8.00	10.000	0.0	10.00	0.500	1.000	60.000
2	STACK AS	4.00	48.00	12.500	0.0	15.00	0.750	2.000	70.000
3	STACK AT	48.00	28.00	20.000	0.0	30.00	1.000	3.000	80.000
SUMS OF THE POINT SOURCE EMISSION RATES				42.500 G/S	0.0	G/S			

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

SCENARIO 1 POINT SOURCE PLUME RISE CALCULATIONS

MIXING HEIGHT:  $h_{mix} = 200.00 \text{ m}$

IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN 200.0 M, THE SOURCE IS IGNORED

POINT SOURCE	EMISSION RATES			HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	DOMINANT INFLUENCE	WIND SPEED AT STACK HEIGHT (M/S)	MAXIMUM EFFECTIVE SOURCE HEIGHT(M)
	SOURCE COORDINATES X(KM)	Y(KM)	Z(KM)						
1	16.00	8.00	10.00	0.0	10.00	0.500	1.000	333.15	18.97
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	29.88
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	50.00

## POLLUTION EPISODIC MODEL

OUTPUT: PFM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

## SCENARIO 2 POINT SOURCE PLUME RISE CALCULATIONS

MIXING HEIGHT: HMIX= 200.00 M

IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN 200.0 M, THE SOURCE IS IGNORED

POINT SOURCE	SOURCE COORDINATES X(KM)	SOURCE COORDINATES Y(KM)	EMISSION RATES POL-1 (G/S)	EMISSION RATES POL-2 (G/S)	HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	EXIT TEMP (DEG K)	DOMINANT INFLUENCE	WIND SPEED AT STACK HEIGHT (M/S)	MAXIMUM EFFECTIVE SOURCE HEIGHT (M)
1	16.00	8.00	10.00	0.0	10.00	0.500	1.000	333.15	BUOYANCY	2.500	18.40
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	BUOYANCY	2.023	28.92
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	BUOYANCY	3.476	48.69

## POLLUTION EPISODIC MODEL

OUTPUT: PFM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

## SCENARIO 3 POINT SOURCE PLUME RISE CALCULATIONS

MIXING HEIGHT: HMIX= 175.00 M  
 IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN 175.0 M, THE SOURCE IS IGNORED

POINT SOURCE	SOURCE COORDINATES X(KM) Y(KM)	EMISSION RATES			HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	DOMINANT INFLUENCE (DEG K)	WIND SPEED AT STACK HEIGHT (M/S)	MAXIMUM EFFECTIVE SOURCE HEIGHT(M)
		POL-1 (G/S)	POL-2 (G/S)							
1	16.00	8.00	10.00	0.0	10.00	0.500	1.000	333.15 BUOYANCY	2.000	19.13
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15 BUOYANCY	2.259	30.11
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15 BUOYANCY	2.781	50.25

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

SCENARIO 4 POINT SOURCE PLUME RISE CALCULATIONS

MIXING HEIGHT: HMIX= 175.00 M

IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN 175.0 M, THE SOURCE IS IGNORED

POINT SOURCE	EMISSION RATES			HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	DOMINANT INFLUENCE	WIND SPEED AT STACK HEIGHT (M/S)	MAXIMUM EFFECTIVE SOURCE HEIGHT(M)
	SOURCE COORDINATES X(KM)	Y(KM)	Z(KM)						
1	16.00	8.00	10.00	0.0	10.00	0.500	1.000	333.15	BUOYANCY
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	BUOYANCY
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	BUOYANCY

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

SCENARIO 5 POINT SOURCE PLUME RISE CALCULATIONS  
 MIXING HEIGHT: HM X= 150.00 M  
 IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN 150.0 M, THE SOURCE IS IGNORED

POINT SOURCE	COORDINATES X(KM) Y(KM)	EMISSION RATES			HEIGHT (M)	DIAMETER (IN)	EXIT VEL (M/S)	DOMINANT INFLUENCE (DEG K)	WIND SPEED AT STACK HEIGHT (M/S)	MAXIMUM EFFECTIVE SOURCE HEIGHT(M)
		POL-1 (G/S)	POL-2 (G/S)							
1	16.00	8.00	10.00	0.0	10.00	0.500	1.000	333.15	2.000	19.29
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	2.259	30.32
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	2.781	50.49

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

SCENARIO 6 POINT SOURCE PLUME RISE CALCULATIONS

MIXING HEIGHT: HMLA= 150.00 M

IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN 150.0 M, THE SOURCE IS IGNORED

POINT SOURCE	SOURCE COORDINATES X(KM) Y(KM)	EMISSION RATES		HEIGHT (M)	DIAMETER (M)	EXIT VEL (M/S)	EXIT TEMP (DEG K)	DOMINANT INFLUENCE	WIND SPEED AT STACK HEIGHT (M/S)	MAXIMUM EFFECTIVE SOURCE HEIGHT (M)
		POL-1 (G/S)	POL-2 (G/S)							
1	16.00	8.00	10.00	0.0	10.00	0.500	1.000	BUOYANCY	2.500	18.69
2	4.00	48.00	12.50	0.0	15.00	0.50	2.000	BUOYANCY	2.823	29.31
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	BUOYANCY	3.476	49.12

PEH OUTPUT: SECTION 1 OF 1, SCENARIO 6 PEH EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION  
 STABILITY=F, WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG, MIXING HT= 150.0 M, AVERAGING TIME= 6 HR,  
 UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00		
96.00	0	0	0	0	0	0	0	0	0	0	0	0	0	96.00	
92.00	0	0	0	0	0	0	0	0	0	0	0	0	0	92.00	
88.00	0	0	0	0	0	0	0	0	0	0	0	0	0	88.00	
84.00	0	0	0	0	0	0	0	0	0	0	0	0	0	84.00	
80.00	0	0	0	0	0	0	0	0	0	0	0	0	0	80.00	
76.00	0	0	0	0	0	0	0	0	0	0	0	0	0	76.00	
72.00	0	0	0	0	0	0	0	0	0	0	0	0	0	72.00	
68.00	0	0	0	0	0	0	0	0	0	0	0	0	0	68.00	
64.00	0	0	0	0	0	0	0	0	0	0	0	0	0	64.00	
60.00	0	0	0	0	0	0	0	0	0	0	0	0	0	60.00	
56.00	0	0	0	0	0	0	0	0	0	0	0	0	0	56.00	
52.00	0	0	0	0	0	0	0	0	0	0	0	0	0	52.00	
48.00	0	145	49	24	13	8	6	4	3	2	1	1	1	48.00	
44.00	0	0	0	0	0	0	0	0	0	0	0	0	0	44.00	
40.00	0	0	0	0	0	0	0	0	0	0	0	0	0	40.00	
36.00	0	0	60	69	72	75	76	76	76	76	76	76	76	36.00	
32.00	0	0	60	69	72	75	76	76	76	76	76	76	76	32.00	
28.00	0	0	60	69	72	75	76	76	76	76	76	76	76	28.00	
24.00	0	0	60	69	72	75	76	76	76	76	76	76	76	24.00	
20.00	0	0	60	69	72	75	76	76	76	76	76	76	76	20.00	
16.00	0	0	0	0	0	0	0	0	0	0	0	0	0	16.00	
12.00	0	0	0	0	0	0	0	0	0	0	0	0	0	12.00	
8.00	0	0	0	0	143	40	18	9	6	4	3	2	1	1	8.00
4.00	0	0	0	0	0	0	0	0	0	0	0	0	0	4.00	
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0	
0.0	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00		

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 6 PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION  
 STABILITY=F, WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG, MIXING HT= 150.0 M, AVERAGING TIME= 6 HR.  
 UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUARE KILOMETER PER HOUR

	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00	
96.00	0	0	0	0	0	0	0	0	0	0	0	0	0	96.00
92.00	0	0	0	0	0	0	0	0	0	0	0	0	0	92.00
88.00	0	0	0	0	0	0	0	0	0	0	0	0	0	88.00
84.00	0	0	0	0	0	0	0	0	0	0	0	0	0	84.00
80.00	0	0	0	0	0	0	0	0	0	0	0	0	0	80.00
76.00	0	0	0	0	0	0	0	0	0	0	0	0	0	76.00
72.00	0	0	0	0	0	0	0	0	0	0	0	0	0	72.00
68.00	0	0	0	0	0	0	0	0	0	0	0	0	0	68.00
64.00	0	0	0	0	0	0	0	0	0	0	0	0	0	64.00
60.00	0	0	0	0	0	0	0	0	0	0	0	0	0	60.00
56.00	0	0	0	0	0	0	0	0	0	0	0	0	0	56.00
52.00	0	0	0	0	0	0	0	0	0	0	0	0	0	52.00
48.00	0	0	5	2	1	0	0	0	0	0	0	0	0	48.00
44.00	0	0	0	0	0	0	0	0	0	0	0	0	0	44.00
40.00	0	0	0	0	0	0	0	0	0	0	0	0	0	40.00
36.00	0	0	2	2	3	3	1	0	0	0	0	0	0	36.00
32.00	0	0	2	2	3	3	1	0	0	0	0	0	0	32.00
28.00	0	0	2	2	3	3	1	0	0	0	0	0	0	28.00
24.00	0	0	2	2	3	3	1	0	0	0	0	0	0	24.00
20.00	0	0	2	2	3	3	1	0	0	0	0	0	0	20.00
16.00	0	0	0	0	0	0	0	0	0	0	0	0	0	16.00
12.00	0	0	0	0	0	0	0	0	0	0	0	0	0	12.00
8.00	0	0	0	0	5	1	1	0	0	0	0	0	0	8.00
4.00	0	0	0	0	0	0	0	0	0	0	0	0	0	4.00
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0
	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00	

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 6 PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION  
 STABILITY-F, WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG, MIXING HT= 150.0 M, AVERAGING TIME= 6 HR.  
 UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00	
96.00	0	0	0	0	0	0	0	0	0	0	0	0	0	96.00
92.00	0	0	0	0	0	0	0	0	0	0	0	0	0	92.00
88.00	0	0	0	0	0	0	0	0	0	0	0	0	0	88.00
84.00	0	0	0	0	0	0	0	0	0	0	0	0	0	84.00
80.00	0	0	0	0	0	0	0	0	0	0	0	0	0	80.00
76.00	0	0	0	0	0	0	0	0	0	0	0	0	0	76.00
72.00	0	0	0	0	0	0	0	0	0	0	0	0	0	72.00
68.00	0	0	0	0	0	0	0	0	0	0	0	0	0	68.00
64.00	0	0	0	0	0	0	0	0	0	0	0	0	0	64.00
60.00	0	0	0	0	0	0	0	0	0	0	0	0	0	60.00
56.00	0	0	0	0	0	0	0	0	0	0	0	0	0	56.00
52.00	0	0	0	0	0	0	0	0	0	0	0	0	0	52.00
48.00	0	0	12	7	4	2	1	1	0	0	0	0	0	48.00
44.00	0	0	0	0	0	0	0	0	0	0	0	0	0	44.00
40.00	0	0	0	0	0	0	0	0	0	0	0	0	0	40.00
36.00	0	0	1	3	4	5	6	5	3	2	1	0	0	36.00
32.00	0	0	1	3	4	5	6	5	3	2	1	0	0	32.00
28.00	0	0	1	3	4	5	6	5	3	2	1	0	0	28.00
24.00	0	0	1	3	4	5	6	5	3	2	1	0	0	24.00
20.00	0	0	1	3	4	5	6	5	3	2	1	0	0	20.00
16.00	0	0	0	0	0	0	0	0	0	0	0	0	0	16.00
12.00	0	0	0	0	0	0	0	0	0	0	0	0	0	12.00
8.00	0	0	0	0	10	4	2	1	1	0	0	0	0	8.00
4.00	0	0	0	0	0	0	0	0	0	0	0	0	0	4.00
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0
	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00	

PEN OUTPUT: SECTION 1 OF 1. SCENARIO 6. PFM EXAMPLE 3. CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION  
 STABILITY=F, WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG., MIXING HT= 150.0 M, AVERAGING TIME= 6 HR.  
 UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQUARE METER PER HOUR

	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00	
96.00	0	0	0	0	0	0	0	0	0	0	0	0	0	96.00
92.00	0	0	0	0	0	0	0	0	0	0	0	0	0	92.00
88.00	0	0	0	0	0	0	0	0	0	0	0	0	0	88.00
84.00	0	0	0	0	0	0	0	0	0	0	0	0	0	84.00
80.00	0	0	0	0	0	0	0	0	0	0	0	0	0	80.00
76.00	0	0	0	0	0	0	0	0	0	0	0	0	0	76.00
72.00	0	0	0	0	0	0	0	0	0	0	0	0	0	72.00
68.00	0	0	0	0	0	0	0	0	0	0	0	0	0	68.00
64.00	0	0	0	0	0	0	0	0	0	0	0	0	0	64.00
60.00	0	0	0	0	0	0	0	0	0	0	0	0	0	60.00
56.00	0	0	0	0	0	0	0	0	0	0	0	0	0	56.00
52.00	0	0	0	0	0	0	0	0	0	0	0	0	0	52.00
48.00	0	0	847	475	287	179	114	74	49	32	22	13	8	5
44.00	0	0	0	0	0	0	0	0	0	0	0	0	0	44.00
40.00	0	0	0	0	0	0	0	0	0	0	0	0	0	40.00
36.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0
32.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0
28.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0
24.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0
20.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0
16.00	0	0	0	0	0	0	0	0	0	0	0	0	0	16.00
12.00	0	0	0	0	0	0	0	0	0	0	0	0	0	12.00
8.00	0	0	0	0	0	0	0	0	0	0	0	0	0	8.00
4.00	0	0	0	0	0	0	0	0	0	0	0	0	0	4.00
0.0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0
	0.0	8.00	16.00	24.00	32.00	40.00	48.00	56.00	64.00	72.00	80.00	88.00	96.00	

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 3    CHEMICAL TRANSFORMATION GAS TO PARTICLE    6-HR AVG CONCENTRATION

HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR EACH SCENARIO

UNCALIBRATED CONCENTRATION IN MICRORAMS PER CUBIC METER - CALIBRATION, POLLUTANT-1:  
CALIBRATION, POLLUTANT-2:

SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	POLLUTANT-1: GAS		POLLUTANT-2: PARTICLE					
		COORDINATES X(KM)	Y(KM)	CONCENTRATION UNCALIBRATED	CONCENTRATION CALIBRATED	COORDINATES X(KM)	Y(KM)	CONCENTRATION UNCALIBRATED	CONCENTRATION CALIBRATED
1	1	8.00	48.00	144.8302	0.0	8.00	48.00	11.7695	0.0

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 3    CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLUTANT FOR EACH SCENARIO

UNCALIBRATED VALUES IN MICROGRAMS PER SQUARE METER PER HOUR - CALIBRATION, POLLUTANT-1;  
CALIBRATION, POLLUTANT-2;

POLLUTANT-1: GAS

SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES X(KM)	COORDINATES Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED	SURFACE DEPOSITION FLUX CALIBRATED
1	1	8.00	48.00	5213.8828	0.0

IHC002I STOP	0
--------------	---

POLLUTANT-2: PARTICLE

SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES X(KM)	COORDINATES Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED	SURFACE DEPOSITION FLUX CALIBRATED
1	1	8.00	48.00	8.00	847.4036

## APPENDIX F

### PEM FORTRAN LISTING

The PEM (Version 82360) computer program was developed and tested on the IBM computers at the Oak Ridge National Laboratory. The program was later modified slightly to run it on the UNIVAC computer at Research Triangle Park. A listing of this UNIVAC-compatible FORTRAN program follows. This listing clearly shows the modifications made to adapt the PEM computer code from the IBM to the UNIVAC. A summary of the statements (identified by their line numbers in the listing) required for each computer is given below:

<u>IBM</u>	<u>UNIVAC</u>
208	209
-	1524
-	1577
-	1639
4362	4359-4361
4389	4386-4388
4415	4412-4414

RAPS\*PEM(1).PROGRAM(4)

1 C 00000010  
2 C 00000020  
3 C 00000030  
4 C \*\*\* PEM (VERSION 82360) \*\*\* 00000040  
5 C 00000050  
6 C 00000060  
7 C POLLUTION EPISODIC MODEL 00000070  
8 C INCLUDING 00000080  
9 C DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION 00000090  
10 C OF POLLUTANTS 00000100  
11 C 00000110  
12 C 00000120  
13 C \*\*\* PEM PROGRAM DEVELOPMENT : --- DECEMBER 1982 00000130  
14 C 00000140  
15 C K. SHANKAR RAO AND MARTHA M. STEVENS 00000150  
16 C ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL) 00000160  
17 C NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION (NOAA) 00000170  
18 C U.S. DEPARTMENT OF COMMERCE 00000180  
19 C P.O. BOX - E 00000190  
20 C OAK RIDGE, TENN 37830 00000200  
21 C 00000210  
22 C PHONE: (615) 576-1238 OR 1241 00000220  
23 C FTS: 626-1238 OR 1241 00000230  
24 C 00000240  
25 C ( THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT 00000250  
26 C BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE 00000260  
27 C NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION ) 00000270  
28 C 00000280  
29 C 00000290  
30 C \*\*\* EXTENDED ABSTRACT : PEM (VERSION 82360). 00000300  
31 C 00000310  
32 C PEM IS AN URBAN SCALE (UPTO 60 KM DISTANCES) AIR QUALITY 00000320  
33 C DISPERSION-DEPOSITION MODEL CAPABLE OF PREDICTING SHORT-TERM 00000330  
34 C (1 TO 24-HOUR) AVERAGE SURFACE CONCENTRATIONS AND DEPOSITION 00000340  
35 C FLUXES OF ONE OR TWO GASEOUS OR PARTICULATE POLLUTANTS AT 00000350  
36 C UP TO A MAXIMUM OF 50X50 GROUND-LEVEL RECEPTORS. PREDICTIONS ARE 00000360  
37 C BASED ON STEADY-STATE GAUSSIAN PLUME HYPOTHESIS, BRIGGS' PLUME 00000370  
38 C RISE FORMULATIONS, AND PASQUILL-GIFFORD (PG) STABILITY CLASS- 00000380  
39 CIFICATION AND DISPERSION PARAMETER CURVES. UP TO 300 INDIVIDUAL 00000390  
40 C POINT SOURCES AND UP TO 50 AREA SOURCES MAY BE INCLUDED IN THE 00000400  
41 C INPUTS TO THE MODEL. CALCULATIONS ARE PERFORMED FOR EACH HOUR 00000410  
42 C USING THE SPECIFIED HOURLY METEOROLOGICAL DATA. UP TO 24 DIFFERENT 00000420  
43 C SETS OF HOURLY METEOROLOGICAL DATA MAY BE SPECIFIED AS INPUT FOR 00000430  
44 C THE DETERMINATION OF AIR QUALITY FOR 24 DISTINCT WEATHER 00000440  
45 C SCENARIOS. POLLUTANT CONCENTRATIONS AND DEPOSITION FLUXES FOR A 00000450  
46 C 2 TO 24 AVERAGING PERIOD ARE CALCULATED BY AVERAGING THE CORRESPONDING 00000460  
47 C VALUES CALCULATED FOR EACH HOUR IN THE PERIOD. 00000470  
48 C 00000480  
49 C PEM IS BASED ON THE TEXAS EPISODIC MODEL (TEM, VERSION 8) 00000490  
50 C DEVELOPED BY THE TEXAS AIR CONTROL BOARD (1979). TEM USES THE 00000500  
51 C GAUSSIAN PLUME CONCENTRATION ALGORITHMS DEVELOPED FOR NON-REACTIVE 00000510  
52 C POLLUTANTS AND A PERFECTLY REFLECTING LOWER BOUNDARY. CHEMICAL 00000520  
53 C AND PHYSICAL DEPLETION PROCESSES ARE THEREFORE IGNORED, EXCEPT FOR 00000530  
54 C AN OPTION WHICH ALLOWS A SIMPLE EXPONENTIAL DECAY OF POLLUTANT 00000540  
55 C WITH TRAVEL TIME. THIS METHOD REQUIRES AN ACCURATE ESTIMATE OF 00000550  
56 C THE POLLUTANT'S HALF-LIFE. 00000560  
57 C 00000570  
58 C IN CONTRAST, PEM EXPLICITLY ACCOUNTS FOR THE DRY DEPOSITION, 00000580  
59 C GRAVITATIONAL SETTLING, AND A FIRST-ORDER CHEMICAL TRANSFORMATION 00000590  
60 C OR DECAY OF GASEOUS OR PARTICULATE POLLUTANTS (OF ANY SIZE) IN 00000600  
61 C THE CONCENTRATION ALGORITHMS. THESE ALGORITHMS, BASED ON EXACT 00000610  
62 C SOLUTIONS OF A GRADIENT-TRANSFER ('K-THEORY') MODEL, WERE GIVEN BY 00000620  
63 C RAO (1981, 1982) AS ANALYTICAL EXTENSIONS OF THE WIDELY-USED 00000630  
64 C GAUSSIAN PLUME DISPERSION ALGORITHMS UNDER VARIOUS ATMOSPHERIC 00000640  
65 C STABILITY AND MIXING CONDITIONS. THUS, PEM TREATS DEPOSITION, 00000650  
66 C SEDIMENTATION, AND CHEMICAL TRANSFORMATION IN A PHYSICALLY REAL- 00000660  
67 C ISTIC AND STRAIGHTFORWARD MANNER, AND IT IS SUBJECT TO THE SAME 00000670  
68 C BASIC ASSUMPTIONS AND LIMITATIONS ASSOCIATED WITH ALL GAUSSIAN- 00000680  
69 C PLUME TYPE MODELS. FOR FURTHER DETAILS REGARDING THE GRADIENT- 00000690  
70 C TRANSFER MODEL FORMULATIONS, ANALYTICAL SOLUTIONS, PARAMETERI- 00000700  
71 C ZATIONS, AND THE DEVELOPMENT OF THE ALGORITHMS FOR PEM, THE USER 00000710  
72 C SHOULD CONSULT THE REPORTS BY RAO (1981, 1982). 00000720  
73 C 00000730  
74 C BASED ON THE NUMBER OF POLLUTANTS (NPOL=1 OR 2) AND THE CHEMI- 00000740  
75 C CAL TRANSFORMATION/DECAY OPTION PARAMETER (ICT=0 OR 1) SPECIFIED 00000750  
76 C IN THE INPUT TO THE MODEL, PEM PROGRAM DOES ONE OF THE FOLLOWING: 00000760

77 C (1) IF NPOL=1 AND ICT=0 OR 1, SURFACE CONCENTRATIONS AND DEPOSI- 00000770  
 78 C TION FLUXES OF ONE GASEOUS OR PARTICULATE POLLUTANT, WITH THE 00000780  
 79 C GIVEN DEPOSITION AND SETTLING VELOCITIES, VD1 AND WI RESPECTI- 00000790  
 80 C VELY, ARE CALCULATED. IF ICT=1, THEN CHEMICAL DECAY OF POLLU- 00000800  
 81 C TANT IS ALSO CONSIDERED IF THE DECAY RATE XKT > 0. IS GIVEN 00000810  
 82 C IN PERCENT PER HOUR. 00000820  
 83 C 00000830  
 84 C 00000840  
 85 C (2) IF NPOL=2 AND ICT=0, SURFACE CONCENTRATIONS AND DEPOSITION 00000850  
 86 C FLUXES OF TWO DIFFERENT AND UNCOUPLED GASEOUS OR PARTICULATE 00000860  
 87 C POLLUTANT SPECIES WITH THE GIVEN DEPOSITION AND SETTLING VELOC- 00000870  
 88 C ITIES VD1 AND WI (FOR SPECIES-1) AND VD2 AND W2 (FOR SPECIES-2) 00000880  
 89 C RESPECTIVELY, ARE CALCULATED. EMISSION RATES FOR BOTH SPECIES 00000890  
 90 C MAY BE DIFFERENT. CHEMICAL DECAY IS NOT CONSIDERED FOR EITHER 00000900  
 91 C SPECIES EVEN IF A VALUE OF XKT > 0. IS SPECIFIED. 00000910  
 92 C 00000920  
 93 C (3) IF NPOL=2 AND ICT=1, THE TWO GASEOUS OR PARTICULATE POLLUTANT 00000930  
 94 C SPECIES ARE COUPLED THROUGH A FIRST-ORDER CHEMICAL TRANSFORMA- 00000940  
 95 C TION. THE SURFACE CONCENTRATIONS AND DEPOSITION FLUXES OF BOTH 00000950  
 96 C THE PRIMARY POLLUTANT (SPECIES-1 OR REACTANT) AS WELL AS THE 00000960  
 97 C SECONDARY POLLUTANT (SPECIES-2 OR REACTION PRODUCT) ARE CALCUL- 00000970  
 98 C ATED. THE CHEMICAL TRANSFORMATION RATE (XKT > 0.) SHOULD BE 00000980  
 99 C GIVEN. BOTH SPECIES MAY BE GIVEN NON-EQUAL DEPOSITION AND SET- 00000990  
 100 C TLING VELOCITIES. A NON-ZERO DIRECT EMISSION RATE FOR THE 00001000  
 101 C SECONDARY POLLUTANT FROM THE POINT AND/OR AREA SOURCES MAY 00001010  
 102 C ALSO BE SPECIFIED AS INPUT FOR THIS CASE. 00001020  
 103 C 00001030  
 104 C FOR FURTHER DETAILS REGARDING THE USE OF THE PEM AND ITS I/O 00001040  
 105 C OPTIONS, INPUT PARAMETERS AND UNITS, AND EXAMPLE PROBLEMS, THE 00001050  
 106 C USER SHOULD CONSULT THE PEM USER'S GUIDE BY RAO AND STEVENS (1982) 00001060  
 107 C 00001070  
 108 C \*\*\* REFERENCES \*\*\* 00001080  
 109 C 00001090  
 110 C (1) STAFF OF THE TEXAS AIR CONTROL BOARD, 1979: USER'S GUIDE : 00001100  
 111 C TEXAS EPISODIC MODEL. TEXAS AIR CONTROL BOARD, PERMITS 00001110  
 112 C SECTION, AUSTIN, TEXAS 78723, 215 PP. 00001120  
 113 C 00001130  
 114 C (2) RAO, K. S., 1981: ANALYTICAL SOLUTIONS OF A GRADIENT-TRANSFER 00001140  
 115 C MODEL FOR PLUME DEPOSITION AND SEDIMENTATION. EPA- , 00001150  
 116 C U.S.E.P.A., RESEARCH TRIANGLE PARK, NC; 00001160  
 117 C NOAA TECH. MEMO. ERL/ARL-109, NOAA-ATDL, OAK RIDGE, TN 37830, 00001170  
 118 C 75 PP. ATDL CONTRIBUTION FILE NO. 81/14. 00001180  
 119 C 00001190  
 120 C (3) RAO, K. S., 1982: GAUSSIAN PLUME CONCENTRATION ALGORITHMS WITH 000001200  
 121 C DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION. 00001210  
 122 C EPA- , RESEARCH TRIANGLE PARK, NC; 00001220  
 123 C NOAA TECH. MEMO. ERL/ARL- , NOAA-ATDL, OAK RIDGE, TN 37830. 00001230  
 124 C ATDL CONTRIBUTION FILE NO. 82/27. 00001240  
 125 C 00001250  
 126 C (4) RAO, K. S., AND M. M. STEVENS, 1982: POLLUTION EPISODIC 00001260  
 127 C MODEL: USER'S GUIDE. EPA- , RESEARCH 00001270  
 128 C TRIANGLE PARK, NC. 00001280  
 129 C NOAA TECH. MEMO. ERL/ARL- , NOAA-ATDL, OAK RIDGE, TN 37830. 00001290  
 130 C ATDL CONTRIBUTION FILE NO. 82/28. 00001300  
 131 C 00001310  
 132 C 00001320  
 133 C 00001330  
 134 C \*\*\* PEM (VERSION 82360) : FORTRAN LISTING. 00001340  
 135 C 00001350  
 136 C 00001360  
 137 C 00001370  
 138 C 00001380  
 139 C 00001390  
 140 C \*\*\* COMMON BLOCKS, DIMENSIONS, AND DATA STATEMENTS. 00001400  
 141 C 00001410  
 142 C 00001420  
 143 C COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00001430  
 144 C 1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00001440  
 145 C 2 XA(50),YA(50),EA(50,2),SIZE(50), 00001450  
 146 C 3 WD(24),WS(24),TA(24),HMIX(24),PEN(24), 00001460  
 147 C 4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00001470  
 148 C 5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLNAM(3,2),CALNAM(7,2), 00001480  
 149 C 6 ITA,IRD,IWR,IDS, D8G,D47,D8047,DIST,DELTA, 00001490  
 150 C 7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS, UINV,WVEC, 00001500  
 151 C 8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS, 00001510  
 152 C 9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCOPT,NMAX, 00001520  
 153 C \* NSTDWN,INTER,NPRINT 130 00001530

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154      C          COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC      00001540
155          COMMON/PARM1A/GAMMA                         00001550
156          COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT       00001560
157          COMMON/PARM2A/AA,BA                         00001570
158          COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2           00001580
159          COMMON/PARM4/V11,V21,V12,V22,V13           00001590
160          COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6 00001600
161          COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42 00001610
162          COMMON/PARM7/QZC1,QZC2                     00001620
163          COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C        00001630
164          COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW     00001640
165          COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX         00001650
166          COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX         00001660
167      C          EXTERNAL FUN3                         00001670
168          REAL*8 FUN3                           00001680
169          REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR,T1A,T2A 00001690
170          DIMENSION IW(102)                      00001700
171          DIMENSION PRL(2,2),DWL(4),ANGLIM(7)        00001710
172          DIMENSION ITABLE(5,10),EPSLIM(10)        00001720
173          DIMENSION AAR(6),BAR(6),CX1(7),DX1(7),CX2(7),DX2(7) 00001730
174          DIMENSION XAI(5),XA2(5),XA2C(5),RCA1(5),RCA2(5) 00001740
175          DIMENSION RCA2CT(5,50),QA2QA1(50),TERMB2(5) 00001750
176          DIMENSION RCA2CT(5,50),QA2QA1(50),TERMB2(5) 00001760
177      C          DATA PRL/4HMOME,4HNTUM,4HBUOY,4HANCY/ 00001770
178          DATA DWL/4H      ,4H      ,4HDOWN,4HWASH/ 00001780
179          DATA EPSLIM/.12427,.16511,.24504,.35884,.46373, 00001790
180          1      .55868,.64350,.69482,.71890,.78540/ 00001800
181          1      0,0,0,0,0,0,0,0,0,1,0,0,0,1,1,0,0,1,1,1,0,0,1,1,2,00001820
182          1      0,1,1,2,2,0,1,1,2,3,0,1,2,2,3,0,1,2,3,3,0,1,2,3,4/00001830
183          1      DATA ANGLIM/0.610865,0.488692,0.366519,0.244346, 00001840
184          1 0.244346,0.183260,0.122173/ 00001850
185          DATA CX1/.495,.310,.197,.122,.122,.0934,.0625/ 00001860
186          DATA DX1/.873,.897,.908,.916,.916,.912,.911/ 00001870
187          DATA CX2/.606,.523,.285,.193,.193,.141,.080/ 00001880
188          DATA DX2/.851,.840,.867,.865,.865,.868,.884/ 00001890
189          DATA AAR/.4,.4,.33,.22,.15,.06/ 00001900
190          DATA BAR/.91,.91,.86,.80,.75,.71/ 00001910
191          DATA BAR/.91,.91,.86,.80,.75,.71/ 00001920
192      C          00001930
193      C          00001940
194      C          00001950
195      C *** DEFINE PROGRAM CONSTANTS. 00001960
196      C          PI=3.14159                         00001970
197          SQPI=SQRT(PI)                         00001980
198          SQRT2=SQRT(2.)                       00001990
199          A1B=1000./(SQRT2*SQPI)                 00002000
200          A1C=2.*SQPI                         00002010
201          AI=0.                                00002020
202          BI=1.                                00002030
203          EPSABS=1.0E-4                         00002040
204          EPSREL=1.0E-4                         00002050
205          LW=800                               00002060
206          NIW=102                             00002070
207          NIW=102                             00002080
208      C          EXPMAX=174.                  00002090
209          EXPMAX= 87.                         00002100
210          EXPMIN=50.                          00002110
211          ETAMAX=SQRT(EXPMAX)                 00002120
212      C          WRITE (IWR,5432)                00002130
213          5432 FORMAT ('1',//46X,'PEM (VERSION 82360)'//    00002140
214          1 45X,'POLLUTION EPISODIC MODEL'//      00002150
215          2 52X,'INCLUDING'//                   00002160
216          3 30X,'DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION'// 00002170
217          4 50X,'OF POLLUTANTS'//              00002180
218          INDEX=0                            00002190
219      C          CALL INPUT MODULE TO READ ALL WEATHER AND SOURCE INFORMATION, 00002200
220          CALL INPUT MODULE TO READ ALL WEATHER AND SOURCE INFORMATION, 00002210
221          DEPOSITION AND SEDIMENTATION VELOCITIES OF POLLUTANT SPECIES, 00002220
222          AND CHEMICAL DECAY OR TRANFORMATION RATE. 00002230
223          INDEX=0                            00002240
224          ***** 00002250
225          CALL INMOD                         00002260
226          ***** 00002270
227          CALL INMOD                         00002280
228          ***** 00002290
229          VD136=VD1*36.                      00002290

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231      VD236=VD2*36.          00002300
232      C                      00002310
233      C                      00002320
234      C *** DETERMINE VALUE OF PARAMETER ISPEC. 00002330
235      C ISPEC IS AN INTERNAL ROUTING PARAMETER USED IN PEM 00002340
236      C TO DETERMINE THE APPROPRIATE CONCENTRATION ALGORITHMS 00002350
237      C TO BE USED FOR A GIVEN PROBLEM. 00002360
238      C VALUE OF ISPEC IS BASED ON NUMBER OF POLLUTANTS, 00002370
239      C AND CHEMICAL TRANSFORMATION OPTION PARAMETER. 00002380
240      C 00002390
241      IF(NPOL.EQ.2) GO TO 41 00002400
242      C ONLY ONE POLLUTANT SPECIES. CHEMICAL DECAY CAN BE CONSIDERED 00002410
243      C BY SETTING ICT = 1 AND XKT > 0. 00002420
244      C ISPEC=1 00002430
245      C GO TO 43 00002440
246      C 00002450
247      C TWO POLLUTANT SPECIES. 00002460
248      41 IF(ICK.EQ.1) GO TO 42 00002470
249      C NO CHEMICAL COUPLING. THE TWO SPECIES ARE INDEPENDENT 00002480
250      C OF EACH OTHER. CHEMICAL DECAY IS NOT CONSIDERED FOR 00002490
251      C EITHER SPECIES. 00002500
252      C ISPEC=2 00002510
253      C GO TO 43 00002520
254      C 00002530
255      C CHEMICAL COUPLING EXISTS BETWEEN SPECIES-1 (REACTANT) 00002540
256      C AND SPECIES-2 (PRODUCT). 00002550
257      42 ISPEC=3 00002560
258      43 CONTINUE 00002570
259      C 00002580
260      C 00002590
261      C 00002600
262      C *** DEFINE TIME-AVERAGING MULTIPLIER CONSTANTS. 00002610
263      C 00002620
264      IF(INTOPT.EQ.1) STCONV = 1. 00002630
265      IF(INTOPT.EQ.2) STCONV= 0.04166667 00002640
266      IF(INTOPT.EQ.3) STCONV= 1.0/FLOAT(NSCEN) 00002650
267      C 00002660
268      INDEX=1 00002670
269      C 00002680
270      C CALL INPUT MODULE TO BRING IN WEATHER DATA FOR ONE SCENARIO 00002690
271      C (NUMBER OF SCENARIO = ISCEN). 00002700
272      C 00002710
273      C ****
274      100 CALL INMOD 00002730
275      C **** 00002740
276      C 00002750
277      C CALCULATE WIND VECTOR (WVEC) FOR SCENARIO. IFLAG IS USED BELOW 00002760
278      C (STMT. 275) TO DETERMINE METHOD OF RESTRICTING THE AREA OF THE 00002770
279      C RECEPTOR GRID AFFECTED BY EACH SOURCE. 00002780
280      C 00002790
281      175 IF(NWDOPT.EQ.1) GO TO 200 00002800
282      DO 180 IWD=1,16 00002810
283      DETA=ABS(IWD(ISCEN)-SECTAN(IWD)) 00002820
284      IF(DETA.LE.0.19634954) GO TO 185 00002830
285      180 CONTINUE 00002840
286      185 GO TO 205 00002850
287      200 WD(ISCEN)=SECTAN(IWD) 00002860
288      205 IF(IWD.LT.8.OR.IWD.GT.10) GO TO 210 00002870
289      IFLAG=1 00002880
290      GO TO 241 00002890
291      210 IF(IWD.NE.11) GO TO 215 00002900
292      IFLAG=2 00002910
293      GO TO 241 00002920
294      215 IF(IWD.LT.12.OR.IWD.GT.14) GO TO 220 00002930
295      IFLAG=3 00002940
296      GO TO 241 00002950
297      220 IF(IWD.NE.15) GO TO 225 00002960
298      IFLAG=4 00002970
299      GO TO 241 00002980
300      225 IF(IWD.LT.16.AND.IWD.GT.2) GO TO 230 00002990
301      IFLAG=5 00003000
302      GO TO 241 00003010
303      230 IF(IWD.NE.3) GO TO 235 00003020
304      IFLAG=6 00003030
305      GO TO 241 00003040
306      235 IF(IWD.LT.4.OR.IWD.GT.6) GO TO 240 00003050
307      IFLAG=7 00003060

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308      GO TO 241                               00003070
309      240  IFLAG=8                           00003080
310      241  WVEC= WD(ISCEN) + 3.14159265    00003090
311          IF(WVEC.GT.6.2831853) WVEC=WVEC - 6.2831853 00003100
312          WDV=4.712388981-WD(ISCEN)           00003110
313          IF(WDV.LT.0.)WDV=WDV+6.283185307  00003120
314          WDPANG=WDV+ANGLIM(ISC)            00003130
315          WDMANG=WDV-ANGLIM(ISC)             00003140
316      C
317      C CALL AUTGRD TO CALCULATE RECEPTOR GRID PARAMETERS AUTOMATICALLY. 00003150
318      C ****
319          IF(IGRID.EQ.1) CALL AUTGRD        00003160
320      C ****
321      C
322      C *** INITIALIZATION.               00003170
323      C
324      C INITIALIZE CONCENTRATION AND SURFACE DEPOSITION FLUX ARRAYS 00003180
325          IF(NTOPT.GT.1.AND.ISCEN.GT.1) GO TO 4 00003190
326          DO 2 I=1,LX                      00003200
327          DO 2 J=1,LY                      00003210
328          CONC(I,J,1)=0.                   00003220
329          SDF(I,J,1)=0.                   00003230
330          IF(ISPEC.EQ.1.AND.NCSOPT.EQ.0) GO TO 2 00003240
331          CONC(I,J,2)=0.                   00003250
332          SDF(I,J,2)=0.                   00003260
333          2 CONTINUE                     00003270
334      C
335      C
336      C
337          4 VGRID= 1./GRID                00003280
338          GRIDSQ= GRID*GRID              00003290
339          ELX= LX                      00003300
340          ELY= LY                      00003310
341          XBL= XSWC + 0.5*GRID          00003320
342          XB2= XSWC + (ELX-0.5)*GRID   00003330
343          YBL= YSWC + 0.5*GRID          00003340
344          YB2= YSWC + (ELY-0.5)*GRID   00003350
345      C
346      C IF NO AREA SOURCES, SKIP AREA SOURCE CALCULATIONS. 00003360
347          IF(NAS.LT.1) GO TO 245        00003370
348      C
349      C
350      C
351      C*** A R E A   S O U R C E   C A L C U L A T I O N S   *** 00003380
352      C
353      C INV HELPS DETERMINE THE PATTERN OF GRID SQUARES AFFECTED BY EACH 00003390
354      C AREA SOURCE. PATTERN DEPENDS ONLY ON WIND DIRECTION. 00003400
355      C EPS IS THE ANGLE BETWEEN THE WIND VECTOR AND THE NEAREST 00003410
356      C COORDINATE AXIS. 00003420
357      C
358          INV= 1 + WVEC/0.78540        00003430
359          GO TO (2411,2412,2413,2414,2415,2416,2417,2418),INV 00003440
360      2411  ITABX=1                  00003450
361          ISIGNX=1                 00003460
362          ISIGNY=1                 00003470
363          EPS= WVEC                00003480
364          GO TO 2419                00003490
365      2412  ITABX=0                  00003500
366          ISIGNX=1                 00003510
367          ISIGNY=1                 00003520
368          EPS= 1.5708 - WVEC       00003530
369          GO TO 2419                00003540
370      2413  ITABX=0                  00003550
371          ISIGNX=1                 00003560
372          ISIGNY=-1                00003570
373          EPS= WVEC - 1.57080     00003580
374          GO TO 2419                00003590
375      2414  ITABX=1                  00003600
376          ISIGNX=1                 00003610
377          ISIGNY=-1                00003620
378          EPS= 3.1416 - WVEC       00003630
379          GO TO 2419                00003640
380      2415  ITABX=1                  00003650
381          ISIGNX=-1               00003660
382          ISIGNY=-1               00003670
383          EPS= WVEC - 3.1416      00003680
384          GO TO 2419                00003690

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385      2416 ITABX=0          00003840
386          ISIGNX=-1        00003850
387          ISIGNY=-1        00003860
388          EPS= 4.7124 - WVEC 00003870
389          GO TO 2419       00003880
390      2417 ITABX=0          00003890
391          ISIGNX=-1        00003900
392          ISIGNY=1          00003910
393          EPS= WVEC - 4.7124 00003920
394          GO TO 2419       00003930
395      2418 ITABX=1          00003940
396          ISIGNX=-1        00003950
397          ISIGNY=1          00003960
398          EPS= 6.2832 - WVEC 00003970
399      2419 IF(ITABX.EQ.0) GO TO 2420 00003980
400          ITABY=0          00003990
401          INCRX=0          00004000
402          INCRY=1          00004010
403          GO TO 2421       00004020
404      2420 ITABY=1          00004030
405          INCRX=1          00004040
406          INCRY=0          00004050
407          DO 2422 L=1,10    00004060
408          IF(EPS.GT.EPSLIM(L)) GO TO 2422 00004070
409          IEPS=L          00004080
410          GO TO 2423       00004090
411      2422 CONTINUE        00004100
412          IEPS=10         00004110
413          C
414          C   REDUCE STABILITY CLASS BY 1 (EXCEPT FOR ISC=1) TO SIMULATE 00004120
415          C   SURFACE TURBULENCE IN URBAN CONDITIONS.                00004130
416          C
417      2423 IA= ISC-1        00004140
418          IF(IA.EQ.0) IA=1        00004150
419          AA= AAR(IA)        00004160
420          BA= BAR(IA)        00004170
421          BA1=2.*(1.-BA)      00004180
422          DXA=1000.*GRID/COS(EPS) 00004190
423          UPL=WS(ISCEN)      00004200
424          UINV=1./UPL        00004210
425          UINV1=UINV/100.      00004220
426          C
427          C   DEFINE NONDIMENSIONAL DEPOSITION AND SEDIMENTATION PARAMETERS. 00004230
428          C
429          C   ISPEC = 1 OR 2 OR 3        00004240
430          BAVDI=0.01*VDI*BA1      00004250
431          VDC1=VDI*UINV1       00004260
432          WC1=W1*UINV1        00004270
433          V11=VDC1-0.5*WC1      00004280
434          V21=VDC1-WC1        00004290
435          IF(V21.EQ.0.) GO TO 44 00004300
436          R11=V11/V21        00004310
437          R21=0.5*WC1/V21      00004320
438          44 IF(ISPEC.EQ.1) GO TO 46 00004330
439          C
440          C   ISPEC = 2 OR 3        00004340
441          BAVD2=0.01*VD2*BA1      00004350
442          VDC2=VD2*UINV1       00004360
443          WC2=W2*UINV1        00004370
444          V12=VDC2-0.5*WC2      00004380
445          V22=VDC2-WC2        00004390
446          IF(V22.EQ.0.) GO TO 45 00004400
447          R12=V12/V22        00004410
448          R22=0.5*WC2/V22      00004420
449          45 IF(ISPEC.EQ.2) GO TO 47 00004430
450          C
451          C   ISPEC = 3          00004440
452          V13=V11-0.5*(WC1-WC2) 00004450
453          IF(V21.EQ.0.) GO TO 46 00004460
454          R13=V13/V21        00004470
455          R23=0.5*WC2/V21      00004480
456          C
457          C   ISPEC = 1 OR 3        00004490
458          46 UTAUC=TAUC*UPL      00004500
459          47 CONTINUE        00004510
460          C

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462 C CALCULATE RELATIVE CONCENTRATIONS AT A RECEPTOR LOCATED AT THE 00004610
463 C CENTER OF THE CALCULATION GRID SQUARE CONTAINING THE AREA SOURCE 00004620
464 C EMISSIONS, AND AT THE CENTER OF EACH OF THE FOUR GRID SQUARES 00004630
465 C IMMEDIATELY DOWNWIND OF THE SOURCE. 00004640
466 C 00004650
467 C FIRST DEFINE DOWNWIND DISTANCES TO THE LEADING AND TRAILING EDGES, 00004660
468 C AND MID-POINTS OF THE FIVE CALCULATION GRID SQUARES. 00004670
469 XA1(1)=0.0 00004680
470 XA2(1)=0.5*DXA 00004690
471 C 00004700
472 DO 102 I=1,5 00004710
473 SZ2=AA*(XA2(I)**BA) 00004720
474 IF(SZ2.GT.5000.) SZ2=5000. 00004730
475 XA2C(I)=XA2(I)/(SQRT2*SZ2) 00004740
476 C 00004750
477 IF(I.EQ.5) GO TO 102 00004760
478 XA1(I+1)=XA2(I) 00004770
479 XA2(I+1)=XA1(I+1)+DXA 00004780
480 102 CONTINUE 00004790
481 C 00004800
482 K=1 00004810
483 IF(ISPEC.NE.3) GO TO 104 00004820
484 C 00004830
485 C START LOOP ON ALL AREA SOURCES IF ISPEC = 3 00004840
486 DO 114 K=1,NAS 00004850
487 IF(EA(K,1).EQ.0.) EA(K,1)=1.E-6 00004860
488 QA2QA1(K)=EA(K,2)/EA(K,1) 00004870
489 IF(K.EQ.1) GO TO 103 00004880
490 IF(QA2QA1(K).EQ.QA2QA1(K-1)) GO TO 112 00004890
491 103 Q2Q1=QA2QA1(K) 00004900
492 G42PX1=Q2Q1 00004910
493 C 00004920
494 104 G41PX1=1. 00004930
495 IF(ISPEC.EQ.2) G42PX1=1. 00004940
496 C 00004950
497 C START LOOP ON FIVE CALCULATION GRID SQUARES WITH RECEPTORS. 00004960
498 DO 111 I=1,5 00004970
499 X1A=XA1(I) 00004980
500 X2A=XA2(I) 00004990
501 X2CA=XA2C(I) 00005000
502 C 00005010
503 C ISPEC = 1 OR 2 OR 3 00005020
504 D31=2.*V11*X2CA 00005030
505 D11=WC1*X2CA 00005040
506 D21=D11*D11 00005050
507 R31=1.+2.*D21 00005060
508 R41=2.*D11/SQPI 00005070
509 IF(ISPEC.EQ.1) GO TO 107 00005080
510 C 00005090
511 C ISPEC = 2 OR 3 00005100
512 D32=2.*V12*X2CA 00005110
513 D12=WC2*X2CA 00005120
514 D22=D12*D12 00005130
515 R32=1.+2.*D22 00005140
516 R42=2.*D12/SQPI 00005150
517 IF(ISPEC.EQ.2) GO TO 107 00005160
518 C 00005170
519 C ISPEC = 3 00005180
520 D33=2.*V13*X2CA 00005190
521 D6=4.*SQPI*(V21-V22)*X2CA 00005200
522 C 00005210
523 107 IF(ICK.EQ.0) XCT=0. 00005220
524 IF(ICK.EQ.1) XCT=X2A/UTAUC 00005230
525 EXCT=EXP(-XCT) 00005240
526 IF(ISPEC.EQ.3) GO TO 108 00005250
527 C 00005260
528 C ISPEC = 1 OR 2 00005270
529 C ****
530 CALL PSG4P(G41PX2,G42PX2) 00005290
531 C ****
532 IF(ICK.EQ.1) GO TO 108 00005310
533 C ISPEC = 1 WITH ICT = 0 OR ISPEC = 2 00005320
534 RCA1(I)=(G41PX1-G41PX2)/BAVD1 00005330
535 IF(RCA1(I).LT.0.) RCA1(I)=0.0 00005340
536 G41PX1=G41PX2 00005350
537 IF(ISPEC.EQ.1) GO TO 111 00005360
538 C ISPEC = 2 00005370

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539      RCA2(I)=(G42PX1-G42PX2)/BAVD2          00005380
540      IF(RCA2(I).LT.0.) RCA2(I)=0.0          00005390
541      G42PX1=G42PX2                      00005400
542      GO TO 111                      00005410
543      C
544      C   ISPEC = 1 WITH ICT = 1 OR ISPEC = 3    00005420
545      108 IF(K.GT.1) GO TO 109          00005430
546      T1A=XIA/UTAUC                      00005440
547      T2A=X2A/UTAUC                      00005450
548      C   COMPUTE INTEGRAL FUNC=F3(T1A,T2A); FUNC IS THE INTEGRAND FUNCTION. 00005460
549      C   *****
550      CALL D01AJF(FUN3,T1A,T2A,EPSABS,EPSREL,RESULT, 00005470
551      1 ABSERR,WORK,LW,IW,NIW,IFAIL)        00005480
552      C   *****
553      FUNC=RESULT                      00005490
554      TERMB1=FUNC                      00005500
555      IF(ISPEC.EQ.1) GO TO 106          00005510
556      TERMB2(I)=GAMMA*FUNC*VDC1/VDC2        00005520
557      IF(ISPEC.EQ.3) GO TO 109          00005530
558      C
559      C   ISPEC = 1 WITH ICT = 1          00005540
560      106 RCA1(I)=((G41PX1-G41PX2)/VDC1-TERMB1)/BA1 00005550
561      IF(RCA1(I).LT.0.) RCA1(I)=0.0          00005560
562      RCA1(I)=RCA1(I)*UINV                00005570
563      G41PX1=G41PX2                      00005580
564      GO TO 111                      00005590
565      C
566      C   ISPEC = 3                      00005600
567      C   *****
568      109 CALL PSG4P(G41PX2,G42PX2)        00005610
569      C   *****
570      IF(K.GT.1) GO TO 110          00005620
571      TERMA1=(G41PX1-G41PX2)/VDC1        00005630
572      DUM1=(TERMA1-TERMB1)/BA1          00005640
573      IF(DUM1.LT.0.) DUM1=0.0          00005650
574      RCA1(I)=DUM1*UINV                00005660
575      G41PX1=G41PX2                      00005670
576      110 TERMA2=(G42PX1-G42PX2)/VDC2        00005680
577      DUM2=(TERMA2+TERMB2(I))/BA1          00005690
578      IF(DUM2.LT.0.) DUM2=0.0          00005700
579      RCA2CT(I,K)=DUM2*UINV                00005710
580      G42PX1=G42PX2                      00005720
581      C
582      111 CONTINUE                      00005730
583      C   END LOOP ON I=1,5 CALCULATION GRID SQUARES. 00005740
584      GO TO 114                      00005750
585      C
586      112 DO 113 I=1,5          00005760
587      RCA2CT(I,K)=RCA2CT(I,K-1)        00005770
588      113 CONTINUE                      00005780
589      C
590      114 CONTINUE                      00005790
591      C   END LOOP ON K=1,NAS AREA SOURCES IF ISPEC = 3 00005800
592      C
593      C
594      C   LOOP THROUGH ALL AREA SOURCES. EMISSIONS FROM EACH AREA SOURCE 00005810
595      C   ARE APPORTIONED AMONG THE RECEPTOR GRID SQUARES WHOLLY OR 00005820
596      C   PARTIALLY COVERED BY THE SOURCE. EACH AFFECTED RECEPTOR GRID 00005830
597      C   SQUARE IS TREATED AS A SOURCE. 00005840
598      C
599      C   START LOOP ON K=1,NAS AREA SOURCES. 00005850
600      DO 2429 K=1,NAS          00005860
601      AREA= SIZE(K)*SIZE(K)          00005870
602      AX1= XA(K)                      00005880
603      AX2= AX1 + SIZE(K)          00005890
604      NX1= (AX1-XSWC)*VGRID + 5.        00005900
605      NX2= (AX2-XSWC)*VGRID + 5.        00005910
606      IF(NX1.GT.LX+8.OR.NX2.LT.1) GO TO 2429 00005920
607      IF(NX1.GE.1) GO TO 32          00005930
608      NX1= 1                      00005940
609      AX1= XSWC - 4.*GRID          00005950
610      32 IF(NX2.LE.LX+8) GO TO 34        00005960
611      NX2= LX+8                      00005970
612      AX2= XSWC + (ELX + 4.)*GRID        00005980
613      34 X1= XSWC + (FLOAT(NX1)-5.)*GRID 00005990
614      X2= XSWC + (FLOAT(NX2)-4.)*GRID        00006000
615      AY1= YA(K)                      00006010

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616      AY2= AY1 + SIZE(K)          00006150
617      NY1= (AY1-YSWC)*VGRID + 5. 00006160
618      NY2= (AY2-YSWC)*VGRID + 5. 00006170
619      IF(NY1.GT.LY+8.OR.NY2.LT.1) GO TO 2429 00006180
620      IF(NY1.GE.1) GO TO 36       00006190
621      NY1= 1                     00006200
622      AY1= YSWC - 4.*GRID       00006210
623      36 IF(NY2.LE.LY+8) GO TO 38 00006220
624      NY2= LY+8                 00006230
625      AY2= YSWC + (ELY + 4.)*GRID 00006240
626      38 Y1= YSWC + (FLOAT(NY1)-5.)*GRID 00006250
627      Y2= YSWC + (FLOAT(NY2)-4.)*GRID 00006260
628      C
629      C START LOOP ON IX=NX1,NX2 COLUMNS OF THE RECEPTOR GRID. 00006270
630      DO 2428 IX=NX1,NX2        00006280
631      IF(NX1.NE.NX2) GO TO 10    00006290
632      DXQ= AX2-AX1             00006300
633      GO TO 13                 00006310
634      10 IF(IX.NE.NX1) GO TO 11 00006320
635      DXQ= GRID+X1-AX1         00006330
636      GO TO 13                 00006340
637      11 IF(IX.NE.NX2) GO TO 12 00006350
638      DXQ= GRID+AX2-X2         00006360
639      GO TO 13                 00006370
640      12 DXQ=GRID             00006380
641      C
642      C START LOOP ON JY=NY1,NY2 ROWS OF THE RECEPTOR GRID. 00006390
643      13 DO 2427 JY=NY1,NY2     00006400
644      IF(NY1.NE.NY2) GO TO 20    00006410
645      DY= AY2-AY1              00006420
646      GO TO 23                 00006430
647      20 IF(JY.NE.NY1) GO TO 21 00006440
648      DY= GRID+Y1-AY1          00006450
649      GO TO 23                 00006460
650      21 IF(JY.NE.NY2) GO TO 22 00006470
651      DY= GRID+AY2-Y2          00006480
652      GO TO 23                 00006490
653      22 DY=GRID              00006500
654      23 SPLIT= DXQ*DY/(AREA*GRIDSQ) 00006510
655      C
656      C LOOP FOR THE FIVE RECEPTORS AFFECTED BY EACH RECEPTOR GRID SQUARE 00006520
657      C CONTAINING EMISSIONS. THE RECEPTORS IN THE FOUR DOWNWIND SQUARES 00006530
658      C AND IN THE SOURCE SQUARE ITSELF ARE AFFECTED. 00006540
659      C
660      DO 2426 L=1,5            00006550
661      NX= IX + ISIGNX*(ITABLE(L,IEPS)*ITABX + (L-1)*INCRX) - 4 00006560
662      IF(NX.LT.1.OR.NX.GT.LX) GO TO 2426 00006570
663      NY= JY + ISIGNY*(ITABLE(L,IEPS)*ITABY + (L-1)*INCRY) - 4 00006580
664      IF(NY.LT.1.OR.NY.GT.LY) GO TO 2426 00006590
665      C
666      C CALCULATE GROUND-LEVEL CONCENTRATIONS CONC (MICROGRAMS PER CUBIC 00006600
667      C METER) AND SURFACE DEPOSITION FLUXES (MICROGRAMS PER SQUARE 00006610
668      C METER PER HOUR) OF POLLUTANTS AT RECEPTOR IN COLUMN NX, ROW NY 00006620
669      C OF THE RECEPTOR GRID DUE TO AREA SOURCE K. 00006630
670      C
671      C ISPEC = 1 OR 2 OR 3        00006640
672      C CINC1=RCA1(L)*EA(K,1)*SPLIT*STCONV 00006650
673      C CONC(NX,NY,1)=CONC(NX,NY,1)+CINC1 00006660
674      C SDF(NX,NY,1)=SDF(NX,NY,1)+VD136*CINC1 00006670
675      C IF(ISPEC.EQ.1) GO TO 2426 00006680
676      C IF(ISPEC.EQ.3) GO TO 2425 00006690
677      C
678      C ISPEC = 2                 00006700
679      C CINC2=RCA2(L)*EA(K,2)*SPLIT*STCONV 00006710
680      C CONC(NX,NY,2)=CONC(NX,NY,2)+CINC2 00006720
681      C SDF(NX,NY,2)=SDF(NX,NY,2)+VD236*CINC2 00006730
682      C GO TO 2426             00006740
683      C
684      C ISPEC = 3                 00006750
685      2425 CINC2=RCA2CT(L,K)*EA(K,1)*SPLIT*STCONV 00006760
686      C CONC(NX,NY,2)=CONC(NX,NY,2)+CINC2 00006770
687      C SDF(NX,NY,2)=SDF(NX,NY,2)+VD236*CINC2 00006780
688      C
689      2426 CONTINUE            00006790
690      C END LOOP ON L=1,5 CALCULATION GRID SQUARES WITH RECEPTORS. 00006800
691      C
692      2427 CONTINUE            00006810
                                         00006820
                                         00006830
                                         00006840
                                         00006850
                                         00006860
                                         00006870
                                         00006880
                                         00006890
                                         00006900
                                         00006910

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693      C      END LOOP ON JY=NY1,NY2 ROWS OF THE RECEPTOR GRID.          00006920
694      C
695      2428  CONTINUE                                              00006930
696      C      END LOOP ON IX=NX1,NX2 COLUMNS OF THE RECEPTOR GRID.    00006940
697      C
698      2429  CONTINUE                                              00006950
699      C      END LOOP ON K=1,NAS AREA SOURCES.                      00006960
700      C
701      C
702      C
703      C *** POINT SOURCES.                                         00006970
704      C
705      C      HPEN= MINIMUM EFFECTIVE SOURCE HEIGHT NECESSARY FOR PLUME TO 00006980
706      C      PENETRATE INVERSION.                                     00006990
707      245   HPEN= PEN(ISCEN)*HMIX(ISCEN)                           00007000
708      C
709      C
710      C      IF NO POINT SOURCES, SKIP POINT SOURCE CALCULATIONS. 00007010
711      C      IF(NPS.LT.1) GO TO 603                                00007020
712      C
713      C
714      C
715      C *** P O I N T   S O U R C E   C A L C U L A T I O N S   *** 00007030
716      C
717      C      LOOP THROUGH ALL POINT SOURCES.                         00007040
718      DO 600 I=1,NPS
719      IF((NWDOPT.GT.1.AND.IWDOPT.GT.1).OR.NTOPT.EQ.2) GO TO 246 00007050
720      IF(NPRINT.EQ.0) GO TO 246                                00007060
721      IF((I-1)/50*50.NE.I-1) GO TO 246                          00007070
722      WRITE(IWR,1005) TT,ISCEN,HMIX(ISCEN),HPEN                00007080
723      WRITE(IWR,1007)
724      246   IPS=I
725      IF(HP(I).GE.HMIX(ISCEN)) GO TO 600
726      IRISE=2
727      IBUOY=1
728      EFF= 2.45*VP(I)*DP(I)*DP(I)*(TP(I)-TA(ISCEN))/TP(I) 00007090
729      IF(EFF.LT.0.) EFF=1.0E-7
730
731      C      CALCULATE INVERSE WIND SPEED (UINV) AT THE PHYSICAL HEIGHT (HP(I)) 00007100
732      C      OF POINT SOURCE I. DO NOT CHANGE IF STACK HEIGHT IS LESS 00007110
733      C      THAN 10 METERS.                                         00007120
734
735      C      UINV = 1./WS(ISCEN)                                     00007130
736      C      IF(HP(I).GT.10.) UINV = UINV*((10./HP(I))**P(ISC)) 00007140
737      C      UPL=1./UINV
738      C      UINV1=UINV/100.                                         00007150
739      C      DEFINE EMISSION RATES (SOURCE STRENGTHS) OF POLLUTANT SPECIES, 00007160
740      C      AND NONDIMENSIONAL DEPOSITION AND SEDIMENTATION PARAMETERS. 00007170
741      C
742      C      ISPEC = 1 OR 2 OR 3
743      C      Q1=EP(I,1)
744      C      VDC1=VD1*UINV1
745      C      WC1=W1*UINV1
746      C      V11=VDC1-0.5*WC1
747      C      V21=VDC1-WC1
748      C      IF(V21.EQ.0.) GO TO 48
749      C      R11=V11/V21
750      C      R21=0.5*WC1/V21
751      C      48 IF(ISPEC.EQ.1) GO TO 50
752
753      C
754      C      ISPEC = 2 OR 3
755      C      Q2=EP(I,2)
756      C      VDC2=VD2*UINV1
757      C      WC2=W2*UINV1
758      C      V12=VDC2-0.5*WC2
759      C      V22=VDC2-WC2
760      C      IF(V22.EQ.0.) GO TO 49
761      C      R12=V12/V22
762      C      R22=0.5*WC2/V22
763      C      49 IF(ISPEC.EQ.2) GO TO 51
764
765      C      ISPEC = 3
766      C      IF(Q1.EQ.0.) Q1=1.E-6
767      C      Q2Q1=Q2/Q1
768      C      V13=V11-0.5*(WC1-WC2)
769      C      IF(V21.EQ.0.) GO TO 50

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770      R13=V13/V21          00007690
771      R23=0.5*WC2/V21      00007700
772      C                   00007710
773      C   ISPEC = 1 OR 3    00007720
774      50 UTAUC=TAUC*UPL   00007730
775      C                   00007740
776      51 KLID=0           00007750
777      C                   00007760
778      C                   00007770
779      C *** PEAK EFFECTIVE SOURCE HEIGHT CALCULATIONS. 00007780
780      C                   00007790
781      IF(ISC.LT.6) GO TO 247 00007800
782      C                   00007810
783      C DETERMINE WHETHER PLUME IS MOMENTUM-DOMINATED (IBUOY=0), 00007820
784      C                      OR BUOYANCY-DOMINATED (IBUOY=1). 00007830
785      C                   00007840
786      C                   00007850
787      C                   00007860
788      C                   00007870
789      IF(ISC.EQ.6) BRIGC=115.28 00007880
790      IF(ISC.EQ.7) BRIGC=87.14 00007890
791      IF(VP(I).GT.BRIGC*(TP(I)-TA(ISCEN))*SQRT(TA(ISCEN))/TP(I)) IBUOY=000007900
792      GO TO 249             00007910
793      247 AF= 21.425         00007920
794      BF= 0.75              00007930
795      IF(EFF.LT.55.) GO TO 248 00007940
796      AF= 38.710            00007950
797      BF= 0.6                00007960
798      248 IF(3.*VP(I)*DP(I).GT.AF*EFF**BF) IBUOY=0 00007970
799      249 CONTINUE           00007980
800      C                   00007990
801      C CALL SUBROUTINE RISE WITH IRISE=2 TO GET PEAK EFFECTIVE SOURCE 00008000
802      C HEIGHT, ESH(2).          00008010
803      C                   00008020
804      C *****          00008030
805      CALL RISE             00008040
806      C *****          00008050
807      IRISE=1               00008060
808      IF(NPRINT.EQ.0) GO TO 1250 00008070
809      IF(NWDOPT.LE.1.OR.IDOPT.LE.1) WRITE(IWR,1010) 00008080
810      1 I,XP(I),YP(I),EP(I,1),EP(I,2),HP(I),DP(I),VP(I),TP(I), 00008090
811      2 PRL(1,IBUOY+1),PRL(2,IBUOY+1),DWL(IDWN),DWL(IDWN+1),UPL,ESH(2) 00008100
812      C                   00008110
813      C CALCULATE DISTANCE AT WHICH PLUME REACHES MAXIMUM HEIGHT (PEAK). 00008120
814      C                   00008130
815      1250 IF(IBUOY.EQ.0) GO TO 252 00008140
816      IF(ISC.LT.6) GO TO 250 00008150
817      PEAK=0.00207148/(UINV*SQRT(DTDZ(ISC-5)*9.8/TA(ISCEN))) 00008160
818      GO TO 253             00008170
819      250 PEAK=0.001*X5        00008180
820      GO TO 253             00008190
821      252 PEAK= 0.             00008200
822      IF(ISC.GE.6) GO TO 253 00008210
823      IF(ABS(VP(I)).LT..000001) GO TO 253 00008220
824      PEAK=(0.004*UINV*(DP(I)*(VP(I) + 3./UINV)**2)/VP(I) 00008230
825      C                   00008240
826      C IF MAXIMUM EFFECTIVE SOURCE HEIGHT EXCEEDS HPEN, PLUME ESCAPES 00008250
827      C THE MIXING LAYER, AND SOURCE IS IGNORED.          00008260
828      C                   00008270
829      253 IF(ESH(2).GT.HPEN) GO TO 600 00008280
830      C                   00008290
831      C IF MAXIMUM EFFECTIVE SOURCE HEIGHT EXCEEDS MIXING HEIGHT BUT 00008300
832      C NOT HPEN, PLUME DOES NOT ESCAPE THE MIXING LAYER, AND MAXIMUM 00008310
833      C EFFECTIVE SOURCE HEIGHT IS SET EQUAL TO THE MIXING HEIGHT. 00008320
834      C                   00008330
835      IF(ESH(2).GT.HMIX(ISCEN)) ESH(2)=HMIX(ISCEN) 00008340
836      C                   00008350
837      C                   00008360
838      C SET LIMITS (XMIN,XMAX,YMIN,YMAX) ON PORTION OF RECEPTOR GRID 00008370
839      C EXAMINED FOR EACH SOURCE. THE EXTENT OF THIS PORTION DEPENDS 00008380
840      C ON SOURCE LOCATION, GRID DIMENSIONS, AND WIND DIRECTION. 00008390
841      C                   00008400
842      275 XMAX= XB2          00008410
843      XMIN= XB1          00008420
844      YMAX= YB2          00008430
845      YMIN= YB1          00008440
846      IF(XP(I)+60.0.LT.XB2) XMAX= XP(I) + 60. 00008450

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847      IF(XP(I)-60.0.GT.XB1) XMIN= XP(I) - 60.          00008460
848      IF(YP(I)+60.0.LT.YB2) YMAX= YP(I) + 60.          00008470
849      IF(YP(I)-60.0.GT.YB1) YMIN= YP(I) - 60.          00008480
850      GO TO (280,285,290,295,300,305,310,315),IFLAG  00008490
851      280   IF(WDPANG.GT.3.14)GOTO282                00008500
852      IF(WDMANG.LT.0)GOTO284                  00008510
853      YMIN=YP(I)                                00008520
854      XL1=XP(I)+(YB2-YP(I))/TAN(WDPANG)        00008530
855      IF(XL1.GT.XMIN)XMIN=XL1                  00008540
856      IF(XL1.GT.XP(I))XMIN=XP(I)              00008550
857      XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG)        00008560
858      IF(XL2.LT.XMAX)XMAX=XL2                  00008570
859      IF(XL2.LT.XP(I))XMAX=XP(I)              00008580
860      GOTO320                                00008590
861      282   YMIN=YP(I)+(XB1-XP(I))*TAN(WDPANG)    00008600
862      XMAX=XP(I)+(YB2-YP(I))/TAN(WDMANG)        00008610
863      GOTO320                                00008620
864      284   YMIN=YP(I)+(XB2-XP(I))*TAN(WDMANG)    00008630
865      XMIN=XP(I)+(YB2-YP(I))/TAN(WDPANG)        00008640
866      GOTO320                                00008650
867      285   XL1=XP(I)+(YB2-YP(I))/TAN(WDPANG)    00008660
868      IF(XL1.GT.XMIN)XMIN=XL1                  00008670
869      IF(XL1.GT.XP(I))XMIN=XP(I)              00008680
870      YL1=YP(I)+(XB2-XP(I))*TAN(WDMANG)        00008690
871      IF(YL1.GT.YMIN)YMIN=YL1                  00008700
872      IF(YL1.GT.YP(I))YMIN=YP(I)              00008710
873      GOTO320                                00008720
874      290   IF(WDPANG.GT.1.57.AND.WDMANG.LT.0.)GOTO292 00008730
875      IF(WDPANG.GT.6.28.AND.WDMANG.LT.4.712)GOTO294 00008740
876      XMIN=XP(I)                                00008750
877      YL1=YP(I)+(XB2-XP(I))*TAN(WDMANG)        00008760
878      IF(YL1.GT.YMIN)YMIN=YL1                  00008770
879      IF(YL1.GT.YP(I))YMIN=YP(I)              00008780
880      YL2=YP(I)+(XB2-XP(I))*TAN(WDPANG)        00008790
881      IF(YL2.LT.YMAX)YMAX=YL2                  00008800
882      IF(YL2.LT.YP(I))YMAX=YP(I)              00008810
883      GOTO320                                00008820
884      292   YMIN=YP(I)+(XB2-XP(I))*TAN(WDMANG)    00008830
885      XMIN=XP(I)+(YB2-YP(I))/TAN(WDPANG)        00008840
886      GOTO320                                00008850
887      294   XMIN=XP(I)+(YB1-YP(I))/TAN(WDMANG)    00008860
888      YMAX=YP(I)+(XB2-XP(I))*TAN(WDPANG)        00008870
889      GOTO320                                00008880
890      295   XL1=XP(I)+(YB1-YP(I))/TAN(WDMANG)    00008890
891      IF(XL1.GT.XMIN)XMIN=XL1                  00008900
892      IF(XL1.GT.XP(I))XMIN=XP(I)              00008910
893      YL2=YP(I)+(XB2-XP(I))*TAN(WDPANG)        00008920
894      IF(YL2.LT.YMAX)YMAX=YL2                  00008930
895      IF(YL2.LT.YP(I))YMAX=YP(I)              00008940
896      GOTO320                                00008950
897      300   IF(WDPANG.GT.6.28)GOTO302            00008960
898      IF(WDMANG.LT.3.14)GOTO304                00008970
899      YMAX=YP(I)                                00008980
900      XL1=XP(I)+(YB1-YP(I))/TAN(WDMANG)        00008990
901      IF(XL1.GT.XMIN)XMIN=XL1                  00009000
902      IF(XL1.GT.XP(I))XMIN=XP(I)              00009010
903      XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)        00009020
904      IF(XL2.LT.XMAX)XMAX=XL2                  00009030
905      IF(XL2.LT.XP(I))XMAX=XP(I)              00009040
906      GOTO320                                00009050
907      302   YMAX=YP(I)+(XB2-XP(I))*TAN(WDPANG)    00009060
908      XMIN=XP(I)+(YB1-YP(I))/TAN(WDMANG)        00009070
909      GOTO320                                00009080
910      304   YMAX=YP(I)+(XB1-XP(I))*TAN(WDMANG)    00009090
911      XMAN=XP(I)+(YB1-YP(I))/TAN(WDPANG)        00009100
912      GOTO320                                00009110
913      305   YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG)    00009120
914      IF(YL2.LT.YMAX)YMAX=YL2                  00009130
915      IF(YL2.LT.YP(I))YMAX=YP(I)              00009140
916      XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)        00009150
917      IF(XL2.LT.XMAX)XMAX=XL2                  00009160
918      IF(XL2.LT.XP(I))XMAX=XP(I)              00009170
919      GOTO320                                00009180
920      310   IF(WDMANG.LT.1.57)GOTO312            00009190
921      IF(WDPANG.GT.4.712)GOTO314                00009200
922      XMAX=XP(I)                                00009210
923      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG)        00009220

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924      IF(YL1.GT.YMIN)YMIN=YL1          00009230
925      IF(YL1.GT.YP(I))YMIN=YP(I)    00009240
926      YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG) 00009250
927      IF(YL2.LT.YMAX)YMAX=YL2        00009260
928      IF(YL2.LT.YP(I))YMAX=YP(I)    00009270
929      GOTO320                      00009280
930      312   XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG) 00009290
931      IF(XL2.LT.XMAX)XMAX=XL2       00009300
932      IF(XL2.LT.XP(I))XMAX=XP(I)    00009310
933      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG) 00009320
934      IF(YL1.GT.YMIN)YMIN=YL1        00009330
935      IF(YL1.GT.YP(I))YMIN=YP(I)    00009340
936      GOTO320                      00009350
937      314   XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG) 00009360
938      IF(XL2.LT.XMAX)XMAX=XL2       00009370
939      IF(XL2.LT.XP(I))XMAX=XP(I)    00009380
940      YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG) 00009390
941      IF(YL2.LT.YMAX)YMAX=YL2        00009400
942      IF(YL2.LT.YP(I))YMAX=YP(I)    00009410
943      GOTO320                      00009420
944      315   XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG) 00009430
945      IF(XL2.LT.XMAX)XMAX=XL2       00009440
946      IF(XL2.LT.XP(I))XMAX=XP(I)    00009450
947      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG) 00009460
948      IF(YL1.GT.YMIN)YMIN=YL1        00009470
949      IF(YL1.GT.YP(I))YMIN=YP(I)    00009480
950      GOTO320                      00009490
951      320   IF(XMIN.GT.XB2.OR.XMAX.LT.XB1.OR.YMIN.GT.YB2.OR.YMAX.LT.YB1) 00009500
952      1 GO TO 600                  00009510
953      IF(XMIN.LT.XB1) XMIN=XB1       00009520
954      IF(XMAX.GT.XB2) XMAX=XB2       00009530
955      IF(YMIN.LT.YB1) YMIN=YB1       00009540
956      IF(YMAX.GT.YB2) YMAX=YB2       00009550
957      C
958      C DETERMINE THE RANGE OF RECEPTOR GRID ROW AND COLUMN NUMBERS (LXMAX, 00009570
959      C LXMIN, LYMAX, LYMIN) CORRESPONDING TO XMAX, ETC. ABOVE - 00009580
960      C
961      LXMAX=(XMAX-XSWC)/GRID + 1. 00009590
962      LXMIN= (XMIN-XSWC)/GRID + 1. 00009600
963      LYMAX= (YMAX-YSWC)/GRID + 1. 00009610
964      LYMIN= (YMIN-YSWC)/GRID + 1. 00009620
965      C
966      C START LOOP ON ALL AFFECTED RECEPTORS. 00009630
967      DO 500 IX=LXMIN,LXMAX          00009640
968      XI=IX                         00009650
969      XG= XSWC + (XI-0.5)*GRID      00009660
970      XD= XG - XP(I) + 0.00001     00009670
971      XDSQ=XD*XD                   00009680
972      DO 500 JY=LYMIN,LYMAX         00009690
973      YJ=JY                         00009700
974      YG= YSWC + (YJ-0.5)*GRID      00009710
975      YD= YG - YP(I) + 0.00001     00009720
976      C DSQ= SQUARE OF SOURCE-RECEPTOR DISTANCE. IF SOURCE-RECEPTOR DISTANCE 00009730
977      C IS GREATER THAN 60 KM., RECEPTOR IS SKIPPED. 00009740
978      DSQ= XDSQ + YD*YD             00009750
979      IF(DSQ.GT.3600.) GO TO 500     00009760
980      DELTA= ATAN(XD/YD)            00009770
981      IF(DELTA.LT.0.) DELTA = DELTA + 3.1415927 00009780
982      IF(XD.LT.0.) DELTA = DELTA + 3.1415927 00009790
983      DELTA= ABS(DELTA - WVEC)      00009800
984      IF(DELTA.GT.3.1415927) DELTA= ABS(6.2831853 - DELTA) 00009810
985      C IF THE CROSSWIND ANGLE (DELTA) EXCEEDS A LIMITING VALUE WHICH 00009820
986      C DEPENDS ON STABILITY CLASS (ANGLIM), THE RECEPTOR IS SKIPPED. 00009830
987      C ANGLIM = 35,28,21,14,14,10.5,AND 7.0 DEGREES FOR 1-HOUR 00009840
988      C FOR STABILITY CLASSES A, B, C, DD, DN, E, AND F RESPECTIVELY. 00009850
989      C
990      IF(DELTA.GT.ANGLIM(ISC)) GO TO 500 00009860
991      C DELTA IS THE ANGLE BETWEEN THE WIND VECTOR AND THE SOURCE-RECEPTOR 00009870
992      C DIRECTION. THE DOWNWIND DISTANCE USED IN THE GAUSSIAN PLUME 00009880
993      C EQUATION IS= DIST= SQRT(DSQ)*COS(DELTA). 00009890
994      DIST=SQRT(DSQ)*COS(DELTA)        00009900
995      IF(DIST.LT.0.002) GO TO 500     00009910
996      C
997      C
998      C *** DETERMINE PROBABILITY DENSITY OF CROSSWIND DISTRIBUTION 00009920
999      C OF CONCENTRATIONS. 00009930
1000     C

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1001      XM=DIST*1000.          00010000
1002      IF(XM.GE.10000.) GO TO 323 00010010
1003      SIGY=CX1(ISC)*(XM**DX1(ISC)) 00010020
1004      GO TO 324 00010030
1005      323 SIGY=CX2(ISC)*(XM**DX2(ISC)) 00010040
1006      324 YM=XM*TAN(DELTA) 00010050
1007      DUMY=YM/SIGY 00010060
1008      ARG=0.5*DUMY*DUMY 00010070
1009      IF(ARG.GE.EXPMIN) GO TO 325 00010080
1010      EXPX=EXP(-ARG) 00010090
1011      GO TO 326 00010100
1012      325 EXPX=1. 00010110
1013      326 PYC=(A1B/SIGY)*EXPA 00010120
1014      C 00010130
1015      C 00010140
1016      C *** DETERMINE PROBABILITY DENSITIES OF VERTICAL DISTRIBUTIONS 00010150
1017      C OF SPECIES-1 AND SPECIES-2 POLLUTANT CONCENTRATIONS. 00010160
1018      C 00010170
1019      IF(DIST.GT.D47) GO TO 330 00010180
1020      C ***** NEAR-SOURCE REGION (DIST .LE. D47). 00010190
1021      C CALCULATE QZC1 AND QZC2 FROM QZCAL (MODULE M=1). 00010200
1022      C ***** 00010210
1023      CALL QZCAL 00010220
1024      C ***** 00010230
1025      GO TO 350 00010240
1026      C 00010250
1027      330 IF(DIST.LT.D80) GO TO 331 00010260
1028      C ***** WELL-MIXED REGION (DIST .GE. D80). 00010270
1029      C CALCULATE QZC1 AND QZC2 FROM QZCAL (MODULE M=2). 00010280
1030      C ***** 00010290
1031      CALL QZCAL 00010300
1032      C ***** 00010310
1033      GO TO 350 00010320
1034      C 00010330
1035      331 IF(KLID.EQ.1) GO TO 337 00010340
1036      C CALCULATE QZC1 AND QZC2 FOR POLLUTANT SPECIES 00010350
1037      C AT DIST=D47 AND DIST=D80 FOR USE IN INTERPOLATION 00010360
1038      C IN PLUME-TRAPPING REGION. 00010370
1039      DUMX=DIST 00010380
1040      DIST=D47 00010390
1041      C ***** 00010400
1042      CALL QZCAL 00010410
1043      C ***** 00010420
1044      QZC11=QZC1 00010430
1045      IF(ISPEC.EQ.1) GO TO 332 00010440
1046      QZC21=QZC2 00010450
1047      C 00010460
1048      332 DIST=D80 00010470
1049      C ***** 00010480
1050      CALL QZCAL 00010490
1051      C ***** 00010500
1052      QZC12=QZC1 00010510
1053      IRC1=1 00010520
1054      IF(QZC11.EQ.0.OR.QZC12.EQ.0.) IRC1=0 00010530
1055      IF(ISPEC.EQ.1) GO TO 333 00010540
1056      QZC22=QZC2 00010550
1057      IRC2=1 00010560
1058      IF(QZC21.EQ.0.OR.QZC22.EQ.0.) IRC2=0 00010570
1059      C 00010580
1060      333 KLID=1 00010590
1061      DIST=DUMX 00010600
1062      IF(IRC1.EQ.0) GO TO 334 00010610
1063      DIFX1=ALOG(D80/D47) 00010620
1064      DIFC1=ALOG(QZC12/QZC11) 00010630
1065      GO TO 335 00010640
1066      334 DIFC1=QZC12-QZC11 00010650
1067      335 IF(ISPEC.EQ.1) GO TO 337 00010660
1068      IF(IRC2.EQ.0) GO TO 336 00010670
1069      DIFX2=ALOG(D80/D47) 00010680
1070      DIFC2=ALOG(QZC22/QZC21) 00010690
1071      GO TO 337 00010700
1072      336 DIFC2=QZC22-QZC21 00010710
1073      C 00010720
1074      C ***** PLUME-TRAPPING REGION (D47 < DIST < D80). 00010730
1075      C CALCULATE QZC1 AND QZC2 BY LINEAR INTERPOLATION 00010740
1076      C (BETWEEN VALUES AT DIST=D47 AND DIST=D80) ON 00010750
1077      C A LOG-LOG PLOT OF QZC VERSUS DOWNWIND DISTANCE. 00010760

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1078 C      IF EITHER OF THE QZC VALUES AT D47 AND D80 ARE          00010770
1079 C      ZERO, USE A LINEAR PLOT FOR INTERPOLATION.          00010780
1080 337 IF(IRC1.EQ.0) GO TO 338                                00010790
1081 RATX1=ALOG(DIST/D47)/DIFX1                                00010800
1082 QZC1L=ALOG(QZC11)+RATX1*DIFC1                            00010810
1083 QZC1=EXP(QZC1L)                                         00010820
1084 GO TO 339                                              00010830
1085 338 RATX1=(DIST-D47)/D8047                            00010840
1086 QZC1=QZC11+RATX1*DIFC1                            00010850
1087 339 IF(ISPEC.EQ.1) GO TO 350                            00010860
1088 C
1089      IF(IRC2.EQ.0) GO TO 340                            00010870
1090 RATX2=ALOG(DIST/D47)/DIFX2                            00010880
1091 QZC2L=ALOG(QZC21)+RATX2*DIFC2                            00010890
1092 QZC2=EXP(QZC2L)                                         00010900
1093 GO TO 350                                              00010910
1094 340 RATX2=(DIST-D47)/D8047                            00010920
1095 QZC2=QZC21+RATX2*DIFC2                            00010930
1096 C
1097 C
1098 C
1099 C      CALCULATE GROUND-LEVEL CONCENTRATIONS CONC (MICROGRAMS PER CUBIC 00010980
1100 C      METER) AND SURFACE DEPOSITION FLUX SDF (MICROGRAMS PER SQUARE 00010990
1101 C      METER PER HOUR) OF POLLUTANTS AT RECEPTOR IN COLUMN IX, ROW JY 00011000
1102 C      OF THE RECEPTOR GRID DUE TO POINT SOURCE I.          00011010
1103 C
1104 C      ISPEC = 1 OR 2 OR 3                                00011020
1105 350 C1=Q1*UINV*PYC*QZC1                                00011030
1106 IF(NCSOPT.EQ.0) GO TO 355                            00011040
1107 CALL WORST(IX,JY,C1)                                00011050
1108 IF(NTOPT.GT.1) CONC(IX,JY,2)=CONC(IX,JY,2) + C1    00011060
1109 355 CINC1=C1*STCONV                                00011070
1110 CONC(IX,JY,1)=CONC(IX,JY,1)+CINC1                  00011080
1111 SDF(IX,JY,1)=SDF(IX,JY,1)+VD136*CINC1            00011090
1112 IF(ISPEC.EQ.1) GO TO 370                            00011100
1113 IF(ISPEC.EQ.3) GO TO 360                            00011110
1114 C
1115 C      ISPEC = 2                                00011120
1116 C2=Q2*UINV*PYC*QZC2                                00011130
1117 GO TO 365                                              00011140
1118 C
1119 C      ISPEC = 3                                00011150
1120 360 C2=Q1*UINV*PYC*QZC2                                00011160
1121 C
1122 365 CINC2=C2*STCONV                                00011170
1123 CONC(IX,JY,2)=CONC(IX,JY,2)+CINC2                  00011180
1124 SDF(IX,JY,2)=SDF(IX,JY,2)+VD236*CINC2            00011190
1125 370 CONTINUE                                         00011200
1126 C
1127 500 CONTINUE                                         00011210
1128 C      END LOOP ON ALL AFFECTED RECEPTORS.          00011220
1129 C
1130 600 CONTINUE                                         00011230
1131 C      END LOOP ON ALL POINT SOURCES.          00011240
1132 C
1133 C
1134 C
1135 C      *** PRINT OUTPUT.                         00011250
1136 C
1137 C      OUTPUT AT END OF EACH SCENARIO OR SUB-SCENARIO 00011260
1138 C
1139 C      TIME AVERAGING: NTOPT=2 OR 3                00011270
1140 C      AT END OF EACH SCENARIO, CALL WROUT TO PRINT OUTPUT FOR 00011280
1141 C      NCSOPT OPTION.                           00011290
1142 C      IF LAST SCENARIO, CALL OUTMOD TO PRINT OUTPUT FOR NLIST, NTAPE, 00011300
1143 C      AND NARRAY OPTIONS. CALL MAXOUT TO PRINT OUTPUT FOR NMAX. 00011310
1144 C      OTHERWISE, GO TO 100 FOR THE NEXT SCENARIO. 00011320
1145 C
1146 C      NO TIME AVERAGING: NTOPT=1                00011330
1147 C      AT END OF EACH SCENARIO (OR SUB-SCENARIO WHEN NWDOPT.GT.1), 00011340
1148 C      CALL OUTMOD TO PRINT OUTPUT FOR NCSOPT, NLIST, NTAPE, 00011350
1149 C      AND NARRAY OPTIONS.                         00011360
1150 C      IF LAST SCENARIO (AND LAST SUB-SCENARIO WHEN NWDOPT.GT.1), 00011370
1151 C      CALL MAXOUT TO PRINT OUTPUT FOR NMAX OPTION. 00011380
1152 C      OTHERWISE, GO TO 100 FOR THE THE NEXT SCENARIO OR SUB-SCENARIO 00011390
1153 C
1154 603 IF(NTOPT.EQ.1) GO TO 620                      00011400

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1155      C          TIME AVERAGING: NTOPT=2 OR 3          00011540
1156      C          IF(NCSOPT.GT.0) CALL WOROUT          00011550
1157      C          IF(ISCEN.NE.NSCEN) GO TO 100          00011560
1158          IF(NCSOPT.GT.0) CALL WOROUT          00011570
1159          IF(ISCEN.NE.NSCEN) GO TO 100          00011580
1160          CALL OUTMOD          00011590
1161          GO TO 999          00011600
1162      C          NO TIME AVERAGING: NTOPT=1          00011610
1163      C          IF(NCSOPT.EQ.0) GO TO 100          00011620
1164      C          CALL OUTMOD          00011630
1165          620 CALL OUTMOD          00011640
1166          IF(ISCEN.NE.NSCEN) GO TO 100          00011650
1167          IF(NWDOPT.LE.1) GO TO 999          00011660
1168          IF(IWDOPT.LT.4) GO TO 100          00011670
1169      C          999 IF(NMAX.GT.0) CALL MAXOUT          00011680
1170      C          STOP          00011690
1171      C          00011700
1172          STOP          00011710
1173      C          00011720
1174      C          00011730
1175          1005 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'//4X,'OUTPUT: ',20A4// 00011740
1176          14X,'SCENARIO',I2,4X,'POINT SOURCE PLUME RISE CALCULATIONS'/ 00011750
1177          221X,'MIXING HEIGHT: HMIX=',F7.2,' M'/
1178          321X,'IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN ',F7.1, 00011760
1179          4' M, THE SOURCE IS IGNORED'/
1180          1007 FORMAT(14X,'SOURCE',8X,'EMISSION RATES',61X,'WIND SPEED AT',4X, 00011770
1181          1 'MAXIMUM'/' POINT',6X,'COORDINATES',4X,'POL-1',6X,'POL-2',4X, 00011780
1182          2 'HEIGHT DIAMETER EXIT VEL EXIT TEMP',6X,'DOMINANT',5X, 00011790
1183          3 'STACK HEIGHT',4X,'EFFECTIVE'/' SOURCE',3X,'X(KM)',4X,'Y(KM)',3X,00011800
1184          4 '(G/S)',6X,'(G/S)',5X,'(M)',6X,'(M)',7X,'(M/S)',4X,'(DEG K)',6X, 00011810
1185          5 'INFLUENCE',8X,'(M/S)',6X,'SOURCE HEIGHT(M)')/ 00011820
1186          1010 FORMAT(1X,I4,2X,F8.2,1X,F8.2,2X,F8.2,2X,F8.2,3X,F7.2,3X,F6.3,3X, 00011830
1187          1 F8.3,3X,F7.2,2X,2A4,1X,2A4,3X,F7.3,8X,F8.2) 00011840
1188          END          00011850
1189      C          00011860
1190      C          00011870
1191      C          SUBROUTINE QZCAL          00011880
1192      C          SUBROUTINE QZCAL (VERSION 82360), PART OF PEM. 00011890
1193          00011900
1194          00011910
1195          00011920
1196          00011930
1197          C          SUBROUTINE QZCAL CALCULATES QZC1 AND QZC2, REPRESENTING THE 00011940
1198          C          PROBABILITY DENSITIES OF VERTICAL DISTRIBUTIONS OF CONCENTRATIONS 00011950
1199          C          OF POLLUTANT SPECIES 1 AND 2, RESPECTIVELY, AT A GIVEN 00011960
1200          C          DISTANCE DOWNWIND OF A POINT SOURCE. 00011970
1201          C          00011980
1202          C          00011990
1203          C          *** PEM ALGORITHMS AND PROGRAM DEVELOPMENT: ---DECEMBER 1982 00012000
1204          C          00012010
1205          C          K. SHANKAR RAO, PHYSICAL RESEARCH SCIENTIST 00012020
1206          C          ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL) 00012030
1207          C          NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION (NOAA) 00012040
1208          C          U.S. DEPARTMENT OF COMMERCE, P.O. BOX - E 00012050
1209          C          OAK RIDGE, TENNESSEE 37830 00012060
1210          C          PHONE: (615) 576-1238 00012070
1211          C          FTS: 626-1238 00012080
1212          C          00012090
1213          C          { THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT 00012100
1214          C          BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE 00012110
1215          C          NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION ) 00012120
1216          C          00012130
1217          C          00012140
1218          C          00012150
1219          C          COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00012160
1220          1 XPC(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00012170
1221          2 XA(50),YA(50),EA(50,2),SIZE(50), 00012180
1222          3 WD(24),WS(24),TA(24),HMIX(24),PEN(24), 00012190
1223          4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00012200
1224          5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLNAM(3,2),CALNAM(7,2), 00012210
1225          6 ITA,IRD,IWR,IDSX, D80,047,D8047,DIST,DELTA, 00012220
1226          7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS, UINV,WVEC, 00012230
1227          8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS, 00012240
1228          9 NTOPT,NWDOPT,NNSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX, 00012250
1229          * NSTDWN,INTER,NPRINT 00012260
1230          COMMON/PARM1/NPOL,ICT,V01,W1,V02,W2,TAUC 00012270
1231          COMMON/PARM1A/GAMMA 00012280
1232          COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT 00012290
1233          00012300

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1232      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2          00012310
1233      COMMON/PARM4/V11,V21,V12,V22,V13          00012320
1234      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6 00012330
1235      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42 00012340
1236      COMMON/PARM7/QZC1,QZC2                    00012350
1237      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C        00012360
1238      COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW    00012370
1239      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX        00012380
1240      EXTERNAL FUN1                            00012390
1241      REAL*8 FUN1                             00012400
1242      REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR 00012410
1243      DIMENSION IW(102)                         00012420
1244      C                                         00012430
1245      C                                         00012440
1246      C                                         00012450
1247      IF(DIST.GE.PEAK) GO TO 5                 00012460
1248      C                                         00012470
1249      C CALL SUBROUTINE RISE FOR EFFECTIVE SOURCE HEIGHT AT DOWNWIND 00012480
1250      C DISTANCE = DIST, LESS THAN DISTANCE TO MAXIMUM HEIGHT (PEAK). 00012490
1251      C *****CALL RISE*****                      00012500
1252      C *****HGT= ESH(1)*****                     00012510
1253      C *****HGT= ESH(2)*****                     00012520
1254      C *****JD=2*****                           00012530
1255      C *****GO TO 6*****                        00012540
1256      C                                         00012550
1257      C USE MAXIMUM EFFECTIVE SOURCE HEIGHT, SINCE DOWNWIND DISTANCE 00012560
1258      C EXCEEDS THE DISTANCE TO MAXIMUM HEIGHT.       00012570
1259      5   HGT= ESH(2)                           00012580
1260      6   JD=2                                00012590
1261      IF(DIST.LT.0.5) JD=1                   00012600
1262      IF(DIST.GT.5.0) JD=3                   00012610
1263      C                                         00012620
1264      C                                         00012630
1265      HL=HMMIX(ISCEN)                         00012640
1266      X=DIST                                 00012650
1267      XM=X*1000.                            00012660
1268      SIGZ= AX(ISC,JD)*(XM**BX(ISC,JD))       00012670
1269      IF(SIGZ.GT.5000.) SIGZ=5000.            00012680
1270      SZ=SIGZ                               00012690
1271      C2=SQRT2*SZ                            00012700
1272      HC=HGT/C2                            00012710
1273      XC=XM/C2                            00012720
1274      C                                         00012730
1275      C ISPEC = 1 OR 2 OR 3                  00012740
1276      D31=2.*V11*XC                          00012750
1277      D11=WC1*XC                           00012760
1278      D21=D11*D11                           00012770
1279      R31=1..+2.*D21                          00012780
1280      R41=2.*D11/SQPI                         00012790
1281      IF(ISPEC.EQ.1) GO TO 9                 00012800
1282      C                                         00012810
1283      C ISPEC = 2 OR 3                      00012820
1284      D32=2.*V12*XC                          00012830
1285      D12=WC2*XC                           00012840
1286      D22=D12*D12                           00012850
1287      R32=1..+2.*D22                          00012860
1288      R42=2.*D12/SQPI                         00012870
1289      IF(ISPEC.EQ.2) GO TO 10                00012880
1290      C                                         00012890
1291      C ISPEC = 3                           00012900
1292      D33=2.*V13*XC                          00012910
1293      D6=4.*SQPI*(V21-V22)*XC              00012920
1294      C                                         00012930
1295      9 TCC=UTAUC/C2                         00012940
1296      10 IF(ICK.EQ.0) XCT=0.                  00012950
1297      IF(ICK.EQ.1) XCT=XC/TCC               00012960
1298      EXCT=EXP(-XCT)                         00012970
1299      C                                         00012980
1300      TERM1=0.                             00012990
1301      TERM2=0.                             00013000
1302      TERM3=0.                             00013010
1303      C                                         00013020
1304      DUM1=D47+0.001                         00013030
1305      DUM2=D80-0.001                         00013040
1306      IF(X.LT.DUM1) GO TO 100               00013050
1307      IF(X.GT.DUM2) GO TO 200               00013060
1308      C                                         00013070

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1309      11 QZC1=0.0          00013080
1310      QZC2=0.0          00013090
1311      RETURN            00013100
1312      C                  00013110
1313      C                  00013120
1314      C ***** NEAR-SOURCE REGION (X .LE. D47). 00013130
1315      C                  00013140
1316      100 M=1           00013150
1317      A1=A1B/SZ         00013160
1318      C3=HC*HC          00013170
1319      IF(C3.GE.EXPMIN) GO TO 11 00013180
1320      A2=1./EXP(C3)     00013190
1321      C                  00013200
1322      C ISPEC = 1 OR 2 OR 3 00013210
1323      C SPECIES-1 (PRIMARY) POLLUTANT: GAS OR PARTICLES. 00013220
1324      ETA1=HC+D31       00013230
1325      ETA1SQ=ETA1*ETA1  00013240
1326      IF(ETA1SQ.GT.EXPMAX) CALL ARGCHK(ETA1,ETA1SQ) 00013250
1327      B11=EXP(ETA1SQ)*ERFC(ETA1) 00013260
1328      ALPHA1=A1C*D31*B11 00013270
1329      SUM=2.-ALPHA1      00013280
1330      IF(SUM) 115,115,116 00013290
1331      115 G21P=0.0       00013300
1332      GO TO 120         00013310
1333      116 IF(WC1.EQ.0.) GO TO 117 00013320
1334      BETA1=-2.*D11*HC+D21 00013330
1335      CALL EXPO(-BETA1,EBT1) 00013340
1336      GO TO 118         00013350
1337      117 EBT1=1.0       00013360
1338      118 G21P=EXCT*EBT1*A2*SUM 00013370
1339      120 QZC1=A1*G21P 00013380
1340      IF(ISPEC.EQ.1) RETURN 00013390
1341      C                  00013400
1342      C                  00013410
1343      C ISPEC = 2 OR 3   00013420
1344      C SPECIES-2 (SECONDARY) POLLUTANT: GAS OR PARTICLES. 00013430
1345      ETA2=HC+D32       00013440
1346      ETA2SQ=ETA2*ETA2  00013450
1347      IF(ETA2SQ.GT.EXPMAX) CALL ARGCHK(ETA2,ETA2SQ) 00013460
1348      B12=EXP(ETA2SQ)*ERFC(ETA2) 00013470
1349      ALPHA2=A1C*D32*B12 00013480
1350      SUM1=2.-ALPHA2    00013490
1351      IF(ISPEC.EQ.3) GO TO 145 00013500
1352      C                  00013510
1353      C ISPEC = 2       00013520
1354      IF(SUM1) 135,135,140 00013530
1355      135 G22P=0.0       00013540
1356      QZC2=0.0          00013550
1357      RETURN            00013560
1358      140 IF(WC2.EQ.0.) GO TO 141 00013570
1359      BETA2=-2.*D12*HC+D22 00013580
1360      CALL EXPO(-BETA2,EBT2) 00013590
1361      GO TO 142         00013600
1362      141 EBT2=1.0       00013610
1363      142 G22P=EBT2*A2*SUM1 00013620
1364      QZC2=A1*G22P      00013630
1365      RETURN            00013640
1366      C                  00013650
1367      C ISPEC = 3       00013660
1368      145 TERM1=(Q2Q1+GAMMA)*A2*SUM1 00013670
1369      C                  00013680
1370      ETA3=HC+D33       00013690
1371      ETA3SQ=ETA3*ETA3  00013700
1372      IF(ETA3SQ.GT.EXPMAX) CALL ARGCHK(ETA3,ETA3SQ) 00013710
1373      B13=EXP(ETA3SQ)*ERFC(ETA3) 00013720
1374      ALPHA3=A1C*D33*B13 00013730
1375      TERM2=-GAMMA*EXCT*A2*(2.-ALPHA3) 00013740
1376      C                  00013750
1377      IF(V21.EQ.V22) GO TO 150 00013760
1378      C COMPUTE INTEGRAL FUNC=F1(XC,0.;HC); FUN1 IS THE INTEGRAND FUNCTION 00013770
1379      CALL D01AJF(FUN1,AI,BI,EPSABS,EPSREL,RESULT, 00013780
1380      1 ABSERR,WORK,LW,IW,NIW,IFAIL) 00013790
1381      RES=RESULT          00013800
1382      FUNC=RES/PI         00013810
1383      TERM3=-GAMMA*D6*FUNC 00013820
1384      C                  00013830
1385      150 SUMT=TERM1+TERM2+TERM3 00013840

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1386      IF(SUMT) 155,155,160          00013850
1387      155 G22P=0.0                 00013860
1388      QZC2=0.0                   00013870
1389      RETURN                      00013880
1390      160 IF(WC2.EQ.0.) GO TO 161  00013890
1391      BETA2=-2.*D12*HC+D22       00013900
1392      CALL EXP0(-BETA2,EBT2)      00013910
1393      GO TO 162                  00013920
1394      161 EBT2=1.0                00013930
1395      162 G22P=EBT2*SUMT        00013940
1396      QZC2=A1*G22P              00013950
1397      RETURN                      00013960
1398      C                           00013970
1399      C                           00013980
1400      C **** WELL-MIXED REGION (X .GE. D80). 00013990
1401      C                           00014000
1402      C     IN THIS REGION, THE CONCENTRATION BELOW THE MIXING HEIGHT IS 00014010
1403      C     UNIFORM REGARDLESS OF THE SOURCE OR RECEPTOR HEIGHTS BECAUSE 00014020
1404      C     OF THOROUGH MIXING OF POLLUTANT BETWEEN THE GROUND AND THE 00014030
1405      C     MIXING HEIGHT.           00014040
1406      C                           00014050
1407      200 M=2                     00014060
1408      A1A=1000./HL               00014070
1409      CALL PSG4P(G41P,G42P)      00014080
1410      QZC1=A1A*G41P             00014090
1411      IF(ISPEC.EQ.1) RETURN    00014100
1412      QZC2=A1A*G42P             00014110
1413      RETURN                      00014120
1414      END                         00014130
1415      C                           00014140
1416      C                           00014150
1417      C     SUBROUTINE PSG4P(G41P,G42P) 00014160
1418      C     SUBROUTINE PSG4P (VERSION 82360), PART OF PEM. 00014170
1419      C                           00014180
1420      C                           00014190
1421      C     THIS SUBROUTINE CALCULATES AND RETURNS VALUES OF G41P AND G42P. 00014200
1422      C     THESE ARE NONDIMENSIONAL VERTICALLY-INTEGRATED PROBABILITY 00014210
1423      C     DENSITY FUNCTIONS USED IN THE WELL-MIXED REGION CONCENTRATION 00014220
1424      C     ALGORITHMS FOR SPECIES-1 AND SPECIES-2, RESPECTIVELY, DOWNWIND 00014230
1425      C     OF A POINT SOURCE. THESE FUNCTIONS ARE INDEPENDENT OF BOTH 00014240
1426      C     SOURCE HEIGHT AND RECEPTOR HEIGHT. THIS SUBROUTINE IS 00014250
1427      C     USED BY BOTH POINT AND AREA SOURCES. FOR AREA SOURCES, 00014260
1428      C     G41P AND G42P REPRESENT SUSPENSION RATIOS OF POLLUTANTS. 00014270
1429      C                           00014280
1430      C                           00014290
1431      C                           00014300
1432      C *** PEM ALGORITHMS AND PROGRAM DEVELOPMENT: --- DECEMBER 1982 00014310
1433      C                           00014320
1434      C     K. SHANKAR RAO, PHYSICAL RESEARCH SCIENTIST 00014330
1435      C     ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL) 00014340
1436      C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION (NOAA) 00014350
1437      C     U.S. DEPARTMENT OF COMMERCE, P.O. BOX - E 00014360
1438      C     OAK RIDGE, TENNESSEE 37830 00014370
1439      C     PHONE : (615) 576-1238 00014380
1440      C     FTS: 626-1238 00014390
1441      C                           00014400
1442      C     ( THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT 00014410
1443      C     BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE 00014420
1444      C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION ) 00014430
1445      C                           00014440
1446      C                           00014450
1447      C                           00014460
1448      C     EXTERNAL FUN2 00014470
1449      REAL*8 FUN2 00014480
1450      REAL*8 WORK(800),AI,BI,EPABS,EPREL,RESULT,ABSERR 00014490
1451      DIMENSION IW(102) 00014500
1452      COMMON/PARM1A/GAMMA 00014510
1453      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT 00014520
1454      COMMON/PARM4/V11,V21,V12,V22,V13 00014530
1455      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6 00014540
1456      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42 00014550
1457      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C 00014560
1458      COMMON/BLOCK2/AI,BI,EPABS,EPREL,LW,NIW 00014570
1459      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX 00014580
1460      C                           00014590
1461      C                           00014600
1462      C     ISPEC = 1 OR 2 OR 3 00014610

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1463 C***** SPECIES-1 (PRIMARY) POLLUTANT: GAS OR PARTICLES. 00014620
1464 C
1465 IF(D21.GT.EXPMAX) CALL ARGCHK(D11,D21) 00014630
1466 B11=EXP(D21)*ERFC(D11) 00014640
1467 IF(V21.EQ.0.) GO TO 201 00014650
1468 D31SQ=D31*D31 00014660
1469 IF(D31SQ.GT.EXPMAX) CALL ARGCHK(D31,D31SQ) 00014670
1470 SUM=R11*(EXP(D31SQ)*ERFC(D31))-R21*B11 00014680
1471 GO TO 202 00014690
1472 201 SUM=R31*B11-R41 00014700
1473 202 IF(SUM.LT.0.) SUM=0.0 00014710
1474 G41P=EXCT*EXP(-D21)*SUM 00014720
1475 IF(ISPEC.EQ.1) RETURN 00014730
1476 C
1477 C ISPEC = 2 OR 3 00014740
1478 C***** SPECIES-2 (SECONDARY) POLLUTANT: GAS OR PARTICLES. 00014750
1479 C
1480 IF(D22.GT.EXPMAX) CALL ARGCHK(D12,D22) 00014760
1481 B12=EXP(D22)*ERFC(D12) 00014770
1482 IF(V22.EQ.0.) GO TO 203 00014780
1483 D32SQ=D32*D32 00014790
1484 IF(D32SQ.GT.EXPMAX) CALL ARGCHK(D32,D32SQ) 00014800
1485 SUM1=R12*(EXP(D32SQ)*ERFC(D32))-R22*B12 00014810
1486 GO TO 204 00014820
1487 203 SUM1=R32*B12-R42 00014830
1488 204 IF(ISPEC.EQ.3) GO TO 205 00014840
1489 C
1490 C ISPEC = 2 00014850
1491 IF(SUM1.LT.0.) SUM1=0.0 00014860
1492 G42P=EXP(-D22)*SUM1 00014870
1493 RETURN 00014880
1494 C
1495 C ISPEC = 3 00014890
1496 205 TERM1=(Q2Q1+GAMMA)*SUM1 00014900
1497 C
1498 IF(V21.EQ.0.) GO TO 206 00014910
1499 D33SQ=D33*D33 00014920
1500 IF(D33SQ.GT.EXPMAX) CALL ARGCHK(D33,D33SQ) 00014930
1501 SUM2=R13*(EXP(D33SQ)*ERFC(D33))-R23*B12 00014940
1502 GO TO 207 00014950
1503 206 SUM2=R32*B12-R42 00014960
1504 207 TERM2=-GAMMA*EXCT*SUM2 00014970
1505 C
1506 IF(V21.EQ.V22) GO TO 208 00014980
1507 C COMPUTE INTEGRAL FUNC=F2(XC); FUN2 IS THE INTEGRAND FUNCTION. 00014990
1508 CALL D01AJF(FUN2,AI,BI,EPSABS,EPSREL,RESULT, 00015000
1509 1 ABSERR,WORK,LW,IW,NIW,IFAIL) 00015010
1510 RES=RESULT 00015020
1511 FUNC=RES/(2.*PI) 00015030
1512 TERM3=-GAMMA*D6*FUNC 00015040
1513 GO TO 209 00015050
1514 208 TERM3=0.0 00015060
1515 C
1516 209 SUMT=TERM1+TERM2+TERM3 00015070
1517 IF(SUMT.LT.0.) SUMT=0.0 00015080
1518 G42P=EXP(-D22)*SUMT 00015090
1519 RETURN 00015100
1520 END 00015110
1521 C
1522 C
1523 DOUBLE PRECISION FUNCTION FUN1(T) 00015120
1524 REAL*8 T,TERM1,TERM2,TERM3
1525 C REAL*8 FUNCTION FUN1(VERSION 82360), PART OF PEM. 00015130
1526 C
1527 C
1528 C INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION IN SUBROUTINE 00015140
1529 C QZCAL (FOR POINT SOURCES) IS DEFINED HERE. 00015150
1530 C
1531 C
1532 C PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982 00015160
1533 C K. SHANKAR RAO 00015170
1534 C NOAA-ATDL, P.O. BOX-E 00015180
1535 C OAK RIDGE, TENN 37830 00015190
1536 C
1537 C
1538 C COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT 00015200
1539 C COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2 00015210

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1540      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6          00015380
1541      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C                00015390
1542      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                 00015400
1543      C                                                 00015410
1544      C                                                 00015420
1545      SQT=SQRT(T)                                         00015430
1546      SQ1T=SQRT(1.-T)                                       00015440
1547      HC1=HC/SQT                                         00015450
1548      C                                                 00015460
1549      ARG1= -(HC1*HC1)-(T*XCT)                           00015470
1550      CALL EXP0(ARG1,EXP1)                                00015480
1551      IF(EXP1.EQ.0.) GO TO 10                            00015490
1552      TERM1= EXP1/(SQT*SQ1T)                            00015500
1553      C                                                 00015510
1554      ETA4=HC1+D33*SQT                                 00015520
1555      ETA4SQ=ETA4*ETA4                                 00015530
1556      IF(ETA4SQ.GT.EXPMAX) CALL ARGCHK(ETA4,ETA4SQ)    00015540
1557      TERM2A= EXP(ETA4SQ)*ERFC(ETA4)                  00015550
1558      HC1SQ=HC1*HC1                                     00015560
1559      IF(HC1SQ.GT.EXPMAX) CALL ARGCHK(HC1,HC1SQ)        00015570
1560      TERM2= 1.-SQPI*(ETA4-HC1)*TERM2A                 00015580
1561      IF(TERM2.LE.0.) GO TO 10                          00015590
1562      C                                                 00015600
1563      ETA5=D32*SQ1T                                    00015610
1564      ETA5SQ=ETA5*ETA5                                00015620
1565      IF(ETA5SQ.GT.EXPMAX) CALL ARGCHK(ETA5,ETA5SQ)    00015630
1566      TERM3=1.-SQPI*ETA5*(EXP(ETA5SQ)*ERFC(ETA5))   00015640
1567      IF(TERM3.LE.0.) GO TO 10                          00015650
1568      C                                                 00015660
1569      FUN1=TERM1*TERM2*TERM3                           00015670
1570      GO TO 11                                         00015680
1571      10 FUN1=0.0                                      00015690
1572      11 RETURN                                       00015700
1573      END                                              00015710
1574      C                                                 00015720
1575      C                                                 00015730
1576      DOUBLE PRECISION FUNCTION FUN2(T)                00015740
1577      REAL*8 T
1578      C                                                 00015750
1579      C                                                 00015760
1580      C                                                 00015770
1581      C                                                 00015780
1582      C INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION IN SUBROUTINE
1583      PSG4P (FOR POINT AND AREA SOURCES) IS DEFINED HERE. 00015790
1584      C                                                 00015800
1585      C PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982 00015810
1586      C K. SHANKAR RAO                                  00015820
1587      C NOAA-ATDL, P.O. BOX-E                         00015830
1588      C OAK RIDGE, TENN 37830                         00015840
1589      C                                                 00015850
1590      C                                                 00015860
1591      C                                                 00015870
1592      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT          00015880
1593      COMMON/PARM4/V11,V21,V12,V22,V13              00015890
1594      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6  00015900
1595      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42 00015910
1596      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C            00015920
1597      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX             00015930
1598      C                                                 00015940
1599      C                                                 00015950
1600      SQT=SQRT(T)                                         00015960
1601      SQ1T=SQRT(1.-T)                                       00015970
1602      ETA4=D33*SQT                                         00015980
1603      ETA5=D32*SQ1T                                       00015990
1604      ETA6=D12*SQ1T                                       00016000
1605      ETA6SQ=ETA6*ETA6                                 00016010
1606      IF(ETA6SQ.GT.EXPMAX) CALL ARGCHK(ETA6,ETA6SQ)    00016020
1607      C                                                 00016030
1608      ARG1=T*XCT                                       00016040
1609      EXP1=EXP(-ARG1)                                 00016050
1610      TERM1=EXP1/SQT                                 00016060
1611      C                                                 00016070
1612      IF(ETA4.EQ.0.) GO TO 10                          00016080
1613      ETA4SQ=ETA4*ETA4                                00016090
1614      IF(ETA4SQ.GT.EXPMAX) CALL ARGCHK(ETA4,ETA4SQ)    00016100
1615      TERM2=1.-SQPI*ETA4*(EXP(ETA4SQ)*ERFC(ETA4))   00016110
1616      IF(TERM2.LT.0.) TERM2=0.                         00016120
1617      GO TO 11                                         00016130

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1617      10 TERM2=1.          00016140
1618      C
1619      11 IF(V22.EQ.0.) GO TO 12 00016150
1620          ETA5SQ=ETA5*ETA5 00016160
1621          IF(ETA5SQ.GT.EXP(MAX) CALL ARGCHK(ETA5,ETA5SQ) 00016170
1622          T3A=EXP(ETA5SQ)*ERFC(ETA5) 00016180
1623          T3B=EXP(ETA6SQ)*ERFC(ETA6) 00016190
1624          TERM3=R12*T3A-R22*T3B 00016200
1625          IF(TERM3.LT.0.) TERM3=0. 00016210
1626          GO TO 13 00016220
1627      C
1628      12 T3A=(1.+2.*ETA6SQ)*(EXP(ETA6SQ)*ERFC(ETA6)) 00016240
1629          T3B=2.*ETA6/SQPI 00016250
1630          TERM3=T3A-T3B 00016260
1631          IF(TERM3.LT.0.) TERM3=0. 00016270
1632      C
1633      13 FUN2=TERM1*TERM2*TERM3 00016280
1634          RETURN 00016300
1635          END 00016320
1636      C
1637      C
1638      DOUBLE PRECISION FUNCTION FUN3(T) 00016330
1639      REAL*8 T
1640      C
1641          REAL*8 FUNCTION FUN3 (VERSION 82360), PART OF PEM. 00016340
1642          C
1643          C
1644          C
1645          C
1646          C
1647          C
1648          C
1649          C
1650          C
1651          C
1652          C
1653          COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT 00016450
1654          COMMON/PARM2A/AA,BA 00016460
1655          COMMON/PARM3/HC,VDC1,WCI,VDC2,WC2 00016470
1656          COMMON/PARM4/V11,V21,V12,V22,V13 00016480
1657          COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42 00016490
1658          COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C 00016500
1659          COMMON/EXPCHK/EXP(MAX),EXP(MIN),ETAMAX 00016510
1660      C
1661      C
1662          DN=SQRT2*AA 00016520
1663          BA1=1.-BA 00016530
1664          UTBA1=(UTAUC)**BA1 00016540
1665          PI=2.*V11*UTBA1/DN 00016550
1666          TBA1=T**BA1 00016560
1667          ETA1=PI*TBA1 00016570
1668          ETA1SQ=ETA1*ETA1 00016580
1669          IF(ETA1SQ.GT.EXP(MAX) CALL ARGCHK(ETA1,ETA1SQ) 00016590
1670          TERM=EXP(ETA1SQ)*ERFC(ETA1) 00016600
1671          EXP1=EXP(-T) 00016610
1672      C
1673          IF(WC1.NE.0.) GO TO 11 00016620
1674      10 SUM=TERM 00016630
1675          GO TO 13 00016640
1676      C
1677      11 IF(V21.EQ.0.) GO TO 12 00016650
1678          P2=WCI*UTBA1/DN 00016660
1679          B1=P2*TBA1 00016670
1680          B1SQ=B1*B1 00016680
1681          IF(B1SQ.GT.EXP(MAX) CALL ARGCHK(B1,B1SQ) 00016690
1682          SUM=EXP(-B1SQ)*(R11*TERM-R21*(EXP(B1SQ)*ERFC(B1))) 00016700
1683          GO TO 13 00016710
1684      C
1685      12 RF1=1.+2.*ETA1SQ 00016720
1686          RS1=2.*ETA1/SQPI 00016730
1687          SUM=EXP(-ETA1SQ)*(RF1*TERM-RS1) 00016740
1688      C
1689      13 IF(SUM.LT.0.) SUM=0.0 00016750
1690          FUN3=EXP1*SUM/VDC1 00016760
1691          RETURN 00016770
1692          END 00016780
1693      C

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1694 C
1695 C      SUBROUTINE EXP0(BX,EX)          00016900
1696 C      SUBROUTINE EXP0 (VERSION 82360), PART OF PEM. 00016910
1697 C
1698 C
1699 C      GIVEN THE ARGUMENT BX, SUBROUTINE EXP0 CALCULATES AND 00016920
1700 C      RETURNS EX=EXP(BX). EXP0 LIMITS THE ARGUMENT TO AVOID 00016930
1701 C      OVERFLOW/UNDERFLOW ERRORS. 00016940
1702 C
1703 C
1704 C      PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982 00016950
1705 C      K. SHANKAR RAO 00017000
1706 C      NOAA-ATDL, P.O. BOX-E 00017010
1707 C      OAK RIDGE, TENN 37830 00017020
1708 C
1709 C
1710 C      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX 00017030
1711 C
1712 C
1713 C      BXABS=ABS(BX) 00017040
1714 C      IF(BX) 5,10,15 00017050
1715 C      5 IF(BXABS-EXPMIN) 6,7,7 00017060
1716 C      6 EX=EXP(BX) 00017070
1717 C      GO TO 20 00017080
1718 C      7 EX=0. 00017090
1719 C      GO TO 20 00017100
1720 C      10 EX=1. 00017110
1721 C      GO TO 20 00017120
1722 C      15 IF(BXABS.GT.EXPMAX) BXABS=EXPMAX 00017130
1723 C      EX=EXP(BXABS) 00017140
1724 C      20 RETURN 00017150
1725 C      END 00017160
1726 C
1727 C
1728 C      SUBROUTINE ARGCHK(E,ESQ) 00017170
1729 C      SUBROUTINE ARGCHK (VERSION 82360), PART OF PEM. 00017180
1730 C
1731 C
1732 C      SUBROUTINE ARGCHK LIMITS THE ARGUMENTS OF EXP(ESQ)*ERFC(E) 00017190
1733 C      TO AVOID OVERFLOW/UNDERFLOW ERRORS. 00017200
1734 C
1735 C
1736 C      PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982 00017210
1737 C      K. SHANKAR RAO 00017220
1738 C      NOAA-ATDL, P.O. BOX-E 00017230
1739 C      OAK RIDGE, TENN 37830 00017240
1740 C
1741 C
1742 C      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX 00017250
1743 C
1744 C
1745 C      ESQ=EXPMAX 00017260
1746 C      IF(E.LT.0.) NSIGN=-1 00017270
1747 C      IF(E.GE.0.) NSIGN=1 00017280
1748 C      E=NSIGN*ETAMAX 00017290
1749 C      RETURN 00017300
1750 C      END 00017310
1751 C
1752 C
1753 C      SUBROUTINE INMOD 00017320
1754 C      SUBROUTINE INMOD (VERSION 82360), PART OF PEM. 00017330
1755 C
1756 C
1757 C      SUBROUTINE INMOD READS IN ALL INPUTS TO THE MODEL, SCREENS THEM, 00017340
1758 C      PRINTS WARNING MESSAGES, AND INSERTS DEFAULT VALUES AS NEEDFD. 00017350
1759 C      THE SUBROUTINE PRINTS OUT LISTS OF THE CONTROL PARAMETERS, 00017360
1760 C      SCENARIO PARAMETERS, AND SOURCE DATA FOR REFERENCE. 00017370
1761 C      INMOD ALSO PROCESSES THE INPUT FOR EACH SCENARIO BEFORE 00017380
1762 C      TRANSMITTING IT TO THE MAIN PROGRAM. 00017390
1763 C
1764 C
1765 C      *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS, 00017400
1766 C      NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830 00017410
1767 C      DECEMBER 1982 00017420
1768 C
1769 C
1770 C      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00017430

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1771      1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),    00017670
1772      2 XA(50),YA(50),EA(50,2),SIZE(50),                                00017680
1773      3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                            00017690
1774      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16),          00017700
1775      5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),  00017710
1776      6 ITA,IRD,IWR,IDS,        D80,D47,D8047,DIST,DELTA,           00017720
1777      7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,   UINV,WVEC,            00017730
1778      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,INDOPT,IWD,ISC,IPS,           00017740
1779      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,  00017750
1780      * NSTDW,INTER,NPRINT                                         00017760
1781      C
1782      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)                   00017770
1783      COMMON/PARM1/NPOL,ICT,V01,W1,V02,W2,TAUC                      00017790
1784      COMMON/PARM1A/GAMMA                                         00017800
1785      C
1786      DIMENSION NAME(2),WDINC(6),SUMAQ(2),SUMPQ(2),SUMAR(2),EAR(2), 00017820
1787      I AMSG(2),CWS(6)                                              00017830
1788      DIMENSION DCR(24,2),NSC(24),NWD(24),NWS(24),ASCALE(2)       00017840
1789      DATA NAME/4H      ,4H      /                               00017850
1790      DATA AMSG/4HVD1 ,4HVD2 /                               00017860
1791      DATA WDINC/1.5707963,0.7853982,0.5235988,0.2617994,        00017870
1792      I          0.1745329,0.08726646/                         00017880
1793      DATA CWS/1.5,2.46,4.47,6.93,9.61,12.52/                  00017890
1794      C
1795      IF(INDEX.NE.0) GO TO 300                                     00017900
1796      C
1797      ISTOP=0                                                 00017920
1798      C
1799      C R E A D   A L L   I N P U T   D A T A .                00017940
1800      C
1801      C ***** READ FIRST CONTROL PARAMETER CARD (TITLE).        00017960
1802      C
1803      READ(IRD,800)TT                                         00017970
1804      WRITE(IWR,900) TT                                       00017980
1805      C
1806      C ***** READ SECOND CONTROL PARAMETER CARD (OPTIONS).    00018010
1807      C
1808      C NTOPT = AVERAGING TIME OPTION (1 OR 2 OR 3).           00018020
1809      C NWDOPT = WIND DIRECTION INPUT OPTION (0 TO 7).         00018030
1810      C NWSOPT = WIND SPEED INPUT OPTION (0 OR 1).           00018040
1811      C NSCEN = NUMBER OF SCENARIOS (1 TO 24).              00018050
1812      C NLIST = OUTPUT OPTION: LISTS OF CONC AND SURF DEP FLUX (0 OR 1) 00018060
1813      C NARRAY = OUTPUT OPTION: MAPS OF CONC AND SURF DEP FLUX (0 TO 3) 00018070
1814      C NTAPE = OUTPUT OPTION: TAPE OF CONC AND SURF DEP FLUX (0 OR 1) 00018080
1815      C NCSOPT = OUTPUT OPTION: POINT SOURCE CULPABILITY LIST (0 OR 1). 00018090
1816      C NMAX = OUTPUT OPTION: MAXIMUM CONC. FOR EACH SCENARIO (0 OR 1). 00018100
1817      C NSTDW = STACK-TIP DOWNWASH OPTION (0 OR 1).             00018110
1818      C INTER = RECEPTOR INTERVAL ON TAPE OUTPUT (1,2,---).       00018120
1819      C NPRINT = OUTPUT OPTION: POINT SOURCE PLUME RISE INFO (0 OR 1) 00018130
1820      C INPTSC = INPUT OPTN: POINT SOURCE DATA ON UNIT IRD OR IDS (1 OR 2) 00018140
1821      C
1822      READ(IRD,805)NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE, 00018150
1823      I NCSOPT,NMAX,NSTDW,INTER,NPRINT,INPTSC                 00018160
1824      C
1825      IF(NTOPT.GE.1 .AND. NTOPT.LE.3) GO TO 2                 00018170
1826      WRITE(IWR,660) NTOPT                                     00018180
1827      NTOPT=1                                               00018190
1828      2 IF(NWDOPT.LE.1) GO TO 6                           00018200
1829      IF(NWDOPT.GT.7) GO TO 5                           00018210
1830      IF(NTOPT.EQ.1 .OR. NWDOPT.LE.1) GO TO 6             00018220
1831      WRITE(IWR,615)                                     00018230
1832      5 NWDOPT=0                                         00018240
1833      6 IF(NWSOPT.GT.1) NWSOPT=0                         00018250
1834      IF(NSCEN.EQ.0) NSCEN=1                           00018260
1835      IF(NTOPT.EQ.2 .AND. NSCEN.NE.24) GO TO 500          00018270
1836      10 IF(NSCEN.GT.24) GO TO 510                     00018280
1837      20 IF(NLIST.EQ.0) GO TO 25                        00018290
1838      IF(NLIST.GT.1) GO TO 22                        00018300
1839      IF(NWDOPT.LE.1) GO TO 25                        00018310
1840      WRITE(IWR,605)                                     00018320
1841      22 NLIST=0                                         00018330
1842      25 IF(NARRAY.GT.3) NARRAY=0                       00018340
1843      IF(NTAPE.EQ.0) GO TO 40                        00018350
1844      IF(NTAPE.GT.1) GO TO 30                        00018360
1845      IF(NWDOPT.LE.1) GO TO 40                        00018370
1846      WRITE(IWR,620)                                     00018380
1847      30 NTAPE=0                                         00018390

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1848      40 IF(NCSOPT.GT.1) NCSOPT=0          00018440
1849      IF(NMAX.GT.1) NMAX=0            00018450
1850      IF(NSTDWN.GT.1) NSTDWN=0        00018460
1851      IF(INTER.EQ.0) INTER=1        00018470
1852      IF(NPRINT.GT.1) NPRINT=0       00018480
1853      IF(INPTSC.LT.1 .OR. INPTSC.GT.2) INPTSC=1  00018490
1854      C                               00018500
1855      C     SET LABEL FOR TIME AVERAGING 00018510
1856      IAV=1                         00018520
1857      IF(NTOPT.EQ.2) IAV=24          00018530
1858      IF(NTOPT.EQ.3) IAV=NSCEN       00018540
1859      C                               00018550
1860      C     **** READ THIRD CONTROL PARAMETER CARD (GRID, DTDZ) 00018560
1861      C                               00018570
1862      C     XRSWC,YRSWC = COORDINATES OF SOUTHWEST CORNER OF RECEPTOR GRID (KM) 00018580
1863      C     LX      = NUMBER OF COLUMNS IN RECEPTOR GRID.           00018590
1864      C     LY      = NUMBER OF ROWS IN RECEPTOR GRID.           00018600
1865      C     GRID    = SPACING BETWEEN ROWS AND COLUMNS OF RECEPTOR GRID (KM) 00018610
1866      C                               00018620
1867      C     DTDZ(1&2) = VERTICAL POTENTIAL TEMPERATURE GRADIENT      00018630
1868      C     FOR STABILITY CLASSES E & F.                      00018640
1869      C                               00018650
1870      C     READ(IRD,810)XRSWC,YRSWC,LX,LY,GRID,DTDZ(1),DTDZ(2) 00018660
1871      C                               00018670
1872      C     IF(LX.EQ.0) LX=1             00018680
1873      C     IF(LY.EQ.0) LY=1             00018690
1874      C     IF(NTAPE.EQ.0) GO TO 115  00018700
1875      C                               00018710
1876      C     NRECS=((LX+1)/INTER)*(LY+1)/INTER)*NSCEN      00018720
1877      C     IF(NTOPT.EQ.2) NRECS= NRECS/4        00018730
1878      C     IF(NTOPT.EQ.3) NRECS= NRECS/NSCEN      00018740
1879      C     IF(NRECS.LT.10000) GO TO 115  00018750
1880      C     WRITE(IWR,600)               00018760
1881      C     NTAPE=0                     00018770
1882      115 CONTINUE                   00018780
1883      C                               00018790
1884      C     **** READ FOURTH CONTROL PARAMETER CARD (POLLUTANTS) 00018800
1885      C                               00018810
1886      C     NPOL   = NUMBER OF POLLUTANTS (1 OR 2)      00018820
1887      C     ICT    = CHEMICAL TRANSFORMATION OR DECAY OPTION (0 OR 1) 00018830
1888      C     VD1    = DEPOSITION VELOCITY FOR POLLUTANT SPECIES-1 (CM/S) 00018840
1889      C     W1     = SETTLING VELOCITY FOR POLLUTANT SPOECIES-1 (CM/S) 00018850
1890      C     VD2    = DEPOSITION VELOCITY FOR POLLUTANT SPECIES-2 (CM/S) 00018860
1891      C     W2     = SETTLING VELOCITY FOR POLLUTANT SPECIES-2 (CM/S) 00018870
1892      C     XKT    = CHEMICAL TRANSFORMATION OR DECAY RATE OF POLLUTANT 00018880
1893      C     SPECIES-1 (PERCENT PER HOUR)                 00018890
1894      C     GAMMA = RATIO OF MOLECULAR WEIGHTS OF SPECIES-2 (PRODUCT) 00018900
1895      C     TO SPECIES-1 (REACTANT) IN CHEMICAL TRANSFORMATION 00018910
1896      C                               00018920
1897      C     NOTE: FOR DEPOSITION TO OCCUR, W SHOULD BE LESS THAN OR EQUAL TO VD. 00018930
1898      C     FOR DEPOSITION OF GASES AND VERY SMALL PARTICLES, W=0.      00018940
1899      C     FOR DEPOSITION OF SMALL PARTICLES, W IS LESS THAN VD.      00018950
1900      C     FOR DEPOSITION OF MEDIUM AND LARGE PARTICLES, W=VD.      00018960
1901      C                               00018970
1902      C     READ (IRD,812) NPOL,ICT,VD1,W1,VD2,W2,XKT,GAMMA 00018980
1903      C                               00018990
1904      C     IF(NPOL.LT.1 .OR. NPOL.GT.2) NPOL=1      00019000
1905      C     IF(NPOL.EQ.1 .OR. NCSOPT.EQ.0) GO TO 116  00019010
1906      C     WRITE(IWR,635)                  00019020
1907      C     NCSOPT=0                     00019030
1908      116 IF(W1.GT.VD1) W1=VD1      00019040
1909      C     IF(NPOL.EQ.2) GO TO 117      00019050
1910      C     VD2=0.0                     00019060
1911      C     W2=0.0                     00019070
1912      C     GO TO 118                  00019080
1913      117 IF(W2.GT.VD2) W2=VD2      00019090
1914      118 IF(IXT.EQ.1) GO TO 119      00019100
1915      C     XKT=0.0                     00019110
1916      C     GAMMA=0.0                   00019120
1917      C     GO TO 122                  00019130
1918      119 IF(XKT.GE.0.1 .AND. XKT.LE.100.) GO TO 120  00019140
1919      C     TXKT=0.1                   00019150
1920      C     IF(XKT.GT.100.) TXKT=100.  00019160
1921      C     WRITE(IWR,640) XKT,TXKT      00019170
1922      C     XKT=TXKT                  00019180
1923      C                               00019190
1924      C     CONVERT CHEMICAL TRANSFORMATION RATE XKT (PERCENT PER HOUR) TO 00019200

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1925      C      THE EQUIVALENT TIME SCALE TAUC (SECONDS).          00019210
1926      120 TAUC=0.36E06/XKT                                00019220
1927      C
1928      122 IF(NCSOPT.EQ.0 .OR. (LX.LE.25 .AND. LY.LE.25)) GO TO 125 00019230
1929          WRITE(IWR,645)
1930          NCSOPT=0
1931      C
1932      C      SHIFT THE RECEPTOR GRID TO THE COMPUTATION GRID. 00019280
1933      125 XSWC= XRSWC - 0.5*GRID                          00019290
1934          YSWC= YRSWC - 0.5*GRID                          00019300
1935      C
1936      130 IF(DTDZ(1).LT.0.00001) DTDZ(1)=0.020           00019310
1937          IF(DTDZ(2).LT.0.00001) DTDZ(2)=0.035           00019320
1938      C
1939      C  IF GRID IS ZERO, SWITCH ON AUTOMATIC GRID OPTION. 00019330
1940          IGRID=0
1941          IF(GRID.LT.1.0E-5) IGRID=1
1942          IF(IGRID.EQ.1.AND.NTOPT.GT.1) GO TO 520
1943      C
1944      C ***** READ 5TH CONTROL PARAMETER CARD (AREA SOURCE SCALING,CALIBRATION) 00019400
1945      C
1946      C      ASCALE(1&2) = AREA SOURCE EMISSION SCALING FACTORS 00019420
1947          FOR EACH POLLUTANT.
1948      C      A(1&2)      = CONCENTRATION CALIBRATION FACTOR (INTERCEPT) 00019430
1949          FOR EACH POLLUTANT.
1950      C      B(1&2)      = CONCENTRATION CALIBRATION FACTOR (SLOPE)    00019440
1951          FOR EACH POLLUTANT.
1952      C
1953      135 READ(IRD,815) ASCALE,A(1),B(1),A(2),B(2)        00019450
1954      C
1955          IF(ASCALE(1).LE.0.) ASCALE(1)=1.0                00019460
1956          IF(ASCALE(2).LE.0.) ASCALE(2)=1.0                00019470
1957      C
1958      C ***** READ CARD 6 (POLLUTANT AND CALIBRATION LABELS) 00019480
1959      C
1960          READ(IRD,817)(POLNAM(I,1),I=1,3),(CALNAM(I,1),I=1,7), 00019490
1961              1 (POLNAM(I,2),I=1,3),(CALNAM(I,2),I=1,7)        00019500
1962      C
1963      C ***** READ ONE TO 24 SCENARIO PARAMETER CARDS.       00019510
1964      C
1965      C      NSC      = STABILITY CLASS NUMBER (1 TO 7)        00019520
1966      C      NWS      = WIND SPEED CLASS NUMBER (1 TO 6)        00019530
1967      C      NWD      = WIND SECTOR NUMBER (1 TO 16)        00019540
1968      C      WS       = WIND SPEED (M/S)                      00019550
1969      C      WD       = WIND DIRECTION (DEGREES)            00019560
1970      C      TA       = AMBIENT TEMPERATURE (DEGREES CELSIUS) 00019570
1971      C      PEN      = INVERSION PENETRATION FACTOR (PEN .GE. 1.0) 00019580
1972      C      HMIX     = MIXING HEIGHT (METERS)                 00019590
1973      C
1974          DO 150 IS=1,NSCEN
1975          READ(IRD,820)NSC(IS),NWS(IS),NWD(IS),WS(IS),WD(IS),TA(IS),
1976              1 PEN(IS),HMIX(IS)                                00019600
1977      C
1978          IF(NSC(IS).GE.1 .AND. NSC(IS).LE.7) GO TO 140
1979          NUM=1
1980          IF(NSC(IS).GT.7) NUM=7
1981          WRITE(IWR,535) IS,NSC(IS),NUM
1982          NSC(IS)=NUM
1983      140 IF(NWSDOPT.EQ.0) GO TO 142
1984          IF(NWS(IS).GE.1 .AND. NWS(IS).LE.6) GO TO 144
1985          NUM=1
1986          IF(NWS(IS).GT.6) NUM=6
1987          WRITE(IWR,545) IS,NWS(IS),NUM
1988          NWS(IS)=NUM
1989          GO TO 144
1990      142 IF(WS(IS).GT.0.) GO TO 144
1991          WRITE(IWR,565) IS,WS(IS)
1992          WS(IS)=1.0
1993      144 IF(NWDOPT.NE.1) GO TO 146
1994          IF(NWD(IS).GE.1 .AND. NWD(IS).LE.16) GO TO 146
1995          NUM=1
1996          IF(NWD(IS).GT.16) NUM=16
1997          WRITE(IWR,555) IS,NWD(IS),NUM
1998          NWD(IS)=NUM
1999      146 IF(PEN(IS).LT.1.0) PEN(IS)=2.0
2000          IF(HMIX(IS).LT.1.0E-5) HMIX(IS)= 9999.9
2001      150 CONTINUE

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2002      C
2003      C PRINT INPUT CONTROL PARAMETERS
2004      C
2005          IF(ISTOP.EQ.1) WRITE(IWR,900) TT
2006          WRITE(IWR,902) NTOPT
2007          WRITE(IWR,904) NWDOPT
2008          WRITE(IWR,906) NWSOFT
2009          WRITE(IWR,908) NSCEN
2010          WRITE(IWR,910) NSTDWN
2011          IF(IGRID.EQ.0) WRITE(IWR,916) LX,LY,GRID,XRSWC,YRSWC
2012          IF(IGRID.EQ.1) WRITE(IWR,914)
2013          WRITE(IWR,920) DTOZ(1),DTOZ(2)
2014          WRITE(IWR,900) TT
2015          WRITE(IWR,922) NPOL,(POLNAM(I,1),I=1,3)
2016          IF(NPOL.EQ.2) WRITE(IWR,923) (POLNAM(I,2),I=1,3)
2017          WRITE(IWR,924) ASCALE(1)
2018          IF(NPOL.EQ.2) WRITE(IWR,935) ASCALE(2)
2019          WRITE(IWR,925) A(1),B(1)
2020          IF(NPOL.EQ.2) WRITE(IWR,926) A(2),B(2)
2021          WRITE(IWR,927) (CALNAM(I,1),I=1,7)
2022          IF(NPOL.EQ.2) WRITE(IWR,921) (CALNAM(I,2),I=1,7)
2023          WRITE(IWR,928) VD1
2024          IF(NPOL.EQ.2) WRITE(IWR,931) VD2
2025          WRITE(IWR,929) W1
2026          IF(NPOL.EQ.2) WRITE(IWR,933) W2
2027          WRITE(IWR,930) ICT
2028          IF(NPOL.EQ.1) WRITE(IWR,932)
2029          IF(NPOL.EQ.2) WRITE(IWR,934)
2030          IF(ICK.EQ.0) GO TO 152
2031          WRITE(IWR,936) XKT
2032          WRITE(IWR,938) GAMMA
2033      152 WRITE(IWR,940)
2034          IF(NLIST.GT.0) WRITE(IWR,942) NLIST
2035          IF(NARRAY.GT.0) WRITE(IWR,944) NARRAY
2036          IF(NARRAY.EQ.1) WRITE(IWR,946)
2037          IF(NARRAY.EQ.2) WRITE(IWR,948)
2038          IF(NARRAY.EQ.3) WRITE(IWR,950)
2039          IF(NTAPE.GT.0) WRITE(IWR,952) NTAPE,INTER
2040          IF(NCSOPT.GT.0) WRITE(IWR,954) NCSOPT
2041          IF(NPRINT.GT.0) WRITE(IWR,956) NPRINT
2042          IF(NMAX.GT.0) WRITE(IWR,958) NMAX
2043      C
2044      C PRINT INPUT PARAMETERS FOR SCENARIOS
2045      C
2046          WRITE(IWR,960) TT
2047          WRITE(IWR,962)
2048          WRITE(IWR,963)
2049          WRITE(IWR,964)
2050      C
2051          DO 160 IS=1,NSCEN
2052          KS=NSC(IS)
2053          WRITE(IWR,966) IS,SCLAB(KS)
2054          IF(NWSOFT.EQ.0) GO TO 153
2055          KW=NWS(IS)
2056          WS(IS)=CWS(KW)
2057          WRITE(IWR,970) KW
2058      153 WRITE(IWR,972) WS(IS)
2059          IF(NWDOPT.EQ.1) GO TO 155
2060          WDOUT=WD(IS)
2061          GO TO 156
2062      155 KD=NWD(IS)
2063          WDOUT=SECTAN(KD) * 180./3.14159265
2064          WRITE(IWR,974) KD
2065      156 WRITE(IWR,978) WDOUT,TA(IS),PEN(IS),HMIX(IS)
2066          WD(IS)= WD(IS)*3.14159265/180.
2067          TA(IS)= TA(IS) + 273.15
2068      C
2069      C FOR EACH SCENARIO, CALCULATE THE CRITICAL DOWNWIND DISTANCES
2070      C AT WHICH VERTICAL MIXING IMPENDS (DCRIT(IS,1)) AND IS COMPLETE
2071      C (DCRIT(IS,2)).
2072          JSC=NSC(IS)
2073          JD=3
2074          IF(AX(JSC,2)*5000.*BX(JSC,2).GT.0.47*HMIX(IS)) JD=2
2075          IF(AX(JSC,1)*500.*BX(JSC,1).GT.0.47*HMIX(IS)) JD=1
2076          DCR(IS,1)=0.001*(0.47*HMIX(IS)/AX(JSC,JD))**(1./BX(JSC,JD))
2077          DCR(IS,2)= DCR(IS,1)*2.
2078      160 CONTINUE

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2079      C
2080      C **** READ UP TO 50 AREA SOURCE CARDS.          00020750
2081      C
2082      C     XA,YA = COORDINATES OF SOUTHWEST CORNER OF AREA SOURCE (KM). 00020760
2083      C     SIZE = LENGTH OF A SIDE OF AREA SOURCE (M).           00020770
2084      C     EA(1&2) = EMISSION RATES OF 2 POLLUTANTS (G/S).        00020780
2085      C
2086      WRITE(IWR,990) TT                           00020790
2087      NAS=1                                         00020800
2088      SUMAQ(1)=0.                                  00020810
2089      SUMAQ(2)=0.                                  00020820
2090      SUMAR(1)=0.                                  00020830
2091      SUMAR(2)=0.                                  00020840
2092      C
2093      170  READ(IRD,825)XA(NAS),YA(NAS),SIZE(NAS),EA(NAS,1),EA(NAS,2) 00020850
2094      C
2095      IF(NPOL.EQ.1) EA(NAS,2)=0.0                00020860
2096      IF((SIZE(NAS)+EA(NAS,1)+EA(NAS,2)).LT.1.0E-04) GO TO 180 00020870
2097      IF(SIZE(NAS).GE.1.0E-4) GO TO 172          00020880
2098      SIZE(NAS)=1.0E-4                            00020890
2099      IF(GRID.NE.0.) SIZE(NAS)=GRID*1000.         00020900
2100      WRITE(IWR,585) NAS,SIZE(NAS)               00020910
2101      172  DO 175 K=1,2                          00020920
2102      EAR(K)=EA(NAS,K)                         00020930
2103      SUMAR(K)=SUMAR(K)+EAR(K)                 00020940
2104      EA(NAS,K)= EA(NAS,K)*ASCALE(K)          00020950
2105      175  SUMAQ(K)=SUMAQ(K)+EA(NAS,K)          00020960
2106      C
2107      C PRINT INPUT PARAMETERS FOR THIS AREA SOURCE 00020970
2108      WRITE(IWR,992)NAS,XA(NAS),YA(NAS),SIZE(NAS),EAR(1),EA(NAS,1), 00020980
2109      1EAR(2),EA(NAS,2)                         00020990
2110      C
2111      SIZE(NAS)=SIZE(NAS)*0.001                00021000
2112      IF(NAS/50*50.EQ.NAS) WRITE(IWR,990)TT       00021010
2113      NAS=NAS+1                                00021020
2114      GO TO 170                                00021030
2115      180  NAS=NAS-1                            00021040
2116      WRITE(IWR,994) SUMAR(1),SUMAQ(1),SUMAR(2),SUMAQ(2) 00021050
2117      C
2118      C IF AREA SOURCE CALCULATIONS ARE TO BE MADE, THEN DEPOSITION VELOCITY 00021060
2119      C VALUE(S) MUST BE GREATER THAN ZERO          00021070
2120      C IF(NAS.LT.1) GO TO 184                  00021080
2121      C IF(VD1.GT.0.) GO TO 181                  00021090
2122      C WRITE(IWR,655) AMSG(1)                  00021100
2123      C VD1=0.01                                 00021110
2124      181  IF(NPOL.EQ.1 .OR. VD2.GT.0.) GO TO 184 00021120
2125      C WRITE(IWR,655) AMSG(2)                  00021130
2126      C VD2=0.01                                 00021140
2127      C
2128      C
2129      C **** READ UP TO 300 POINT SOURCES        00021150
2130      C
2131      C     XP,YP = COORDINATES OF POINT SOURCE (KM). 00021160
2132      C     EP(1&2) = EMISSION RATES OF 2 POLLUTANTS (G/S). 00021170
2133      C     HP = SOURCE HEIGHT (M).              00021180
2134      C     DP = INSIDE DIAMETER (M).            00021190
2135      C     VP = VELOCITY (M/S).                00021200
2136      C     TP = TEMPERATURE (DEGREES CELSIUS). 00021210
2137      C     NAME = IDENTIFICATION.            00021220
2138      C
2139      184  WRITE(IWR,980) TT                   00021230
2140      C     NPS=1                               00021240
2141      C     SUMPQ(1)=0.                         00021250
2142      C     SUMPQ(2)=0.                         00021260
2143      C
2144      185  IF(INPTSC.EQ.2)READ(IDSK,830)XP(NPS),YP(NPS),EP(NPS,1),EP(NPS,2), 00021270
2145      C     1 HP(NPS),DP(NPS),VP(NPS),TP(NPS),NAME(1),NAME(2) 00021280
2146      C     IF(INPTSC.EQ.1) READ(IRD,830)XP(NPS),YP(NPS),EP(NPS,1),EP(NPS,2), 00021290
2147      C     1 HP(NPS),DP(NPS),VP(NPS),TP(NPS),NAME(1),NAME(2) 00021300
2148      C
2149      C     IF(NPOL.EQ.1) EP(NPS,2)=0.0          00021310
2150      C     IF(HP(NPS)+DP(NPS)+VP(NPS)+TP(NPS).LT.1.0E-4) GO TO 190 00021320
2151      C     IF(DP(NPS).GT.0.0) GO TO 187          00021330
2152      C     WRITE(IWR,575) NPS                  00021340
2153      C     DP(NPS)=1.0E-4                      00021350
2154      C
2155      C PRINT INPUT PARAMETERS FOR THIS POINT SOURCE 00021360

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2156      187 WRITE(IWR,984) NPS,NAME(1),NAME(2),XP(NPS),YP(NPS),EP(NPS,1),
2157          1 EP(NPS,2),HP(NPS),DP(NPS),VP(NPS),TP(NPS)                      00021520
2158      C
2159          TP(NPS)=TP(NPS)+273.15                                         00021530
2160          IF(NPS/50*50.EQ.NPS) WRITE(IWR,980)TT                           00021550
2161          SUMPQ(1)=SUMPQ(1)+EP(NPS,1)                                     00021560
2162          SUMPQ(2)=SUMPQ(2)+EP(NPS,2)                                     00021570
2163          NPS=NPS+1                                                 00021580
2164          GO TO 185                                              00021590
2165      190  NPS= NPS-1                                             00021600
2166          WRITE(IWR,986) SUMPQ(1),SUMPQ(2)                           00021620
2167      C
2168      C   IF THERE WERE SERIOUS ERRORS IN INPUT PARAMETERS, STOP        00021630
2169          IF(ISTOP.EQ.0) GO TO 195                                     00021640
2170          WRITE(IWR,630)                                           00021650
2171          STOP                                                 00021660
2172      C
2173      C   INITIALIZE FOR FIRST CALL TO INMOD FOR SCENARIO PREPARATION 00021670
2174      195 IWDOPT= 0                                               00021680
2175          ISCEN=0                                              00021690
2176          RETURN                                              00021700
2177      C
2178      C
2179      C   P R E P A R E   S C E N A R I O   I N F O R M A T I O N . 00021710
2180      C
2181      300  IF(NWDOPT.LE.1) GO TO 350                                00021720
2182          IF(ISCEN.EQ.0.OR.IWDOPT.GE.4) GO TO 320                  00021730
2183          IWDOPT= IWDOPT + 1                                         00021740
2184          WD(ISCEN)= WD(ISCEN) + WDINC(NWDOPT-1)                   00021750
2185          IF(WD(ISCEN).GE.6.2831853) WD(ISCEN)=WD(ISCEN) - 6.2831853 00021760
2186          GO TO 353                                              00021770
2187      320  ISCEN= ISCEN + 1                                         00021780
2188          IWDOPT= 1                                              00021790
2189          GO TO 353                                              00021800
2190      350  ISCEN= ISCEN + 1                                         00021810
2191      353  ISC=NSC(ISCEN)                                         00021820
2192          IWD=NWD(ISCEN)                                         00021830
2193          D47= DCR(ISCEN,1)                                         00021840
2194          D80= DCR(ISCEN,2)                                         00021850
2195          D8047= D80 - D47                                         00021860
2196          IF(NCSOPT.EQ.0) GO TO 400                                00021870
2197          DO 380 I=1,25                                         00021880
2198          DO 380 J=1,25                                         00021890
2199          DO 380 K=1,5                                         00021900
2200          NWORST(I,J,K)=0                                         00021910
2201      380  CWORST(I,J,K)=0.                                         00021920
2202          RETURN                                              00021930
2203      C
2204      C   E R R O R   M E S S A G E S                            00021940
2205      C
2206          500 WRITE(IWR,505)                                         00021950
2207          505 FORMAT(1HO,'WHEN TIME AVG OPTION NTOPT=2, NUMBER OF SCENARIOS MUST00022030
2208              1 =24')                                              00021960
2209          ISTOP=1                                              00021970
2210          GO TO 10                                              00021980
2211          510 WRITE(IWR,515) NSCEN                                         00021990
2212          515 FORMAT(1HO,'MAXIMUM NUMBER OF SCENARIOS ALLOWED IS 24. NSCEN=',I4)00022080
2213          ISTOP=1                                              00022090
2214          GO TO 20                                              00022100
2215          520 WRITE(IWR,525)                                         00022110
2216          525 FORMAT(1HO,'AUTOGRID MAY NOT BE USED WITH TIME AVG OPTION NTOPT>1'00022120
2217              1)                                              00022130
2218          ISTOP=1                                              00022140
2219          GO TO 135                                             00022150
2220          535 FORMAT(1HO,'IN SCENARIO',I3,' STABILITY CLASS NUMBER NSC=',I2, 00022160
2221              1' IS OUT OF RANGE. NSC SET TO ',I2)                     00022170
2222          545 FORMAT(1HO,'IN SCENARIO',I3,' WIND SPEED CLASS NUMBER NWS=',I2, 00022180
2223              1' IS OUT OF RANGE. NWS SET TO ',I2)                     00022190
2224          555 FORMAT(1HO,'IN SCENARIO',I3,' WIND DIRECTION SECTOR NUMBER NWD=', 00022200
2225              1 I3,' IS OUT OF RANGE. NWD SET TO ',I3)                 00022210
2226          565 FORMAT(1HO,'IN SCENARIO',I3,' SPECIFIED WIND SPEED MUST BE GREATER00022220
2227              1 THAN ZERO. WS SET TO 1.0 M/S')                         00022230
2228          575 FORMAT(1HO,'POINT SOURCE',I4,':: INSIDE DIAMETER MUST BE GREATER T00022240
2229              1HAN ZERO. DP SET TO .0001 M')                          00022250
2230          585 FORMAT(1HO,'AREA SOURCE',I3,':: LENGTH OF SIDE MUST BE GREATER THA00022260
2231              1N ZERO. SIZE SET TO ',F9.2)                           00022270
2232          600 FORMAT(1HO,'RUN REQUESTED WOULD PRODUCE OVER 10000 RECORDS ON TAPE00022280

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2233      1'/' OUTPUT OPTION NTAPE HAS BEEN SET TO ZERO')          00022290
2234 605 FORMAT(1H0,'OUTPUT OPTION NLIST MAY NOT BE USED WITH AUTOMATIC WIN00022300
2235      1D SHIFT OPTION (NWDOPT>1)'' NLIST HAS BEEN SET TO ZERO')    00022310
2236 615 FORMAT(1H0,'AUTOMATIC WIND SHIFT OPTION (NWDOPT>1) MAY NOT BE USED00022320
2237      1 WITH TIME AVG OPTION NTOPT>1'' NWDOPT HAS BEEN SET TO ZERO') 00022330
2238 620 FORMAT(1H0,'OUTPUT OPTION NTAPE MAY NOT BE USED WITH AUTOMATIC WIN00022340
2239      1D SHIFT OPTION (NWDOPT>1)'' NTAPE HAS BEEN SET TO ZERO')    00022350
2240 630 FORMAT(1H1//' SERIOUS ERROR(S) IN INPUT PARAMETERS',5X,        00022360
2241      1 'RUN CANNOT BE CONTINUED')                                00022370
2242 635 FORMAT(1H0,'CONTROL STRATEGY OUTPUT OPTION NCSOPT MAY NOT BE USED 00022380
2243      1WITH TWO POLLUTANTS'' NCSOPT HAS BEEN SET TO ZERO')       00022390
2244 640 FORMAT(1H0,'CHEMICAL TRANSFORMATION RATE XKT=',F7.3,' IS OUT OF RA00022400
2245      INGE'' XKT HAS BEEN SET TO ',F8.3)                         00022410
2246 645 FORMAT(1H0,'CONTROL STRATEGY OUTPUT OPTION NCSOPT MAY NOT BE USED 00022420
2247      1WHEN NUMBER OF COLUMNS OR ROWS IN RECEPTOR GRID IS GREATER THAN 2500022430
2248      2'' NCSOPT HAS BEEN SET TO ZERO')                           00022440
2249 655 FORMAT(1H0,'AREA SOURCE CALCULATIONS REQUIRE DEPOSITION VELOCITY S00022450
2250      1REATR THAN ZERO.',4X,A4,'HAS BEEN SET TO 0.01')           00022460
2251 660 FORMAT(1H0,'TIME AVERAGING OPTION NTOPT=',I2,' IS OUT OF RANGE. N00022470
2252      1TOPT SET TO 1')                                         00022480
2253 C
2254 C   INPUT FORMATS                                         00022490
2255 C
2256 800  FORMAT(20A4)                                         00022520
2257 805  FORMAT(13I5)                                         00022530
2258 810  FORMAT(2F10.0,2I10,3F10.0)                         00022540
2259 812  FORMAT(2I5,6F10.0)                                     00022550
2260 815  FORMAT(6F10.0)                                       00022560
2261 817  FORMAT(3A4,7A4,3A4,7A4)                         00022570
2262 820  FORMAT(3I5,5F10.0)                                     00022580
2263 825  FORMAT(5F10.0)                                       00022590
2264 830  FORMAT(8F9.0,2A4)                                     00022600
2265 C
2266 C   OUTPUT FORMATS                                         00022610
2267 C
2268 900 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT CONTROL PARA00022640
2269      1METERS: ',20A4//)                                      00022650
2270 902 FORMAT(10X,'AVERAGING TIME OPTION: NTOPT=',I1//        00022660
2271      1 18X,'A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR'// 00022670
2272      2 13X,'1 1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO'// 00022680
2273      3 13X,'2 24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE 00022690
2274      4AVERAGED'//3X,'3 VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN 00022700
2275      5NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED'//)        00022710
2276 904 FORMAT(10X,'WIND DIRECTION OPTION: NWDOPT=',I1//        00022720
2277      113X,'0 DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO'// 00022730
2278      213X,'1 SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO'// 00022740
2279      312X,'2-7 DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOU00022750
2280      4R SUB-SCENARIOS.'//7X,'FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRE00022760
2281      5CTION IS AUTOMATICALLY INCREASED'//7X,'BY 90,45,30,15,10,OR 5 DEGR00022770
2282      6EES, DEPENDING ON THE OPTION NUMBER SELECTED.'//)       00022780
2283 906 FORMAT(10X,'WIND SPEED OPTION: NWSOPT=',I1//        00022790
2284      113X,'0 SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO'// 00022800
2285      213X,'1 WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO'00022810
2286      3//)                                              00022820
2287 908 FORMAT(10X,'NUMBER OF SCENARIOS: NSCEN=',I2//)        00022830
2288 910 FORMAT(10X,'STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=',I1// 00022840
2289      1 13X,'0 ALGORITHM IS IN EFFECT'//                  00022850
2290      2 13X,'1 ALGORITHM IS NOT USED'//)                   00022860
2291 914 FORMAT(10X,'AUTOMATIC RECEPTOR GRID OPTION IS IN EFFECT'//) 00022870
2292 916 FORMAT(10X,'RECEPTOR GRID:',          00022880
2293      16X,'COLUMNS: LX=',I3,4X,'ROWS: LY=',I3/          00022890
2294      230X,'SPACING: GRID=',F7.3,' KM'//               00022900
2295      330X,'SOUTHWEST CORNER XRSWC= ',F8.3,' KM W'// 00022910
2296      450X,'YRSWC= ',F8.3,' KM S'//)                   00022920
2297 920 FORMAT(10X,'POTENTIAL TEMPERATURE GRADIENT: DTDZ(1)= ',F7.3, 00022930
2298      1' DEG/M STABILITY CLASS E'//                      00022940
2299      242X,'DTDZ(2)= ',F7.3,' DEG/M STABILITY CLASS F'//) 00022950
2300 921 FORMAT(1H+,85X,7A4)                                    00022960
2301 922 FORMAT(10X,'NUMBER OF POLLUTANTS: NPOL=',I1/        00022970
2302      1 51X,'POLLUTANT-1: ',3A4)                         00022980
2303 923 FORMAT(1H+,85X,'POLLUTANT-2: ',3A4)                00022990
2304 924 FORMAT(/10X,'AREA SOURCE SCALING FACTOR:',17X,'ASCALE=',F9.3) 00023000
2305 925 FORMAT(10X,'CALIBRATION COEFFICIENTS:',          00023010
2306      1 16X,'A=',F10.3,' B=',F10.3)                   00023020
2307 926 FORMAT(1H+,85X,'A=',F10.3,' B=',F10.3)           00023030
2308 927 FORMAT(10X,'CALIBRATION IDENTIFICATION:',14X,7A4,6X,7A4) 00023040
2309 928 FORMAT(10X,'DEPOSITION VELOCITY (CM/S):',20X,'VD1=',F8.3) 00023050

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2310 929 FORMAT(10X,'SETTLING VELOCITY (CM/S):',23X,'W1=',F8.3) 00023060
2311 930 FORMAT(//10X,'CHEMICAL TRANSFORMATION OPTION: ICT=',I1/) 00023070
2312 931 FORMAT(1H+,9IX,'VD2=',F8.3) 00023080
2313 932 FORMAT(13X,'NPOL=1'/
2314   215X,'ICT=0 CHEMICAL TRANSFORMATION LOSS OF POLLUTANT IS IGNORED'/00023100
2315   315X,'ICT=1 FIRST-ORDER CHEMICAL TRANSFORMATION LOSS OF POLLUTANT 00023110
2316   4IS CONSIDERED'//)
2317 933 FORMAT(1H+,92X,'W2=',F8.3) 00023130
2318 934 FORMAT(13X,'NPOL=2'/
2319   215X,'ICT=0 CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED'00023150
2320   3/15X,'ICT=1 FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO00023160
2321   4 POLLUTANT-2 IS CONSIDERED'//)
2322 935 FORMAT(1H+,88X,'ASCALE=',F9.3) 00023180
2323 936 FORMAT(10X,'CHEMICAL TRANSFORMATION RATE: XKT=',F7.3, 00023190
2324   1' PERCENT/HR'//)
2325 938 FORMAT(10X,'RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO00023210
2326   1 POLLUTANT-1 (REACTANT): GAMMA=',F6.3/) 00023220
2327 940 FORMAT(//9X,'OUTPUT OPTIONS SELECTED:'//) 00023230
2328 942 FORMAT(13X,'NLIST=',I1,3X,'LISTS OF CONCENTRATION AND SURFACE DEPO00023240
2329   1SITION FLUX AT EACH RECEPTOR IN THE GRID,'/24X,'ONE COLUMN PER PAG00023250
2330   2E')
2331 944 FORMAT(13X,'NARRAY=',I1,2X,'MAPS OF CONCENTRATION AND SURFACE DEP00023270
2332   1SITION FLUX AT EACH RECEPTOR IN THE GRID,') 00023280
2333 946 FORMAT(24X,'CALIBRATED AND UNCALIBRATED') 00023290
2334 948 FORMAT(24X,'UNCALIBRATED ONLY') 00023300
2335 950 FORMAT(24X,'CALIBRATED ONLY') 00023310
2336 952 FORMAT(13X,'NTAPE=',I1,3X,'TAPE CONTAINING COORDINATES, CONCENTRAT00023320
2337   1ION, AND SURFACE DEPOSITION FLUX'/24X,'AT EACH RECEPTOR IN THE GRI00023330
2338   2D'/13X,'INTER=',I2,2X,'INTERVAL OF RECEPOTRS WHICH WILL BE WRITTEN00023340
2339   3 ON TAPE')
2340 954 FORMAT(13X,'NCOPT=',I1,2X,'LIST OF POINT SOURCE CULPABILITY FOR C00023360
2341   1ONCENTRATION AND SURFACE DEPOSITION FLUX'/24X,'AT EACH RECEPTOR IN00023370
2342   2 THE GRID')
2343 956 FORMAT(13X,'NPRINT=',I1,2X,'LIST OF POINT SOURCE PARAMETERS AND EF00023390
2344   1FFECTIVE STACK HEIGHTS'/24X,'PRINTED AT BEGINNING OF EACH SCENARIO'00023400
2345   2)
2346 958 FORMAT(13X,'NMAX=',I1,4X,'LIST OF RECEPOTRS WITH HIGHEST CONCENTRA00023420
2347   1TION AND SURFACE DEPOSITION FLUX'/24X,'FOR EACH SCENARIO - PRINTED00023430
2348   2 AT END OF RUN')
2349 960 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'//4X,'INPUT SCENARIO PAR00023450
2350   1AMETERS: ',20A4//26X,'WIND DIRECTIONS',27X,'WIND SPEED CLASSES', 00023460
2351   212X,'STABILITY CLASSES')
2352 962 FORMAT(10X,'SECTOR DIRECTION',6X,'SECTOR DIRECTION',9X, 00023480
2353   1'CLASS SPEED CLASS',15X,'CLASS'/
2354   210X,'NUMBER',8X,'(DEG)',6X,'NUMBER',8X,'(DEG)',9X,'INDEX (M/S) 00023500
2355   3 INTERVAL(KT)',9X,'INDEX CLASS'//13X,'1 N',7X,'0.0',9X,'9 00023510
2356   4S',5X,'180.0'/13X,'2 NNE 22.5',8X,'10 SSW 202.5',11X, 00023520
2357   5'1',6X,'1.50',7X,'0-3',16X,'1',7X,'A'/13X,'3 NE',5X,'45.0',8X, 00023530
2358   6'11 SW 225.0',11X,'2',6X,'2.46',7X,'4-6',16X,'2',7X,'B') 00023540
2359 963 FORMAT(13X,'4 ENE 67.5',8X,'12 WSW 247.5',11X,'3',6X, 00023550
2360   1'4.47',7X,'7-10',15X,'3',7X,'C'/13X,'5 E',6X,'90.0',8X,'13 W00023560
2361   2',5X,'270.0',11X,'4',6X,'6.93',6X,'11-16',15X,'4',7X,'00 (DAY)'/ 00023570
2362   313X,'6 ESE 112.5',8X,'14 WNW 292.5',11X,'5',6X,'9.61', 00023580
2363   46X,'17-21',15X,'5',7X,'DN (NIGHT)'/13X,'7 SE 135.0',8X,'15 00023590
2364   5 NW 315.0',11X,'6',5X,'12.52 OVER 21',15X,'6',7X,'E'/. 00023600
2365   613X,'8 SSE 157.5',8X,'16 NNN 337.5',48X,'7',7X,'F'//) 00023610
2366 964 FORMAT(5X,'SCENARIO',3X,'STABILITY',3X,'WIND SPEED',5X,'WIND',8X, 00023620
2367   1'WIND',6X,'WIND',8X,'AMBIENT',9X,'INVERSION',8X,'MIXING'/
2368   26X,'NUMBER',6X,'CLASS',7X,'CLASS',8X,'SPEED',6X,'SECTOR',3X, 00023640
2369   3'DIRECTION',3X,'TEMPERATURE',3X,'PENETRATION FACTOR',3X,'HEIGHT'/
2370   443X,'(M/S)',17X,'(DEG)',7X,'(DEG C)',27X,'(M)')/ 00023660
2371 966 FORMAT(8X,I2,10X,A2) 00023670
2372 970 FORMAT(1H+,31X,I1) 00023680
2373 972 FORMAT(1H+,42X,F6.3) 00023690
2374 974 FORMAT(1H+,55X,I2) 00023700
2375 978 FORMAT(1H+,63X,F6.2,7X,F7.2,11X,F6.3,8X,F7.1) 00023710
2376 980 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'//4X,'INPUT POINT SOURCE00023720
2377   1 PARAMETERS: ',20A4//'
2378   26X,'POINT SOURCE',10X,'COORDINATES',9X,'EMISSION RATE', 00023740
2379   36X,'EMISSION RATE',5X,'HEIGHT',4X,'DIAMETER',4X,'EXIT VEL',5X, 00023750
2380   4'EXIT TEMP'/5X,'NUMBER',3X,'LABEL',7X,'X(KM)',5X,'Y(KM)',6X, 00023760
2381   5'POLLUTANT-1 (G/S)',2X,'POLLUTANT-2 (G/S)',3X,'(M)',8X,'(M)',8X, 00023770
2382   6'(M/S)',8X,'(DEG C)'/) 00023780
2383 984 FORMAT(6X,I3,3X,2A4,3X,F8.2,2X,F8.2,10X,F9.3,10X,F9.3,6X,F6.2,5X, 00023790
2384   1F6.3,6X,F7.3,6X,F8.3) 00023800
2385 986 FORMAT(1H0,5X,'SUMS OF THE POINT SOURCE EMISSION RATES',6X,F9.3, 00023810
2386   1' G/S',6X,F9.3,' G/S') 00023820

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2387 990 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'//4X,'INPUT AREA SOURCE 00023830
2388 1PARAMETERS: ',20A4/// 00023840
2389 270X,'POLLUTANT-1',17X,'POLLUTANT-2'/5X,'AREA SOURCE',8X, 00023850
2390 3'COORDINATES',9X,'LENGTH OF SIDE',11X,'EMISSION RATE',15X, 00023860
2391 4'EMISSION RATE' / 00023870
2392 57X,'NUMBER',9X,'X(KM)',5X,'Y(KM)',13X,'(M)',12X,'INPUT (G/S)', 00023880
2393 64X,'SCALED',7X,'INPUT (G/S)',4X,'SCALED') / 00023890
2394 992 FORMAT(9X,I2,8X,F8.2,2X,F8.2,10X,F8.2,9X,F9.3,4X,F9.3,6X, 00023900
2395 1 F9.3,4X,F9.3) 00023910
2396 994 FORMAT(1H0,5X,'SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN' 00023920
2397 1,8X,F9.3,4X,F9.3,6X,F9.3,4X,F9.3) 00023930
2398 END 00023940
2399 C 00023950
2400 C 00023960
2401 SUBROUTINE OUTMOD 00023970
2402 C SUBROUTINE OUTMOD (VERSION 82360), PART OF PEM. 00023980
2403 C 00023990
2404 C 00024000
2405 C SUBROUTINE OUTMOD COORDINATES OUTPUT OF THE CONCENTRATION(S) 00024010
2406 C AND SURFACE DEPOSITION FLUX(ES) CALCULATED FOR EACH RECEPTOR 00024020
2407 C IN THE GRID FOR EACH SCENARIO. 00024030
2408 C ON OPTION, THE OUTPUT MAY BE IN THE FORM OF LISTS, ARRAY 00024040
2409 C MAPS, OR TAPE. 00024050
2410 C OUTMOD CALLS SUBROUTINE SCENMX TO DETERMINE AND STORE THE 00024060
2411 C RECEPTORS WITH MAXIMUM CONCENTRATION(S) AND SURFACE DEPOSITION 00024070
2412 C FLUX(ES) FOR THE SCENARIO. 00024080
2413 C 00024090
2414 C 00024100
2415 C *** PEM MODIFICATIONS AND FORMATS BY MARTHA M. STEVENS, 00024110
2416 C NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830 00024120
2417 C DECEMBER 1982 00024130
2418 C 00024140
2419 C 00024150
2420 COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00024160
2421 1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00024170
2422 2 XA(50),YA(50),EA(50,2),SIZE(50), 00024180
2423 3 WD(24),WS(24),TA(24),HMIX(24),PEN(24), 00024190
2424 4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00024200
2425 5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLNAM(3,2),CALNAM(7,2), 00024210
2426 6 ITA,IRD,IMR,IDS, D80,047,D8047,DIST,DELTA, 00024220
2427 7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS, UINV,WVEC, 00024230
2428 8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS, 00024240
2429 9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCOPT,NMAX, 00024250
2430 * NSTDWN,INTER,NPRINT 00024260
2431 C 00024270
2432 COMMON/PARMI/NPOL,ICT,VD1,W1,VD2,W2,TAUC 00024280
2433 DIMENSION CON(2),CALCON(2),SD(2),CALSD(2) 00024290
2434 C 00024300
2435 C 00024310
2436 WOUT= WD(ISCEN)*180./3.1415927 00024320
2437 C 00024330
2438 C CONTROL STRATEGY RESULTS OUTPUT BY SUBROUTINE WROUT 00024340
2439 IF(NCOPT.GT.0.AND.NTOPT.EQ.1) CALL WROUT 00024350
2440 C 00024360
2441 C PRINT AND/OR WRITE-ON-TAPE LISTS OF CONCENTRATION(S) AND 00024370
2442 C SURFACE DEPOSITION FLUX(ES) 00024380
2443 IF(NLIST.EQ.0 .AND. NTAP.EQ.0) GO TO 350 00024390
2444 IF(NTAPE.EQ.1) WRITE(ITA,900)TT 00024400
2445 NREP=0 00024410
2446 C 00024420
2447 C BEGIN LOOP ON COLUMNS 00024430
2448 100 DO 325 I=1,LX 00024440
2449 IF(NLIST.EQ.0) GO TO 250 00024450
2450 ISKIP=0 00024460
2451 DO 125 JM=1,LY 00024470
2452 DO 125 KM=1,2 00024480
2453 IF(CONC(I,JM,KM).NE.0.) GO TO 130 00024490
2454 125 CONTINUE 00024500
2455 ISKIP=1 00024510
2456 IF(NTAPE.EQ.0) GO TO 325 00024520
2457 GO TO 250 00024530
2458 130 IF(NREP.EQ.1) GO TO 150 00024540
2459 WRITE(IWR,905)TT,ISCEN,SCLAB(ISC),WS(ISCEN),WOUT, 00024550
2460 1 HMIX(ISCEN),IAV 00024560
2461 WRITE(IWR,910)(CALNAM(L,1),L=1,7),(CALNAM(L,2),L=1,7), 00024570
2462 1 (POLNAM(L,1),L=1,3),(POLNAM(L,2),L=1,3),(POLNAM(L,1),L=1,3), 00024580
2463 2 (POLNAM(L,2),L=1,3) 00024590

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2464      GO TO 250                                         00024600
2465 150 WRITE(IWR,907) TT,ISCEN,SCLAB(ISC),WS(ISCEN),WOUT,    00024610
2466     1 HMIX(ISCEN),IAV                                00024620
2467     WRITE(IWR,912) (CALNAM(L,1),L=1,7), (CALNAM(L,2),L=1,7), 00024630
2468     1 (POLNAM(L,1),L=1,3),(POLNAM(L,2),L=1,3),(POLNAM(L,1),L=1,3), 00024640
2469     2 (POLNAM(L,2),L=1,3)                            00024650
2470 C
2471   250 XI=I                                         00024660
2472     X=XSWC+(XI-0.5)*GRID                           00024670
2473 C BEGIN LOOP ON ROWS IN THIS COLUMN                  00024690
2474     DO 300 J=1,LY                                    00024700
2475     YJ=J                                         00024710
2476     Y=YSWC+(YJ-0.5)*GRID                           00024720
2477 C
2478 C INITIALIZE CONCENTRATION AND SDF VARIABLES       00024730
2479     DO 260 K=1,2                                    00024740
2480     CON(K)=0.                                       00024750
2481     CALCON(K)=0.                                     00024760
2482     SD(K)=0.                                       00024770
2483     CALSD(K)=0.                                     00024780
2484 260 CONTINUE                                         00024790
2485 C SET CONCENTRATION AND SDF - APPLY CALIBRATION COEFFICIENTS 00024800
2486     DO 280 K=1,NPOL                                00024810
2487     IF(NREP.EQ.1) GO TO 270                         00024820
2488     CON(K)=CONC(I,J,K)                            00024830
2489     CALCON(K)= A(K) + B(K) * CON(K)                00024840
2490     SD(K)=SDF(I,J,K)                             00024850
2491     CALSD(K)= A(K) + B(K) * SD(K)                 00024860
2492 280 CONTINUE                                         00024870
2493 C
2494     IF(NLIST.EQ.0 .OR. ISKIP.EQ.1) GO TO 290        00024880
2495     IF(NREP.EQ.0) WRITE(IWR,970) I,J,X,Y,CON(1),CON(2), 00024890
2496     1 CALCON(1),CALCON(2)                           00024900
2497     IF(NREP.EQ.1) WRITE(IWR,970) I,J,X,Y,SD(1),SD(2), 00024910
2498     1 CALSD(1),CALSD(2)                            00024920
2499 290 IF(NTAPE.EQ.0 .OR. NREP.EQ.1) GO TO 300        00024930
2500     IF(((I-1)/INTER)*INTER.NE.(I-1).OR.((J-1)/INTER)*INTER.NE. 00024940
2501     1 (J-1)) GO TO 300                            00024950
2502     WRITE(ITA,975)X,Y,(CON(K),SD(K),CALCON(K),CALSD(K),K=1,2) 00024960
2503 300 CONTINUE                                         00024970
2504 325 CONTINUE                                         00024980
2505 C
2506     IF(NLIST.EQ.0 .OR. NREP.EQ.1) GO TO 350        00024990
2507 C
2508     C IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT 00025000
2509     IF(VD1.LE.0.01 .AND. VD2.LE.0.01) GO TO 350        00025010
2510     NREP=1                                         00025020
2511     GO TO 100                                         00025030
2512 C
2513 C PRINT ARRAY MAPS OF CONCENTRATIONS               00025040
2514 350 IF(NARRAY.GT.0) CALL ARRAY                     00025050
2515 C
2516 C DETERMINE MAXIMUM PREDICTED CONCENTRATION(S) FOR SCENARIO VIA SCENMX 00025060
2517     IF(NMAX.GT.0.AND.(NTOPT.EQ.1.OR.ISCEN.EQ.NSCEN)) CALL SCENMX 00025070
2518 C
2519     RETURN                                         00025080
2520 C
2521 900 FORMAT(20A4)                                     00025090
2522     905 FORMAT(1H1,'PEM OUTPUT: PREDICTED CONCENTRATION: ', 00025100
2523     120A4/' SCENARIO ',I2,', STABILITY=',A2,', WIND SPEED=',F5.2,' M/S, 00025110
2524     2 WIND DIRECTION=',F6.2,' DEG, MIXING HEIGHT=',F7.1,' M, AVERAGING 00025120
2525     3TIME=',I3,' HR//')                           00025130
2526     907 FORMAT(1H1,'PEM OUTPUT: PREDICTED SURFACE DEPOSITION FLUX: ', 00025140
2527     120A4/' SCENARIO ',I2,', STABILITY=',A2,', WIND SPEED=', 00025150
2528     2F5.2,' M/S, WIND DIRECTION=',F6.2,' DEG, MIXING HEIGHT=',F7.1, 00025160
2529     3' M, AVERAGING TIME='.I3,' HR//')             00025170
2530     910 FORMAT(33X,'UNCALIBRATED CONCENTRATION',11X,'CALIBRATED CONCENTRAT 00025180
2531     1ION POL-1: ',7A4/16X,'RECEPTOR',9X,'(MICROGRAMS PER CUBIC METER)' 00025190
2532     2,9X,'CALIBRATED CONCENTRATION POL-2: ',7A4/15X,'COORDINATES',7X, 00025200
2533     3' POLLUTANT-1',5X,'POLLUTANT-2',10X,'POLLUTANT-1',5X,'POLLUTANT-2'/ 00025210
2534     4' COL ROW',6X,'X(KM)',4X,'Y(KM)',5X,3A4,4X,3A4,9X,3A4,4X,3A4) 00025220
2535     912 FORMAT(32X,'UNCALIBRATED SURFACE DEPOSITION FLUX',4X,'CALIBRATED V 00025230
2536     1ALUE POLLUTANT-1: ',7A4/16X,'RECEPTOR',9X,'(MICROGRAMS PER SQ MET 00025240
2537     2ER PER HOUR)',5X,'CALIBRATED VALUE POLLUTANT-2: ',7A4/ 00025250
2538     315X,'COORDINATES',7X,'POLLUTANT-1',5X,'POLLUTANT-2',12X, 00025260
2539     4' POLLUTANT-1',5X,'POLLUTANT-2//' COL ROW',6X,'X(KM)',4X,'Y(KM)', 00025270
2540     55X,3A4,4X,3A4,11X,3A4,4X,3A4)                00025280

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2541      970 FORMAT(2(2X,I2),2X,F9.2,F9.2,6X,F11.4,5X,F11.4,10X,F11.4,5X,F11.4)00025370
2542      975 FORMAT(10F8.2)
2543      END
2544      C
2545      SUBROUTINE ARRAY
2546      C
2547      C          SUBROUTINE ARRAY (VERSION 82360), PART OF PEM. 00025430
2548      C
2549      C
2550      C          SUBROUTINE ARRAY CREATES ARRAY MAPS OF THE CONCENTRATIONS AND 00025460
2551      C          SURFACE DEPOSITION FLUXES IN THE RECEPTOR GRID AND 00025470
2552      C          PRINTS THEM AT THE END OF EACH SCENARIO. 00025480
2553      C          UNCALIBRATED AND CALIBRATED CONCENTRATIONS OF EACH POLLUTANT 00025490
2554      C          APPEAR ON SEPARATE MAPS OF UP TO FOUR SECTIONS (PAGES) EACH. 00025500
2555      C
2556      C
2557      C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS, 00025530
2558      C          NOAA-ATDL, P.O. BOX E, OAK RIDGE, TN 37830 00025540
2559      C          DECEMBER 1982 00025550
2560      C
2561      C
2562      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00025580
2563      1 XPC(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00025590
2564      2 XA(50),YA(50),EA(50,2),SIZE(50), 00025600
2565      3 WD(24),WS(24),TA(24),HMIX(24),PEN(24), 00025610
2566      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00025620
2567      5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLNAM(3,2),CALNAM(7,2), 00025630
2568      6 ITA,IRD,IWR,IDSX, D80,D47,D8047,DIST,DELTA, 00025640
2569      7 ESH(2),PEAK,IBUOY,IRISE,IDLW,EFF,XS, UINV,WVEC, 00025650
2570      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS, 00025660
2571      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCOPT,NMAX, 00025670
2572      * NSTDWN,INTER,NPRINT 00025680
2573      C
2574      COMMON/PARML/NPOL,ICT,VD1,W1,VD2,W2,TAUC 00025690
2575      DIMENSION X(50),CC(50),SSDF(50),DV(2) 00025700
2576      INTEGER CC,SSDF 00025710
2577      C
2578      DV(1)=VD1 00025720
2579      DV(2)=VD2 00025730
2580      WOUT= WD(ISCEN)*180./3.1415927 00025740
2581      NLX=1 00025750
2582      NLY=1 00025760
2583      IF(LX.GT.25) NLX=2 00025770
2584      IF(LY.GT.25) NLY=2 00025780
2585      NSECT=NLX*NLY 00025790
2586      C
2587      100 ISECT=0 00025800
2588      DO 700 JLX=1,NLX 00025810
2589      MX2= JLX*25 00025820
2590      IF(MX2.GT.LX) MX2=LX 00025830
2591      MX1=1 00025840
2592      IF(JLX.EQ.2) MX1=26 00025850
2593      DO 125 I=MX1, MX2 00025860
2594      XI=I 00025870
2595      125 X(I)= XSWC + (XI-0.5)*GRID 00025880
2596      DO 600 JLY=1,NLY 00025890
2597      ISECT=ISECT+1 00025900
2598      IF(JLY.EQ.1) GO TO 150 00025910
2599      MY1=26 00025920
2600      MY2=LY 00025930
2601      GO TO 175 00025940
2602      150 MY1=1 00025950
2603      MY2=25 00025960
2604      IF(LY.LT.25) MY2=LY 00025970
2605      175 DO 500 N=1,NPOL 00025980
2606      NREP=0 00025990
2607      180 IF(NARRAY.EQ.3) GO TO 320 00026000
2608      WRITE(IWR,900)ISECT,NSECT,ISCEN,TT 00026010
2609      WRITE(IWR,902)SCLAB(ISC),WS(ISCEN),WOUT,HMIX(ISCEN),IAV, 00026020
2610      1 N,(POLNAM(L,N),L=1,3) 00026030
2611      IF(NREP.EQ.0) GO TO 185 00026040
2612      C          LOOP THROUGH SDF ARRAY TO FIND ANY VALUE GE 1000. IN THAT CASE, 00026050
2613      C          SET FLAG TO SCALE SDF VALUES AS THEY ARE SET IN SSDF ARRAY 00026060
2614      C          IFLAG=0 00026070
2615      DO 182 NX=1,LX 00026080
2616      DO 182 NY=1,LY 00026090
2617      IF(SDF(NX,NY,N).GT.999.49) GO TO 184 00026100

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2618    182 CONTINUE          00026140
2619        WRITE(IWR,905)      00026150
2620        GO TO 190         00026160
2621    184 IFLAG=1           00026170
2622        WRITE(IWR,910)      00026180
2623        GO TO 190         00026190
2624    185 WRITE(IWR,904)      00026200
2625    190 WRITE(IWR,915) (X(I),I=MX1,MX2,2) 00026210
2626        DO 300 J=MY1,MY2 00026220
2627        IY= MY2 + MY1 - J 00026230
2628        Y=IY              00026240
2629        Y= YSWC + (Y-0.5)*GRID 00026250
2630    C
2631        IF(NREP.EQ.1) GO TO 240 00026260
2632        DO 230 I=MX1,MX2 00026270
2633        CC(I)= CONC(I,IY,N) + 0.5 00026280
2634        WRITE(IWR,920)Y,(CC(I),I=MX1,MX2) 00026290
2635        GO TO 300         00026300
2636    240 DO 250 I=MX1,MX2 00026310
2637        IF(IFLAG.EQ.0) GO TO 245 00026320
2638        SSDF(I)=SDF(I,IY,N)*1.0E-03 + 0.5 00026330
2639        GO TO 250         00026340
2640        245 SSDF(I)= SDF(I,IY,N) + 0.5 00026350
2641    250 CONTINUE          00026360
2642        WRITE(IWR,920) Y,(SSDF(I),I=MX1,MX2) 00026370
2643    300 WRITE(IWR,925)Y 00026380
2644        WRITE(IWR,915)(X(I),I=MX1,MX2,2) 00026390
2645    320 IF(NARRAY.EQ.2) GO TO 450 00026400
2646        WRITE(IWR,900)ISECT,NSECT,ISCEN,TT 00026410
2647        WRITE(IWR,902)SCLAB(ISC),WS(ISCEN),WOUT,HMIX(ISCEN),IAV, 00026420
2648        1 N,(POLNAM(L,N),L=1,3) 00026430
2649        IF(NREP.EQ.0) WRITE(IWR,906)(CALNAM(L,N),L=1,7),A(N),B(N) 00026440
2650        IF(NREP.EQ.1) WRITE(IWR,907) (CALNAM(L,N),L=1,7),A(N),B(N) 00026450
2651        WRITE(IWR,915)(X(I),I=MX1,MX2,2) 00026460
2652        DO 400 J=MY1,MY2 00026470
2653        IY= MY2 + MY1 - J 00026480
2654        Y=IY              00026490
2655        Y= YSWC + (Y-0.5)*GRID 00026500
2656    C
2657        IF(NREP.EQ.1) GO TO 340 00026510
2658        DO 330 I=MX1,MX2 00026520
2659        330 CC(I)= A(N) + B(N)*CONC(I,IY,N) + 0.5 00026530
2660        WRITE(IWR,920)Y,(CC(I),I=MX1,MX2) 00026540
2661        GO TO 400         00026550
2662    340 DO 350 I=MX1,MX2 00026560
2663        350 SSDF(I)= A(N) + B(N) * SDF(I,IY,N) + 0.5 00026570
2664        WRITE(IWR,920) Y,(SSDF(I),I=MX1,MX2) 00026580
2665    400 WRITE(IWR,925)Y 00026590
2666        WRITE(IWR,915)(X(I),I=MX1,MX2,2) 00026600
2667    450 IF(NREP.EQ.1) GO TO 500 00026610
2668    C  IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT 00026620
2669        IF(DV(N).LE.0.01) GO TO 500 00026630
2670        NREP=1             00026640
2671        GO TO 180         00026650
2672    500 CONTINUE          00026660
2673    600 CONTINUE          00026670
2674    700 CONTINUE          00026680
2675    C
2676        RETURN            00026690
2677    C
2678    900 FORMAT(1H1,'PEM OUTPUT: ','SECTION ',I1,' OF ',I1,', SCENARIO ', 00026700
2679        1 I2.2X,20A4)      00026710
2680    902 FORMAT(' STABILITY=',A2,', WIND SPD=',F5.2,' M/S, WIND DIR=',F6.2,00026720
2681        1 ' DEG, MIXING HT=',F7.1,' M, AVERAGING TIME=',I3,' HR.',',6X, 00026730
2682        2 ' POLLUTANT-',I1,': ',3A4) 00026740
2683    904 FORMAT(' UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER')00026750
2684    905 FORMAT(' UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQU00026760
2685        IARE METER PER HOUR') 00026770
2686    906 FORMAT(' CALIBRATED CONCENTRATION - ',7A4,18X,'CALIBRATION COEFFIC00026780
2687        1IENTS: A =',F11.4,', B =',F11.4) 00026790
2688    907 FORMAT(' CALIBRATED SURFACE DEPOSITION FLUX - ',7A4,10X, 00026800
2689        1'CALIBRATION COEFFICIENTS: A=',F10.4,5X,'B=',F10.4) 00026810
2690    910 FORMAT(' UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUA00026820
2691        1RE KILOMETER PER HOUR') 00026830
2692    915 FORMAT(1H0,14X,13F8.2) 00026840
2693    920 FORMAT(1H0,4X,F8.2,4X,25I4) 00026850
2694    925 FORMAT(1H+,122X,F8.2) 00026860

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2695      END                               00026910
2696      C
2697      C
2698      C      SUBROUTINE WORST(I,J,CHI)        00026920
2699      C      SUBROUTINE WORST (VERSION 82360), PART OF PEM. 00026930
2700      C
2701      C
2702      C      SUBROUTINE WORST DETERMINES THE FIVE POINT SOURCES CONTRIBUTING THE 00026940
2703      C      MOST TO THE TOTAL CONCENTRATION AT EACH RECEPTOR. SOURCE 00026950
2704      C      IDENTIFICATIONS AND CONTRIBUTIONS ARE STORED IN NWORST AND CWORST 00026960
2705      C      RESPECTIVELY, FOR OUTPUT BY SUBROUTINE WROUT. 00026970
2706      C
2707      C
2708      C      *** PEM MODIFICATIONS BY M.M. STEVENS, 00026980
2709      C      NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830 00026990
2710      C      DECEMBER 1982 00027000
2711      C
2712      C
2713      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00027010
2714      1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00027020
2715      2 XA(50),YA(50),EA(50,2),SIZE(50), 00027030
2716      3 WD(24),WS(24),TA(24),HMIX(24),PEN(24), 00027040
2717      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00027050
2718      5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLNAM(3,2),CALNAM(7,2), 00027060
2719      6 ITA,IRD,IWR,IDS, D80,D47,D8047,DIST,DELTA, 00027070
2720      7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS, UINV,WVEC, 00027080
2721      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS, 00027090
2722      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCOPT,NMAX, 00027100
2723      * NSTDWN,INTER,NPRINT 00027110
2724      C
2725      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5) 00027200
2726      C
2727      C
2728      IF(CHI.LE.CWORST(I,J,5)) RETURN 00027210
2729      IF(CHI.GT.CWORST(I,J,4)) GO TO 205 00027220
2730      CWORST(I,J,5)= CHI 00027230
2731      NWORST(I,J,5)= IPS
2732      RETURN
2733      205 IF(CHI.GT.CWORST(I,J,3)) GO TO 210 00027240
2734      NW=1 00027250
2735      GO TO 225 00027260
2736      210 IF(CHI.GT.CWORST(I,J,2)) GO TO 215 00027270
2737      NW=2 00027280
2738      GO TO 225 00027290
2739      215 IF(CHI.GT.CWORST(I,J,1)) GO TO 220 00027300
2740      NW=3 00027310
2741      GO TO 225 00027320
2742      220 NW=4 00027330
2743      225 DO 250 IW=1,NW 00027340
2744      CWORST(I,J,6-IW)= CWORST(I,J,5-IW) 00027350
2745      250 NWORST(I,J,6-IW)= NWORST(I,J,5-IW) 00027360
2746      CWORST(I,J,5-NW)= CHI 00027370
2747      NWORST(I,J,5-NW)= IPS 00027380
2748      RETURN 00027390
2749      END
2750      C
2751      C
2752      SUBROUTINE WROUT 00027400
2753      C      SUBROUTINE WROUT (VERSION 82350), PART OF PEM. 00027410
2754      C
2755      C
2756      C      SUBROUTINE WROUT PRINTS A CULPABILITY LIST OF THE IDENTIFICATIONS 00027420
2757      C      AND CONTRIBUTIONS OF THE FIVE POINT SOURCES CONTRIBUTING THE MOST 00027430
2758      C      TO THE TOTAL CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH 00027440
2759      C      RECEPTOR, USING DATA COMPILED BY SUBROUTINE WORST 00027450
2760      C
2761      C
2762      C      *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS, 00027460
2763      C      NOAA-ATDL, P.O. BOX E, OAK RIDGE, TN 37830 00027470
2764      C      DECEMBER 1982 00027480
2765      C
2766      C
2767      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00027490
2768      1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00027500
2769      2 XA(50),YA(50),EA(50,2),SIZE(50), 00027510
2770      3 WD(24),WS(24),TA(24),HMIX(24),PEN(24), 00027520
2771      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00027530

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2772      5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),    00027680
2773      6 ITA,IRD,IWR,IDS,        D80,D47,D8047,DIST,DELTA,          00027690
2774      7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,   UINV,WVEC,           00027700
2775      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,         00027710
2776      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCOSOPT,NMAX,  00027720
2777      * NSTDWN,INTER,NPRINT          00027730
2778      C
2779      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)                  00027740
2780      C
2781      C
2782      WOUT= WD(ISCEN)*180./3.1415927                         00027750
2783      N=1
2784      IF(NTOPT.EQ.1) GO TO 250                         00027760
2785      N=2
2786      250 DO 400 I=1,LX                         00027770
2787      C IF ALL CONCENTRATION VALUES ARE ZERO IN THIS COL, SKIP IT 00027780
2788      DO 275 JM=1,LY                         00027790
2789      IF(CONC(I,JM,N).NE.0.) GO TO 280             00027800
2790      275 CONTINUE                         00027810
2791      GO TO 400
2792      C
2793      280 WRITE(IWR,905) TT,(POLNAM(L,1),L=1,3)            00027820
2794      WRITE(IWR,910) ISCEN,WOUT,WS(ISCEN),SCLAB(ISC),HMIX(ISCEN),IAV 00027830
2795      WRITE(IWR,915)
2796      XI=I
2797      X= XSWC + (XI-0.5)*GRID                   00027840
2798      DO 400 J=1,LY                         00027850
2799      IF(CONC(I,J,N).LT.1.0E-5) GO TO 303       00027860
2800      DO 300 L=1,5                         00027870
2801      300 CWORST(I,J,L)= CWORST(I,J,L)*100./CONC(I,J,N) 00027880
2802      303 YJ=J
2803      Y= YSWC + (YJ-0.5)*GRID                   00027890
2804      WRITE(IWR,925) I,J,X,Y,NWORST(I,J,1),CWORST(I,J,1),NWORST(I,J,2), 00027900
2805      1 CWORST(I,J,2),NWORST(I,J,3),CWORST(I,J,3),NWORST(I,J,4), 00027910
2806      2 CWORST(I,J,4),NWORST(I,J,5),CWORST(I,J,5),CONC(I,J,N),SDF(I,J,N) 00027920
2807      400 CONTINUE                         00027930
2808      C
2809      RETURN
2810      C
2811      905 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'//4X,'OUTPUT: ',20A4// 00027940
2812      14X,'LIST OF THE FIVE POINT SOURCES WHICH PRODUCE THE HIGHEST VALUE 00027950
2813      25 OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR'//00027960
2814      34X,'POLLUTANT: ',3A4,' - CONCENTRATION IN MICROGRAMS PER CUBIC METER 00027970
2815      4ETER'/32X,'SURFACE DEPOSITION FLUX IN MICROGRAMS PER SQUARE METER 00027980
2816      5PER HOUR')                           00027990
2817      910 FORMAT(4X,'SCENARIO',6X,'WIND DIRECTION',6X,'WIND SPEED',6X,'STABI00028000
2818      1ILITY CLASS',6X,'MIXING HEIGHT',6X,'AVERAGING TIME'/
2819      25X,'NUMBER',11X,'(DEG)',13X,'(M/S)',34X,'(M)',17X,'(HR)'// 00028010
2820      37X,I2,13X,F5.1,13X,F5.2,15X,A2,15X,F7.2,15X,I3/) 00028020
2821      915 FORMAT(45X,'POINT SOURCE SEQUENCE NUMBER AND PERCENT'/
2822      115X,'COORDINATES',15X,'OF TOTAL CONCENTRATION AND SURFACE DEPOSITI00028030
2823      20N FLUX',14X,'TOTAL',8X,'TOTAL SURFACE'/
2824      3' COL ROW',4X,'X (KM)',4X,'Y (KM)',9X,'HIGHEST',6X,'SECOND',8X, 00028040
2825      4'THIRD',7X,'FOURTH',8X,'FIFTH',6X,'CONCENTRATION',3X,'DEPOSITION F00028050
2826      5LUX')/
2827      925 FORMAT(2(2X,I2),3X,F8.2,2X,F8.2,3X,5(3X,I3,F7.2),6X,F8.2,9X,F8.2) 00028060
2828      C
2829      END
2830      C
2831      C
2832      SUBROUTINE SCENMX
2833      SUBROUTINE SCENMX (VERSION 82360), PART OF PEM. 00028070
2834      C
2835      C
2836      C SUBROUTINE SCENMX LOCATES AND STORES THE COORDINATES, CONCENTRATION, 00028080
2837      C AND SURFACE DEPOSITION FLUX AT THE RECEPTOR GRID POINTS RECORDING 00028090
2838      C THE HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX OF EACH 00028100
2839      C POLLUTANT IN EACH SCENARIO. STORED VALUES ARE PRINTED BY SUBROUTINE 00028110
2840      C MAXOUT AT THE END OF THE RUN. 00028120
2841      C
2842      C
2843      C *** PEM MODIFICATIONS BY M.M. STEVENS, 00028130
2844      C NOAA-ATDL, P.O.BOX - E, OAK RIDGE, TN 37830 00028140
2845      C DECEMBER 1982 00028150
2846      C
2847      C
2848      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00028160

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2849      1 XPC(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),    00028450
2850      2 XA(50),YA(50),EA(50,2),SIZE(50),                                00028460
2851      3 WD(24),WS(24),TA(24),HMX(24),PEN(24),                            00028470
2852      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16),          00028480
2853      5 XSWC,YSWC,GRID,LX,LY,   A(2),B(2),POLNAM(3,2),CALNAM(7,2),  00028490
2854      6 ITA,IRD,IWR,IDS,   D80,D47,D8047,DIST,DELTA,                  00028500
2855      7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,   UINV,WVEC,            00028510
2856      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,             00028520
2857      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,    00028530
2858      * NSTDWN,INTER,NPRINT                                         00028540
2859      C
2860      COMMON/MAX/XMX(24,4,2),YMX(24,4,2),ZMX(24,4,2),SMX(24,4,2) 00028550
2861      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                         00028570
2862      C
2863      C
2864      IF(NTOPT.EQ.1) GO TO 120                                     00028600
2865      I= 1                                                       00028610
2866      GO TO 130                                                 00028620
2867      120     I= ISCEN                                         00028630
2868      130     IF(NWDOPT.LE.1) GO TO 140                           00028640
2869      J= IWDOPT                                         00028650
2870      GO TO 150                                                 00028660
2871      140     J= 1                                               00028670
2872      150     DO 400 K=1,NPOL                               00028680
2873      Z= 0.                                                 00028690
2874      DO 350 NX=1,LX                                         00028700
2875      DO 350 NY=1,LY                                         00028710
2876      IF(CONC(NX,NY,K).LT.Z) GO TO 350                      00028720
2877      Z= CONC(NX,NY,K)                                       00028730
2878      ZS=SDF(NX,NY,K)                                       00028740
2879      ZX=NX                                              00028750
2880      ZY=NY                                              00028760
2881      350     CONTINUE                                         00028770
2882      ZMX(I,J,K)= Z                                         00028780
2883      SMX(I,J,K)=ZS                                         00028790
2884      XMX(I,J,K)= XSWC + (ZX - 0.5)*GRID                 00028800
2885      YMX(I,J,K)= YSWC + (ZY - 0.5)*GRID                 00028810
2886      400     CONTINUE                                         00028820
2887      RETURN                                              00028830
2888      END                                                 00028840
2889      C
2890      C
2891      SUBROUTINE MAXOUT                                      00028850
2892      C
2893      C
2894      C
2895      C
2896      C
2897      C
2898      C
2899      C
2900      C
2901      C
2902      C
2903      C
2904      C
2905      C
2906      C
2907      C
2908      1 XPC(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00029030
2909      2 XA(50),YA(50),EA(50,2),SIZE(50),                                00029040
2910      3 WD(24),WS(24),TA(24),HMX(24),PEN(24),                            00029050
2911      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16),          00029060
2912      5 XSWC,YSWC,GRID,LX,LY,   A(2),B(2),POLNAM(3,2),CALNAM(7,2),  00029070
2913      6 ITA,IRD,IWR,IDS,   D80,D47,D8047,DIST,DELTA,                  00029080
2914      7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,   UINV,WVEC,            00029090
2915      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,             00029100
2916      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,    00029110
2917      * NSTDWN,INTER,NPRINT                                         00029120
2918      C
2919      COMMON/MAX/XMX(24,4,2),YMX(24,4,2),ZMX(24,4,2),SMX(24,4,2) 00029130
2920      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                         00029140
2921      DIMENSION ZC(2),ZS(2)                                         00029150
2922      C
2923      C
2924      CHECK WHETHER SURF DEP FLUX WAS CALCULATED AND SET FLAG        00029160
2925      NREP=1                                         00029170
2926      IF(VD1.LE.0.01 .AND. VD2.LE.0.01) NREP=0                         00029180
2927

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2926      C          IF(NWDOPT.GT.1) GO TO 300          00029220
2927      C          J=1                          00029230
2928      C          N=1                          00029240
2929      C          IF(NTOPT.EQ.1) N=NSCEN          00029250
2930      C          PRINT HIGHEST CONCENTRATIONS 00029260
2931      C          WRITE(IWR,900) TT             00029270
2932      C          WRITE(IWR,902) (CALNAM(L,1),L=1,7) 00029280
2933      C          IF(NPOL.EQ.2) WRITE(IWR,903) (CALNAM(L,2),L=1,7) 00029290
2934      C          WRITE(IWR,910) (POLNAM(L,1),L=1,3) 00029300
2935      C          IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3) 00029310
2936      C          WRITE(IWR,912)                00029320
2937      C          WRITE(IWR,915)                00029330
2938      C          DO 200 I=1,N                  00029340
2939      C          DO 120 K=1,NPOL              00029350
2940      C          120 ZC(K)= A(K) + B(K)*ZMX(I,1,K) 00029360
2941      C          WRITE(IWR,920)                00029370
2942      C          WRITE(IWR,925) I,J,(XMX(I,1,K),YMX(I,1,K),ZMX(I,1,K),ZC(K), 00029380
2943      C          1 K=1,NPOL                  00029390
2944      C          200 CONTINUE                 00029400
2945      C          PRINT SURFACE DEPOSITION FLUX VALUES 00029410
2946      C          IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT 00029420
2947      C          IF(NREP.EQ.0) RETURN          00029430
2948      C          WRITE(IWR,900) TT             00029440
2949      C          WRITE(IWR,932) (CALNAM(L,1),L=1,7) 00029450
2950      C          IF(NPOL.EQ.2) WRITE(IWR,933) (CALNAM(L,2),L=1,7) 00029460
2951      C          WRITE(IWR,910) (POLNAM(L,1),L=1,3) 00029470
2952      C          IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3) 00029480
2953      C          WRITE(IWR,942)                00029490
2954      C          WRITE(IWR,915)                00029500
2955      C          DO 250 I=1,N                  00029510
2956      C          DO 220 K=1,NPOL              00029520
2957      C          220 ZS(K)= A(K) + B(K)*SMX(I,1,K) 00029530
2958      C          WRITE(IWR,920)                00029540
2959      C          WRITE(IWR,925) I,J,(XMX(I,1,K),YMX(I,1,K),SMX(I,1,K),ZS(K), 00029550
2960      C          1 K=1,NPOL                  00029560
2961      C          250 CONTINUE                 00029570
2962      C          RETURN                     00029580
2963      C          PRINT FOR CASE OF NWDOPT>1 - SUB-SCENARIOS 00029590
2964      C          300 N=NSCEN                  00029600
2965      C          PRINT HIGHEST CONCENTRATIONS 00029610
2966      C          DO 500 I=1,N                  00029620
2967      C          IF(((I-1)/8)*8.NE.I-1) GO TO 310 00029630
2968      C          WRITE(IWR,900) TT             00029640
2969      C          WRITE(IWR,902) (CALNAM(L,1),L=1,7) 00029650
2970      C          IF(NPOL.EQ.2) WRITE(IWR,903) (CALNAM(L,2),L=1,7) 00029660
2971      C          WRITE(IWR,910) (POLNAM(L,1),L=1,3) 00029670
2972      C          IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3) 00029680
2973      C          WRITE(IWR,912)                00029690
2974      C          WRITE(IWR,915)                00029700
2975      C          310 WRITE(IWR,920)            00029710
2976      C          DO 400 J=1,4                  00029720
2977      C          DO 320 K=1,NPOL              00029730
2978      C          320 ZC(K)= A(K) + B(K)*ZMX(I,J,K) 00029740
2979      C          WRITE(IWR,925) I,J,(XMX(I,J,K),YMX(I,J,K),ZMX(I,J,K),ZC(K), 00029750
2980      C          1 K=1,NPOL                  00029760
2981      C          400 CONTINUE                 00029770
2982      C          500 CONTINUE                 00029780
2983      C          PRINT SURFACE DEPOSITION FLUX VALUES 00029790
2984      C          IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT 00029800
2985      C          IF(NREP.EQ.0) RETURN          00029810
2986      C          DO 600 I=1,N                  00029820
2987      C          IF(((I-1)/8)*8.NE.I-1) GO TO 510 00029830
2988      C          WRITE(IWR,900) TT             00029840
2989      C          WRITE(IWR,932) (CALNAM(L,1),L=1,7) 00029850
2990      C          IF(NPOL.EQ.2) WRITE(IWR,933) (CALNAM(L,2),L=1,7) 00029860
2991      C          IF(NREP.EQ.0) RETURN          00029870
2992      C          DO 600 I=1,N                  00029880
2993      C          IF(((I-1)/8)*8.NE.I-1) GO TO 510 00029890
2994      C          WRITE(IWR,900) TT             00029900
2995      C          WRITE(IWR,910) (POLNAM(L,1),L=1,3) 00029910
2996      C          IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3) 00029920
2997      C          WRITE(IWR,942)                00029930
2998      C          WRITE(IWR,915)                00029940
2999      C          510 WRITE(IWR,920)            00029950
3000      C          WRITE(IWR,915)                00029960
3001      C          00 550 J=1,4                  00029970
3002      C          00 550 J=1,4                  00029980

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3003      DO 520 K=1,NPOL          00029990
3004      520 ZS(K)= A(K) + B(K)*SMX(I,J,K)          00030000
3005      WRITE(IWR,925) I,J,(XMX(I,J,K),YMX(I,J,K),SMX(I,J,K),ZS(K),    00030010
3006      1 K=1,NPOL)          00030020
3007      550 CONTINUE          00030030
3008      600 CONTINUE          00030040
3009      C                      00030050
3010      700 RETURN          00030060
3011      C                      00030070
3012      900 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'//4X,'OUTPUT: ',20A4//)00030080
3013      902 FORMAT(4X,'HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR E00030090
3014      1ACH SCENARIO'//4X,'UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CU00030100
3015      2BIC METER - CALIBRATION, POLLUTANT-1: ',7A4)          00030110
3016      903 FORMAT(65X,'CALIBRATION, POLLUTANT-2: ',7A4)          00030120
3017      910 FORMAT(//40X,'POLLUTANT-1: ',3A4)          00030130
3018      911 FORMAT(1H+,93X,'POLLUTANT-2: ',3A4)          00030140
3019      912 FORMAT(/' SCENARIO WIND DIRECTION',7X,'COORDINATES',14X,    00030150
3020      1'CONCENTRATION',16X,'COORDINATES',14X,'CONCENTRATION')    00030160
3021      915 FORMAT(2X,'NUMBER',4X,'SUB-SCENARIO',6X,'X(KM)',5X,'Y(KM)',6X, 00030170
3022      1'UNCALIBRATED',4X,'CALIBRATED',7X,'X(KM)',5X,'Y(KM)',6X,    00030180
3023      2'UNCALIBRATED',4X,'CALIBRATED')          00030190
3024      920 FORMAT(1X)          00030200
3025      925 FORMAT(4X,I2,11X,I2,8X,F9.2,1X,F9.2,5X,F11.4,4X,F11.4,4X,F9.2,1X, 00030210
3026      1F9.2,5X,F11.4,4X,F11.4)          00030220
3027      932 FORMAT(4X,'HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLU00030230
3028      ITANT FOR EACH SCENARIO'//4X,'UNCALIBRATED VALUES IN MICROGRAMS PER00030240
3029      2 SQUARE METER PER HOUR - CALIBRATION, POLLUTANT-1: ',7A4)          00030250
3030      933 FORMAT(68X,'CALIBRATION, POLLUTANT-2: ',7A4)          00030260
3031      942 FORMAT(/' SCENARIO WIND DIRECTION',7X,'COORDINATES',9X,    00030270
3032      1'SURFACE DEPOSITION FLUX',11X,'COORDINATES',9X,'SURFACE DEPOSITION00030280
3033      2 FLUX')          00030290
3034      END          00030300
3035      C          00030310
3036      C          00030320
3037      SUBROUTINE RISE          00030330
3038      C          SUBROUTINE RISE (VERSION 82360), PART OF PEM. 00030340
3039      C          00030350
3040      C          00030360
3041      C          SUBROUTINE RISE CALCULATES PLUME RISE VIA ONE OF SIX EQUATIONS 00030370
3042      C          (BRIGGS,1969). IF IRISE=1, DISTANCE DEPENDENT EFFECTIVE SOURCE 00030380
3043      C          HEIGHT (ESH(1)) IS RETURNED. IF IRISE=2, MAXIMUM EFFECTIVE SOURCE 00030390
3044      C          HEIGHT (ESH(2)) IS RETURNED. RISE IS CALLED ONCE PER SOURCE PER 00030400
3045      C          SCENARIO WITH IRISE=2. IT IS CALLED WITH IRISE=1 WHENEVER THE 00030410
3046      C          DOWNWIND DISTANCE (DIST) IS LESS THAN THE DISTANCE TO MAXIMUM 00030420
3047      C          PLUME RISE (PEAK).          00030430
3048      C          00030440
3049      C          00030450
3050      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20),          00030460
3051      1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300), 00030470
3052      2 XA(50),YA(50),EA(50,2),SIZE(50),          00030480
3053      3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),          00030490
3054      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00030500
3055      5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLNAM(3,2),CALNAM(7,2), 00030510
3056      6 ITA,IRD,IWR,IDS, D80,D47,D8047,DIST,DELTA,          00030520
3057      7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS, UINV,WVEC, 00030530
3058      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS, 00030540
3059      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX, 00030550
3060      * NSTDWN,INTER,NPRINT          00030560
3061      C          00030570
3062      IDWN=1          00030580
3063      IF(IRISE.EQ.1) GO TO 300          00030590
3064      DWNSH= 1.0          00030600
3065      IF(IBUOY.EQ.0) GO TO 205          00030610
3066      IF(EFF.GE.55.) GO TO 150          00030620
3067      C          00030630
3068      XS,CTB, AND CTMU ARE INDEPENDENT OF DISTANCE, AND ARE THEREFORE 00030640
3069      C          CALCULATED ONCE PER SOURCE PER SCENARIO (WHEN IRISE=2). 00030650
3070      XS= 49.*EFF**0.625          00030660
3071      GO TO 160          00030670
3072      150 XS=119.*EFF**0.4          00030680
3073      160 CTB= 1.6*UINV*EFF**0.333333          00030690
3074      IF(ISC.GE.6) GO TO 170          00030700
3075      C          00030710
3076      C          PEAK PLUME RISE: BUOYANCY-DOMINATED PLUME, UNSTABLE AIR (A-D). 00030720
3077      DELTAH= CTB*XS**0.666667          00030730
3078      GO TO 250          00030740
3079      C          00030750

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3080      C PEAK PLUME RISE: BUOYANCY-DOMINATED PLUME, STABLE AIR (E,F).          00030760
3081      170 DELTAH= 2.6*(EFF*UINV*TA(ISCEN)/(9.8*DTDZ(ISC-5)))*0.333333            00030770
3082          GO TO 250                                         00030780
3083      205 IF(ISC.GE.6) GO TO 230                                         00030790
3084          CTMU= 1.89*(VP(IPS)*VP(IPS)*DP(IPS)*UINV/(VP(IPS)+3./UINV))*0.66600030800
3085          1667                                         00030810
3086      C                                         00030820
3087      C PEAK PLUME RISE: MOMENTUM-DOMINATED PLUME, UNSTABLE AIR (A-D).        00030830
3088          DELTAH= 3.0*VP(IPS)*DP(IPS)*UINV                                         00030840
3089          GO TO 250                                         00030850
3090      C                                         00030860
3091      C PEAK PLUME RISE: MOMENTUM-DOMINATED PLUME, STABLE AIR (E,F).        00030870
3092      230 DELTAH= 1.5*(0.5*VP(IPS)*DP(IPS))*0.666667*UINV*0.333333            00030880
3093          1 *(TA(ISCEN)/(DTDZ(ISC-5)*9.8))*0.166667                         00030890
3094      250 IF(NSTDWN.EQ.1) GO TO 270                                         00030900
3095          IF(VP(IPS)*UINV.GT.1.5) GO TO 270                                         00030910
3096          COELH= 2.0*(1.5 - VP(IPS)*UINV)*DP(IPS)                                00030920
3097          IDWN=3                                         00030930
3098          IF(COELH.GE.DELTAH) GO TO 260                                         00030940
3099          DWNWSH= (DELTAH-COELH)/DELTAH                                         00030950
3100          GO TO 270                                         00030960
3101      260 DWNWSH= 0.                                         00030970
3102      270 ESH(2)= HP(IPS) + DELTAH*DWNWSH                                         00030980
3103          RETURN                                         00030990
3104      C                                         00031000
3105      300 IF(IBUOY.EQ.0) GO TO 500                                         00031010
3106      C                                         00031020
3107      C DISTANCE-DEPENDENT PLUME RISE: BUOYANCY-DOMINATED PLUME,          00031030
3108      C ANY STABILITY (A-F).                                         00031040
3109          ESH(1)= DWNWSH*CTB*(DIST*1000.)*0.666667 + HP(IPS)                  00031050
3110          IF(ESH(1).GT.ESH(2)) ESH(1)=ESH(2)                               00031060
3111          RETURN                                         00031070
3112      C                                         00031080
3113      C DISTANCE-DEPENDENT PLUME RISE: MOMENTUM-DOMINATED PLUME,          00031090
3114      C UNSTABLE AIR (A-D).                                         00031100
3115      500 ESH(1)= DWNWSH*CTMU*(DIST*1000.)*0.333333 + HP(IPS)                  00031110
3116          IF(ESH(1).GT.ESH(2)) ESH(1)=ESH(2)                               00031120
3117          RETURN                                         00031130
3118      C                                         00031140
3119      C THERE IS NO DISTANCE-DEPENDENT PLUME RISE GIVEN FOR A          00031150
3120      C MOMENTUM-DOMINATED PLUME IN STABLE AIR. DISTANCE TO MAXIMUM PLUME 00031160
3121      C RISE FOR THIS SITUATION IS SET EQUAL TO ZERO IN THE MAIN PROGRAM, 00031170
3122      C SO THE MAXIMUM HEIGHT, ESH(2), IS USED AT ALL DISTANCES.          00031180
3123          END                                         00031190
3124      C                                         00031200
3125      C                                         00031210
3126      C                                         00031220
3127          SUBROUTINE AUTGRD                                         00031230
3128      C SUBROUTINE AUTGRD (VERSION 82360), PART OF PEM.                      00031240
3129      C                                         00031250
3130      C                                         00031260
3131      C SUBROUTINE AUTGRID CALCULATES THE FIVE PARAMETERS DEFINING THE 00031270
3132      C RECEPTOR GRID (XSWC,YSWC,LX,LY,GRID) WHEN THE AUTOMATIC GRID 00031280
3133      C OPTION IS USED. THIS IS DONE BY SETTING GRID=0.0 IN THE INPUT 00031290
3134      C DATA. GRID PARAMETERS WILL BE CHOSEN FOR EACH SCENARIO SO AS 00031300
3135      C TO INSURE GOOD COVERAGE BY RECEPTORS NEAR THE POINT OF 00031310
3136      C MAXIMUM CONCENTRATION. THIS POINT IS DETERMINED USING GAUSSIAN 00031320
3137      C PLUME ALGORITHMS WITHOUT POLLUTANT REMOVAL MECHANISMS. THIS 00031330
3138      C POINT IS THEREFORE ONLY APPROXIMATE FOR PROBLEMS WHICH INCLUDE 00031340
3139      C DEPOSITION, SEDIMENTATION, AND CHEMICAL DECAY/TRANSFORMATION. 00031350
3140      C THE OPTIMUM RECEPTOR GRID IN THIS CASE SHOULD BE DETERMINED BY 00031360
3141      C TRIAL AND ERROR, USING THE RECEPTOR GRID DEFINED BY AUTGRD AS 00031370
3142      C THE FIRST APPROXIMATION.                                         00031380
3143      C                                         00031390
3144      C                                         00031400
3145          COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20),                00031410
3146          1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),    00031420
3147          2 XA(50),YA(50),EA(50,2),SIZE(50),                           00031430
3148          3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                         00031440
3149          4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16),           00031450
3150          5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLHAM(3,2),CALNAM(7,2),    00031460
3151          6 ITA,IRD,IWR,IDSX, D80,D47,D8047,DIST,DELTA,                   00031470
3152          7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS, UINV,WVEC,                 00031480
3153          8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,               00031490
3154          9 NTOPT,NWDOPT,NWSOFT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,     00031500
3155          * NSTDWN,INTER,NPRINT                                         00031510
3156      C                                         00031520

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3157      C          00031530
3158      DIMENSION XCRNR(4),YCRNR(4),HL(2),DL(2),XTM(2) 00031540
3159      DIMENSION AG(7,2),BG(7,2),DG(7)               00031550
3160      DATA AG/.0383,.1393,.112,.0856,.0818,.1094,.05645, 00031560
3161      1       .0002539,.04396,.1014,.2591,.2527,.2452,.1930/ 00031570
3162      DATA BG/1.281,.9467,.9100,.865,.8155,.7657,.805, 00031580
3163      1       2.089,1.114,.926,.6869,.6341,.6358,.6072/ 00031590
3164      DATA DG/.873,.897,.908,.916,.916,.912,.911/ 00031600
3165      C          00031610
3166      C          00031620
3167      E= 1.570796 -WVEC 00031630
3168      SINEE= SIN(E) 00031640
3169      COSNE= COS(E) 00031650
3170      GX1= XP(1)*COSNE + YP(1)*SINEE 00031660
3171      GX2= GX1 00031670
3172      GY1= YP(1)*COSNE - XP(1)*SINEE 00031680
3173      GY2= GY1 00031690
3174      DO 200 I=1,NPS 00031700
3175      XT= XP(I)*COSNE + YP(I)*SINEE 00031710
3176      YT= YP(I)*COSNE - XP(I)*SINEE 00031720
3177      IBUOY=1 00031730
3178      IF(VP(I).GT.90.67*(TP(I)-TA(ISCEN))*SQRT(TA(ISCEN))/TP(I)) IBUOY=000031740
3179      IRISE=2 00031750
3180      UINV = 1./WS(ISCEN) 00031760
3181      IF(HP(I).GT.10.) UINV = UINV*((10./HP(I))*P(ISC)) 00031770
3182      EFF= 2.45*VP(I)*DP(I)*DP(I)*(TP(I)-TA(ISCEN))/TP(I) 00031780
3183      IPS=I 00031790
3184      HL(1)= HP(I) 00031800
3185      CALL RISE 00031810
3186      HL(2)= ESH(2) 00031820
3187      DO 170 J=1,2 00031830
3188      DL(J)=(BG(ISC,2)*HL(J)*HL(J)/(AG(ISC,2)*AG(ISC,2)*(BG(ISC,2)+DG(ISC))))**0.5/BG(ISC,2)*0.001 00031850
3189      1C)))**(0.5/BG(ISC,2))*0.001 00031860
3190      IF(DL(J).GE.400.) GO TO 170 00031870
3191      DL(J)=(BG(ISC,1)*HL(J)*HL(J)/(AG(ISC,1)*AG(ISC,1)*(BG(ISC,1)+DG(ISC))))**0.5/BG(ISC,1)*0.001 00031880
3192      1C)))**(0.5/BG(ISC,1))*0.001 00031890
3193      170     XTM(J)= XT + DL(J) 00031890
3194      IF(XTM(2).GT.GX2) GX2= XTM(2) 00031900
3195      IF(XTM(1).LT.GX1) GX1= XTM(1) 00031910
3196      IF(YT.GT.GY2) GY2= YT 00031920
3197      IF(YT.LT.GY1) GY1= YT 00031930
3198      200     CONTINUE 00031940
3199      XCRNR(1)= GX1 00031950
3200      XCRNR(2)= GX2 00031960
3201      XCRNR(3)= GX2 00031970
3202      XCRNR(4)= GX1 00031980
3203      YCRNR(1)= GY1 00031990
3204      YCRNR(2)= GY1 00032000
3205      YCRNR(3)= GY2 00032010
3206      YCRNR(4)= GY2 00032020
3207      DO 300 J=1,4 00032030
3208      XCRNRT= XCRNR(J) 00032040
3209      XCRNR(J)= XCRNR(J)*COSNE - YCRNR(J)*SINEE 00032050
3210      300     YCRNR(J)= YCRNR(J)*COSNE + XCRNRT*SINEE 00032060
3211      XSWC= XCRNR(1) 00032070
3212      XNEC= XSWC 00032080
3213      YSWC= YCRNR(1) 00032090
3214      YNEC= YSWC 00032100
3215      DO 400 I=2,4 00032110
3216      IF(XCRNR(I).GT.XNEC) XNEC= XCRNR(I) 00032120
3217      IF(XCRNR(I).LT.XSWC) XSWC= XCRNR(I) 00032130
3218      IF(YCRNR(I).GT.YNEC) YNEC= YCRNR(I) 00032140
3219      400     IF(YCRNR(I).LT.YSWC) YSWC= YCRNR(I) 00032150
3220      XT= XNEC - XSWC 00032160
3221      YT= YNEC - YSWC 00032170
3222      DMAX= XT 00032180
3223      IF(YT.GT.XT) DMAX= YT 00032190
3224      IF(DMAX.LT.10.) GO TO 500 00032200
3225      IF(XT.GT.YT) GO TO 420 00032210
3226      LY= 50 00032220
3227      GRID= YT/50. 00032230
3228      LX= XT/GRID 00032240
3229      IF(LX.LT.50) LX= LX+1 00032250
3230      GO TO 600 00032260
3231      420     LX= 50 00032270
3232      GRID= XT/50. 00032280
3233      LY= YT/GRID 00032290

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3234      IF(LY.LT.50) LY=LY+1                               00032300
3235      GO TO 600                                         00032310
3236 500   IF(DMAX.LT.5.) GO TO 540                      00032320
3237      GRID= 0.2                                         00032330
3238      LX= XT/GRID                                       00032340
3239      LY= YT/GRID                                       00032350
3240      IF(LX.LT.50) LX=LX+1                           00032360
3241      IF(LY.LT.50) LY=LY+1                           00032370
3242      GO TO 600                                         00032380
3243 540   IF(DMAX.LT.0.25) GO TO 580                  00032390
3244      IF(XT.GT.YT) GO TO 560                         00032400
3245      LY= 25                                           00032410
3246      GRID= YT/25.                                     00032420
3247      LX= XT/GRID                                       00032430
3248      IF(LX.LT.25) LX=LX+1                           00032440
3249      GO TO 600                                         00032450
3250 560   LX= 25                                         00032460
3251      GRID= XT/25.                                     00032470
3252      LY= YT/GRID                                       00032480
3253      IF(LY.LT.25) LY=LY+1                           00032490
3254      GO TO 600                                         00032500
3255 580   GRID= 0.01                                       00032510
3256      LX= XT/GRID                                       00032520
3257      LY= YT/GRID                                       00032530
3258      IF(LX.LT.25) LX=LX+1                           00032540
3259      IF(LY.LT.25) LY=LY+1                           00032550
3260 600   XSWC= XSWC - 0.5*GRID                      00032560
3261      YSWC= YSWC - 0.5*GRID                      00032570
3262      IF(NCSOPT.LT.1.OR.(LX.LE.25.AND.LY.LE.25)) GO TO 700 00032580
3263      XL=LX                                         00032590
3264      YL=LY                                         00032600
3265      IF(LX.GT.LY) GO TO 640                         00032610
3266      DELG= YL/25.                                    00032620
3267      LY=25                                         00032630
3268      GRID= GRID*DELG                            00032640
3269      LX= XL/DELG                                00032650
3270      IF(LX.LT.25) LX=LX+1                           00032660
3271      GO TO 700                                         00032670
3272 640   DELG= XL/25.                                00032680
3273      LX=25                                         00032690
3274      GRID= GRID*DELG                            00032700
3275      LY= YL/DELG + 1.                           00032710
3276 700   CONTINUE                                      00032720
3277      WRITE(IWR,900)ISCEN,INDOPT,TT                00032730
3278      XRSWC=XSWC+0.5*GRID                      00032740
3279      YRSWC=YSWC+0.5*GRID                      00032750
3280      WRITE(IWR,905)LX,LY,GRID,XRSWC,YRSWC        00032760
3281 900   FORMAT(IHI,'PEM: AUTOMATICALLY GENERATED RECEPTOR GRID PARAMETER'// 00032770
3282 IS FOR SCENARIO ',I2,' (WIND DIRECTION SUB-SCENARIO ',I2,')'// 00032780
3283 221X,20A4/1X,120('-'')// 00032790
3284 905   FORMAT(' RECEPTOR GRID CONSISTS OF ',I2,' COLUMNS AND ',I2,' ROWS 00032800
3285 10F SPACING =',F7.4,' KM. SOUTHWEST CORNER OF GRID =',F8.3,' KM W, 00032810
3286 2',F8.3,' KM S.')                                00032820
3287      RETURN                                         00032830
3288      END                                            00032840
3289      C                                              00032850
3290      C                                              00032860
3291      C                                              00032870
3292      BLOCK DATA                                     00032880
3293      C                                              BLOCK DATA (VERSION 82360), PART OF PEM. 00032890
3294      C                                              00032900
3295      C                                              00032910
3296      C                                              00032920
3297      C THIS SUBPROGRAM INITIALIZES VARIABLES IN COMMON/PEMCOM/ 00032930
3298      C                                              00032940
3299      C *** PEM MODIFICATIONS BY M.M.STEVENS, 00032950
3300      C NOAA-ATDL, P.O.BOX-E, OAK RIDGE, TENN 37830 00032960
3301      C DECEMBER 1982                                00032970
3302      C                                              00032980
3303      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2), TT(20), 00032990
3304      1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300), 00033000
3305      2 XA(50),YA(50),EA(50,2),SIZE(50), 00033010
3306      3 WD(24),WS(24),TA(24),HMIX(24),PEN(24), 00033020
3307      4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2), SECTAN(16), 00033030
3308      5 XSWC,YSWC,GRID,LX,LY, A(2),B(2),POLNAM(3,2),CALNAM(7,2), 00033040
3309      6 ITA,IRD,IWR,IDS, D80,D47,D8047,DIST,DELTA, 00033050
3310      7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS, UINV,WVEC, 00033060

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3311      8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,          00033070
3312      9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCOPT,NMAX, 00033080
3313      * NSTOWN,INTER,NPRINT                                     00033090
3314      C                                                       00033100
3315      C                                                       00033110
3316      DATA INDEX,NAS,NPS/0,0,0/                                00033120
3317      DATA ITA,IRD,IWR,IDSX/1,5,6,8/                            00033130
3318      DATA SCLAB/2HA ,2HB ,2HC ,2HDD,2HDN,2HE ,2HF /           00033140
3319      DATA P/0.1,0.15,0.2,0.25,0.25,0.3,0.3/                  00033150
3320      DATA AX/.0383,.1393,.112,.0856,.0818,.1094,.05645,    00033160
3321      1 .0002539,.04936,.1014,.2591,.2527,.2452,.1930,     00033170
3322      2 .0002539,.04936,.1154,.7368,1.297,.9204,1.505/       00033180
3323      DATA BX/1.281,.9467,.9100,.865,.8155,.7657,.805,      00033190
3324      1 2.089,1.114,.926,.6869,.6341,.6358,.6072,            00033200
3325      2 2.089,1.114,.9109,.5642,.4421,.4805,.3662/           00033210
3326      DATA SECTAN/0.,.39270,.78540,1.17810,1.57080,1.96350,2.35620, 00033220
3327      1 2.74890,3.14159,3.53429,3.92699,4.31969,4.71239,5.10509, 00033230
3328      2 5.49779,5.89049/                                       00033240
3329      C                                                       00033250
3330      END                                                     00033260
3331      C                                                       00033270
3332      C                                                       00033280
3333      C                                                       00033290
3334      SUBROUTINE D01AJF(F, A, B, EPSABS, EPSREL, RESULT, ABSERR,WORK, 00033300
3335      * LWORK, IWORK, LIWORK, IFAIL)                           00033310
3336      C                                                       00033320
3337      C                                                       00033330
3338      C                                                       00033340
3339      C                                                       00033350
3340      C                                                       00033360
3341      C DOIAJF IS A GENERAL PURPOSE INTEGRATOR WHICH CALCULATES 00033370
3342      C AN APPROXIMATION TO THE INTEGRAL OF A FUNCTION OVER A FINITE 00033380
3343      C INTERVAL (A,B). THIS ROUTINE CAN BE USED WHEN THE INTEGRAND 00033390
3344      C HAS SINGULARITIES, ESPECIALLY WHEN THESE ARE OF ALGEBRAIC OR 00033400
3345      C LOGARITHMIC TYPE. D01AJF IS AN ADAPTIVE ROUTINE, USING THE 00033410
3346      C GAUSS 10-POINT AND KRONROD 21-POINT RULES. THE ALGORITHM 00033420
3347      C INCORPORATES A GLOBAL ACCEPTANCE CRITERION TOGETHER WITH 00033430
3348      C EPS-ALGORITHM TO PERFORM EXTRAPOLATION. THE LOCAL ERROR IS 00033440
3349      C ESTIMATED.                                         00033450
3350      C                                                       00033460
3351      C THE GENERAL PURPOSE INTEGRATOR D01AJF INCLUDES THE FOLLOWING: 00033470
3352      C SUBROUTINES (1) D01AJF, (2) D01AJV, (3) D01AJX, (4) D01AJY, 00033480
3353      C (5) D01AJZ, INTEGER FUNCTION P01AAF, DOUBLE PRECISION FUNCTIONS 00033490
3354      C (1) X02AAF, (2) X02ABF, (3) X02ACF, AND SUBROUTINE X04AAF. 00033500
3355      C THE PROGRAM LISTINGS FOR THESE SUBROUTINES AND FUNCTIONS, COPIED 00033510
3356      C HERE FROM ORNL - NAG LIBRARY, FOLLOW. THESE ARE DEVELOPED BY 00033520
3357      C NUMERICAL ALGORITHMS GROUP (NAG)                         00033530
3358      C 1131 WARREN AVENUE                                     00033540
3359      C WHICH HOLDS THE COPYRIGHT (NAG FORTRAN MINI MANUAL, MARK8, 1980). 00033550
3360      C THESE PROGRAM LISTINGS ARE INCLUDED HERE WITH PERMISSION FROM 00033560
3361      C COMPUTER SCIENCES DEPARTMENT                         00033570
3362      C OAK RIDGE NATIONAL LABORATORY (ORNL)                 00033580
3363      C OAK RIDGE, TENNESSEE 37830                          00033590
3364      C EXCLUSIVELY FOR PEM. THESE LIBRARY SUBROUTINES AND PROGRAMS 00033600
3365      C SHOULD NOT BE USED FOR ANY OTHER PURPOSE WITHOUT PRIOR APPROVAL 00033610
3366      C FROM NAG AND ORNL.                                    00033620
3367      C                                                       00033630
3368      C                                                       00033640
3369      C D01AJF ITSELF IS ESSENTIALLY A DUMMY ROUTINE WHOSE FUNCTION IS TO 00033650
3370      C PARTITION THE WORK ARRAYS WORK AND IWORK FOR USE BY D01AJV. 00033660
3371      C WORK IS PARTITIONED INTO 4 ARRAYS EACH OF SIZE LWORK/4.        00033670
3372      C IWORK IS A SINGLE ARRAY IN D01AJV.                      00033680
3373      C                                                       00033690
3374      C .. SCALAR ARGUMENTS ..                               00033700
3375      C DOUBLE PRECISION A, ABSERR, B, EPSABS, EPSREL, RESULT 00033710
3376      C INTEGER IFAIL, LIWORK, LWORK                         00033720
3377      C .. ARRAY ARGUMENTS ..                                00033730
3378      C DOUBLE PRECISION WORK(LWORK)                        00033740
3379      C INTEGER IWORK(LIWORK)                             00033750
3380      C .. FUNCTION ARGUMENTS ..                            00033760
3381      C DOUBLE PRECISION F                                00033770
3382      C .. 00033780
3383      C .. LOCAL SCALARS ..                                00033790
3384      C $P 1 DOUBLE PRECISION SRNAME                      00033800
3385      C INTEGER IBL, IEL, IER, IRL, LIMIT                00033810
3386      C .. FUNCTION REFERENCES ..                         00033820
3387      C .. 00033830

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3388      INTEGER P01AAF          00033840
3389      C .. SUBROUTINE REFERENCES .. 00033850
3390      C D01AJV                00033860
3391      C ..
3392      C EXTERNAL F              00033880
3393      C DATA SRNAME /8H D01AJF / 00033890
3394      C CHECK THAT MINIMUM WORKSPACE REQUIREMENTS ARE MET 00033900
3395      C IF (LWORK.LT.4) GO TO 20 00033910
3396      C IF (LIWORK.LT.LWORK/8+2) GO TO 20 00033920
3397      C LIMIT = UPPER BOUND ON NUMBER OF SUBINTERVALS 00033930
3398      C LIMIT = LWORK/4          00033940
3399      C SET UP BASE ADDRESSES FOR WORK ARRAYS 00033950
3400      C IBL = LIMIT + 1         00033960
3401      C IEL = LIMIT + IBL       00033970
3402      C IRL = LIMIT + IEL       00033980
3403      C PERFORM INTEGRATION    00033990
3404      C CALL D01AJV(F, A, B, DABS(EPSABS), DABS(EPSREL), WORK(1), WORK(IBL) 00034000
3405      * , WORKIEL), WORK(IRL), LIMIT, IWORK, LIWORK, RESULT, ABSERR, IER) 00034010
3406      C IF (IER.NE.0) GO TO 40 00034020
3407      C IFAIL = 0               00034030
3408      C GO TO 60               00034040
3409      C ERROR 6 = INSUFFICIENT WORKSPACE 00034050
3410      C 20 IER = 6               00034060
3411      C 40 IFAIL = P01AAF(IFAIL,IER,SRNAME) 00034070
3412      C 60 RETURN              00034080
3413      C END                     00034090
3414      C                         00034100
3415      C                         00034110
3416      C SUBROUTINE D01AJV(F, A, B, EPSABS, EPSREL, ALIST, BLIST, ELIST, 00034120
3417      * RLIST, LIMIT, IORD, LIORD, RESULT, ABSERR, IER) 00034130
3418      C                         SUBROUTINE D01AJV, PART OF PEM (VERSION 82360). 00034140
3419      C                         00034150
3420      C MARK 8 RELEASE. NAG COPYRIGHT 1979 00034160
3421      C BASED ON QUADPACK ROUTINE DQAGS (FORMERLY QAGS) 00034170
3422      C **** 00034180
3423      C                         00034190
3424      C PURPOSE                 00034200
3425      C THE ROUTINE CALCULATES AN APPROXIMATION 00034210
3426      C /RESULT/ TO A GIVEN DEFINITE INTEGRAL I = 00034220
3427      C INTEGRAL OF /F/ OVER (A,B), HOPEFULLY 00034230
3428      C SATISFYING FOLLOWING CLAIM FOR ACCURACY . 00034240
3429      C ABS(I-RESULT) .LE. MAX(EPSABS,EPSREL*ABS(I)). 00034250
3430      C                         00034260
3431      C CALLING SEQUENCE        00034270
3432      C CALL D01AJV (F,A,B,EPSABS,EPSREL,ALIST,BLIST,ELIST, 00034280
3433      C RLIST,LIMIT,IORD,LIORD,RESULT,ABSERR,IER) 00034290
3434      C                         00034300
3435      C PARAMETERS              00034310
3436      C F - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND 00034320
3437      C FUNCTION F(X). THE ACTUAL NAME FOR F 00034330
3438      C NEEDS TO BE DECLARED E X T E R N A L 00034340
3439      C IN THE DRIVER PROGRAM 00034350
3440      C                         00034360
3441      C A - LOWER LIMIT OF INTEGRATION 00034370
3442      C                         00034380
3443      C B - UPPER LIMIT OF INTEGRATION 00034390
3444      C                         00034400
3445      C EPSABS - ABSOLUTE ACCURACY REQUESTED 00034410
3446      C                         00034420
3447      C EPSREL - RELATIVE ACCURACY REQUESTED 00034430
3448      C                         00034440
3449      C ALIST,BLIST,ELIST,RLIST 00034450
3450      C - WORK ARRAYS (FUNCTIONS DESCRIBED BELOW) 00034460
3451      C                         00034470
3452      C LIMIT - UPPER BOUND FOR NUMBER OF SUBINTERVALS 00034480
3453      C                         00034490
3454      C IORD - WORK ARRAY 00034500
3455      C                         00034510
3456      C LIORD - LENGTH OF IORD (AT LEAST LIMIT/2 + 2) 00034520
3457      C                         00034530
3458      C RESULT - APPROXIMATION TO THE INTEGRAL 00034540
3459      C                         00034550
3460      C ABSERR - ESTIMATE OF THE MODULUS OF THE ABSOLUTE ERROR, 00034560
3461      C WHICH SHOULD EQUAL OR EXCEED ABS(I-RESULT) 00034570
3462      C                         00034580
3463      C IER - IER = 0 NORMAL AND RELIABLE 00034590
3464      C TERMINATION OF THE ROUTINE. 00034600

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3465	C	IT IS ASSUMED THAT THE	00034610
3466	C	REQUESTED ACCURACY HAS BEEN	00034620
3467	C	ACHIEVED.	00034630
3468	C	- IER .NE. 0 ABNORMAL TERMINATION OF	00034640
3469	C	THE ROUTINE. THE ESTIMATES	00034650
3470	C	FOR INTEGRAL AND ERROR ARE	00034660
3471	C	LESS RELIABLE. IT IS ASSUMED	00034670
3472	C	THAT THE REQUESTED ACCURACY	00034680
3473	C	HAS NOT BEEN ACHIEVED.	00034690
3474	C	= 1 MAXIMUM NUMBER OF SUBDIVISIONS ALLOWED	00034700
3475	C	HAS BEEN ACHIEVED. THE USER CAN	00034710
3476	C	ALLOW MORE SUB DIVISIONS BY	00034720
3477	C	INCREASING THE DIMENSIONS OF THE	00034730
3478	C	WORK ARRAYS WORK AND IWORK.	00034740
3479	C	HOWEVER, THIS MAY	00034750
3480	C	YIELD NO IMPROVEMENT, AND IT	00034760
3481	C	IS RATHER ADVISED TO HAVE A	00034770
3482	C	CLOSE LOOK AT THE INTEGRAND,	00034780
3483	C	IN ORDER TO DETERMINE THE	00034790
3484	C	INTEGRATION DIFFICULTIES. IF	00034800
3485	C	THE POSITION OF A LOCAL	00034810
3486	C	DIFFICULTY CAN BE DETERMINED	00034820
3487	C	(I.E. SINGULARITY,	00034830
3488	C	DISCONTINUITY WITHIN THE	00034840
3489	C	INTERVAL) ONE WILL PROBABLY	00034850
3490	C	GAIN FROM SPLITTING UP THE	00034860
3491	C	INTERVAL AT THIS POINT AND	00034870
3492	C	CALLING THE INTEGRATOR ON THE	00034880
3493	C	SUB-RANGES. IF POSSIBLE, AN	00034890
3494	C	APPROPRIATE SPECIAL-PURPOSE	00034900
3495	C	INTEGRATOR SHOULD BE USED	00034910
3496	C	WHICH IS DESIGNED FOR	00034920
3497	C	HANDLING THE TYPE OF	00034930
3498	C	DIFFICULTY INVOLVED.	00034940
3499	C	= 2 THE OCCURRENCE OF ROUND OFF	00034950
3500	C	ERROR IS DETECTED WHICH	00034960
3501	C	PREVENTS THE REQUESTED	00034970
3502	C	TOLERANCE FROM BEING	00034980
3503	C	ACHIEVED. THE ERROR MAY BE	00034990
3504	C	UNDER-ESTIMATED.	00035000
3505	C	= 3 EXTREMELY BAD INTEGRAND BEHAVIOUR	00035010
3506	C	OCURRS AT SOME INTERIOR POINTS OF THE	00035020
3507	C	INTEGRATION INTERVAL.	00035030
3508	C	= 4 IT IS PRESUMED THAT THE REQUESTED	00035040
3509	C	TOLERANCE CANNOT BE ACHIEVED,	00035050
3510	C	AND THAT THE RETURNED RESULT	00035060
3511	C	IS THE BEST WHICH CAN BE	00035070
3512	C	OBTAINED.	00035080
3513	C	= 5 THE INTEGRAL IS PROBABLY DIVERGENT, OR	00035090
3514	C	SLOWLY CONVERGENT. IT MUST BE NOTED	00035100
3515	C	THAT DIVERGENCE CAN OCCUR	00035110
3516	C	WITH ANY OTHER VALUE OF IER.	00035120
3517	C	*****	00035130
3518	C	.. SCALAR ARGUMENTS ..	00035140
3519	C	DOUBLE PRECISION A, ABSERR, B, EPSABS, EPSREL, RESULT	00035150
3520	C	INTEGER IER, LIMIT, LIORD	00035160
3521	C	.. ARRAY ARGUMENTS ..	00035170
3522	C	DOUBLE PRECISION ALIST(LIMIT), BLIST(LIMIT), ELIST(LIMIT),	00035180
3523	*	* RLIST(LIMIT)	00035190
3524	C	INTEGER IORD(LIORD)	00035200
3525	C	.. FUNCTION ARGUMENTS ..	00035210
3526	C	DOUBLE PRECISION F	00035220
3527	C	..	00035230
3528	C	.. SCALARS IN COMMON ..	00035240
3529	C	INTEGER JUPBND	00035250
3530	C	..	00035260
3531	C	.. LOCAL SCALARS ..	00035270
3532	C	DOUBLE PRECISION A1, A2, ABSEPS, AREA12, AREA1, AREA2, AREA, B1,	00035280
3533	*	* B2,CORREC, DEFAB1, DEFAB2, DEFABS, DRES, EPMACH, ERLARG, ERLAST,	00035290
3534	*	* ERRBND, ERRMAX, ERRO12, ERRO1, ERROR1, ERROR2, ERRSUM,ERTEST, OFLOW,	00035300
3535	*	* RESABS, RESEPS, SMALL, UFLW	00035310
3536	*	* INTEGER ID, IERRO, IROFF1, IROFF2, IROFF3, K, KSGN, KTMN,LASTI,	00035320
3537	*	* LAST, MAXERR, NRES, NRMAX, NUMRL2	00035330
3538	*	* LOGICAL EXTRAP, NOEXT	00035340
3539	C	.. LOCAL ARRAYS ..	00035350
3540	C	DOUBLE PRECISION RES3LA(3), RLIST2(52)	00035360
3541	C		00035370

3542	C	.. FUNCTION REFERENCES ..	00035380
3543		DOUBLE PRECISION X02AAF, X02ABF, X02ACF	00035390
3544	C	.. SUBROUTINE REFERENCES ..	00035400
3545	C	D01AJX, D01AJY, D01AJZ	00035410
3546	C	..	00035420
3547		EXTERNAL F	00035430
3548		COMMON /AD01AJ/ JUPBND	00035440
3549	C		00035450
3550	C	THE DIMENSION OF /RLIST2/ IS DETERMINED BY	00035460
3551	C	DATA /LIMEXP/ IN SUBROUTINE D01AJY (/RLIST2/	00035470
3552	C	SHOULD BE OF DIMENSION (LIMEXP+2) AT LEAST).	00035480
3553	C		00035490
3554		EPMACH = X02AAF(1.0D0)	00035500
3555		UFLOW = X02ABF(1.0D0)	00035510
3556		OFLW = X02ACF(1.0D0)	00035520
3557	C		00035530
3558	C	LIST OF MAJOR VARIABLES	00035540
3559	C	-----	00035550
3560	C		00035560
3561	C	ALIST - LIST OF LEFT END-POINTS OF ALL SUBINTERVALS	00035570
3562	C	CONSIDERED UP TO NOW	00035580
3563	C		00035590
3564	C	BLIST - LIST OF RIGHT END-POINTS OF ALL SUBINTERVALS	00035600
3565	C	CONSIDERED UP TO NOW	00035610
3566	C		00035620
3567	C	RLIST(I) - APPROXIMATION TO THE INTEGRAL OVER	00035630
3568	C	(ALIST(I),BLIST(I))	00035640
3569	C		00035650
3570	C	RLIST2 - ARRAY OF DIMENSION AT LEAST LIMEXP+2	00035660
3571	C	CONTAINING THE PART OF THE EPSILON TABLE	00035670
3572	C	WHICH IS STILL NEEDED FOR FURTHER	00035680
3573	C	COMPUTATIONS	00035690
3574	C		00035700
3575	C	ELIST(I) - ERROR ESTIMATE APPLYING TO RLIST(I)	00035710
3576	C		00035720
3577	C	MAXERR - POINTER TO THE INTERVAL WITH LARGEST ERROR	00035730
3578	C	ESTIMATE	00035740
3579	C		00035750
3580	C	ERRMAX - ELIST(MAXERR)	00035760
3581	C		00035770
3582	C	ERLAST - ERROR ON THE INTERVAL CURRENTLY SUBDIVIDED	00035780
3583	C	(BEFORE THAT SUBDIVISION HAS TAKEN PLACE)	00035790
3584	C		00035800
3585	C	AREA - SUM OF THE INTEGRALS OVER THE SUBINTERVALS	00035810
3586	C		00035820
3587	C	ERRSUM - SUM OF THE ERRORS OVER THE SUBINTERVALS	00035830
3588	C		00035840
3589	C	ERRBND - REQUESTED ACCURACY MAX(EPSABS,EPSREL*	00035850
3590	C	ABS(RESULT))	00035860
3591	C		00035870
3592	C	*****1 - VARIABLE FOR THE LEFT INTERVAL	00035880
3593	C		00035890
3594	C	*****2 - VARIABLE FOR THE RIGHT INTERVAL	00035900
3595	C		00035910
3596	C	LAST - INDEX FOR SUBDIVISION	00035920
3597	C		00035930
3598	C	NRES - NUMBER OF CALLS TO THE EXTRAPOLATION ROUTINE	00035940
3599	C		00035950
3600	C	NUMRL2 - NUMBER OF ELEMENTS CURRENTLY IN	00035960
3601	C	RLIST2. IF AN APPROPRIATE	00035970
3602	C	APPROXIMATION TO THE COMPOUNDED	00035980
3603	C	INTEGRAL HAS BEEN OBTAINED IT IS	00035990
3604	C	PUT IN RLIST2(NUMRL2) AFTER NUMRL2	00036000
3605	C	HAS BEEN INCREASED BY ONE.	00036010
3606	C		00036020
3607	C	SMALL - LENGTH OF THE SMALLEST INTERVAL CONSIDERED	00036030
3608	C	UP TO NOW, MULTIPLIED BY 1.5	00036040
3609	C		00036050
3610	C	ERLARG - SUM OF THE ERRORS OVER THE INTERVALS LARGER	00036060
3611	C	THAN THE SMALLEST INTERVAL	00036070
3612	C	CONSIDERED UP TO NOW	00036080
3613	C	EXTRAP - LOGICAL VARIABLE DENOTING THAT THE	00036090
3614	C	ROUTINE IS ATTEMPTING TO PERFORM	00036100
3615	C	EXTRAPOLATION. I.E. BEFORE	00036110
3616	C	SUBDIVIDING THE SMALLEST INTERVAL	00036120
3617	C	WE TRY TO DECREASE THE VALUE OF	00036130
3618	C	ERLARG	00036140

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3619      C      NOEXT      - LOGICAL VARIABLE DENOTING THAT EXTRAPOLATION      00036150
3620      C      IS NO LONGER ALLOWED(/TRUE/ VALUE)                      00036160
3621      C
3622      C      FIRST APPROXIMATION TO THE INTEGRAL                         00036170
3623      C      -----
3624      C
3625      LAST1 = 1                                         00036200
3626      IER = 0                                         00036210
3627      IERRO = 0                                        00036220
3628      CALL D01AJZ(F, A, B, RESULT, ABSERR, DEFABS, RESABS) 00036230
3629      C
3630      C      TEST ON ACCURACY                                     00036240
3631      C
3632      DRES = DABS(RESULT)                                 00036250
3633      ERRBND = DMAX1(EPSABS, EPSREL*DRES)                00036260
3634      IF (ABSERR.LE.1.0D+02*EPMACH*DEFABS .AND. ABSERR.GT.ERRBND) IER = 200036270
3635      IF (LIMIT.LT.2 .AND. ABSERR.GT.ERRBND) IER = 1          00036280
3636      IF (IER.NE.0 .OR. ABSERR.LE.ERRBND) GO TO 320        00036290
3637      C
3638      C      INITIALIZATION                                00036300
3639      C      -----
3640      C
3641      ALIST(1) = A                                       00036310
3642      BLIST(1) = B                                       00036320
3643      RLIST(1) = RESULT                                 00036330
3644      RLIST2(1) = RESULT                               00036340
3645      ERRMAX = ABERR                                 00036350
3646      MAXERR = 1                                      00036360
3647      AREA = RESULT                                 00036370
3648      ERRSUM = ABERR                                 00036380
3649      ABSERR = OFLOW                                 00036390
3650      NRMAX = 1                                      00036400
3651      NRES = 0                                       00036410
3652      NUMRL2 = 2                                      00036420
3653      KTMIN = 0                                       00036430
3654      EXTRAP = .FALSE.                                00036440
3655      NOEXT = .FALSE.                                00036450
3656      IROFF1 = 0                                      00036460
3657      IROFF2 = 0                                      00036470
3658      IROFF3 = 0                                      00036480
3659      KSGN = -1                                      00036490
3660      IF (DRES.GE.(0.1D+01-0.5D+02*EPMACH)*DEFABS) KSGN = 1 00036500
3661      C
3662      C      MAIN DO-LOOP                                00036510
3663      C      -----
3664      C
3665      IF (LIMIT.LT.2) GO TO 220                      00036520
3666      DO 200 LAST=2,LIMIT                           00036530
3667      C
3668      C      BISECT THE SUBINTERVAL WITH THE NRMAX-TH LARGEST 00036540
3669      C      ERROR ESTIMATE                            00036550
3670      C
3671      LAST1 = LAST                                 00036560
3672      A1 = ALIST(MAXERR)                            00036570
3673      B1 = 0.5D+00*(ALIST(MAXERR)+BLIST(MAXERR)) 00036580
3674      A2 = B1                                       00036590
3675      B2 = BLIST(MAXERR)                            00036600
3676      ERLAST = ERRMAX                             00036610
3677      CALL D01AJZ(F, A1, B1, AREA1, ERROR1, RESABS, DEFAB1) 00036620
3678      CALL D01AJZ(F, A2, B2, AREA2, ERROR2, RESABS, DEFAB2) 00036630
3679      C
3680      C      IMPROVE PREVIOUS APPROXIMATION OF INTEGRAL 00036640
3681      C      AND ERROR AND TEST FOR ACCURACY           00036650
3682      C
3683      AREA12 = AREA1 + AREA2                         00036660
3684      ERRO12 = ERROR1 + ERROR2                       00036670
3685      ERRSUM = ERRSUM + ERRO12 - ERRMAX            00036680
3686      AREA = AREA + AREA12 - RLIST(MAXERR)         00036690
3687      IF (DEFAB1.EQ.ERROR1 .OR. DEFAB2.EQ.ERROR2) GO TO 40 00036700
3688      IF (DABS(RLIST(MAXERR)-AREA12).GT.0.1D-04*DABS(AREA12) .OR. 00036710
3689      * ERRO12.LT.0.99D+00*ERRMAX) GO TO 20          00036720
3690      IF (EXTRAP) IROFF2 = IROFF2 + 1              00036730
3691      IF (.NOT.EXTRAP) IROFF1 = IROFF1 + 1          00036740
3692      20 IF (LAST.GT.10 .AND. ERRO12.GT.ERRMAX) IROFF3 = IROFF3 + 1 00036750
3693      40 RLIST(MAXERR) = AREA1                      00036760
3694      RLIST(LAST) = AREA2                        00036770
3695      ERRBND = DMAX1(EPSABS, EPSREL*DABS(AREA))    00036780

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3696      IF (ERRSUM.LE.ERRBND) GO TO 280          00036920
3697      C
3698      C      TEST FOR ROUND OFF ERROR AND EVENTUALLY 00036930
3699      C      SET ERROR FLAG                      00036940
3700      C
3701      IF (IROFF1+IROFF2.GE.10 .OR. IROFF3.GE.20) IER = 2 00036950
3702      IF (IROFF2.GE.5) IERRO = 3                 00036960
3703      C
3704      C      SET ERROR FLAG IN THE CASE THAT THE NUMBER OF INTERVAL 00036970
3705      C      BISECTIONS EXCEEDS /LIMIT/
3706      C
3707      IF (LAST.EQ.LIMIT) IER = 1                00036980
3708      C
3709      C      SET ERROR FLAG IN THE CASE OF BAD INTEGRAND BEHAVIOUR 00036990
3710      C      AT INTERIOR POINTS OF INTEGRATION RANGE           00037000
3711      C
3712      IF (DMAX1(DABS(A1),DABS(B2)).LE.(0.1D+01+0.1D+03*EPMACH)* 00037010
3713      * (DABS(A2)+0.1D+04*UFLOW)) IER = 4            00037020
3714      IF (IER.NE.0) GO TO 220                  00037030
3715      C
3716      C      APPEND THE NEWLY-CREATED INTERVALS TO THE LIST 00037040
3717      C
3718      IF (ERROR2.GT.ERROR1) GO TO 60            00037050
3719      ALIST(LAST) = A2                         00037060
3720      BLIST(MAXERR) = B1                         00037070
3721      BLIST(LAST) = B2                         00037080
3722      ELIST(MAXERR) = ERROR1                   00037090
3723      ELIST(LAST) = ERROR2                   00037100
3724      GO TO 80                                00037110
3725      60      ALIST(MAXERR) = A2             00037120
3726      ALIST(LAST) = A1                         00037130
3727      BLIST(LAST) = B1                         00037140
3728      RLIST(MAXERR) = AREA2                   00037150
3729      RLIST(LAST) = AREAL                     00037160
3730      ELIST(MAXERR) = ERROR2                   00037170
3731      ELIST(LAST) = ERROR1                   00037180
3732      C
3733      C      CALL SUBROUTINE D01AJX TO MAINTAIN THE 00037190
3734      C      DESCENDING ORDERING IN THE LIST OF ERROR 00037200
3735      C      ESTIMATES AND SELECT THE SUBINTERVAL WITH 00037210
3736      C      NRMAX-TH LARGEST ERROR ESTIMATE (TO BE BISECTED 00037220
3737      C      NEXT)                           00037230
3738      C
3739      80      CALL D01AJX(LIMIT, LAST, MAXERR, ERRMAX, ELIST, IORD, LIORD, 00037240
3740      *      NRMAX)
3741      IF (LAST.EQ.2) GO TO 180                  00037250
3742      IF (NOEXT) GO TO 200                     00037260
3743      ERLARG = ERLARG - ERLAST                00037270
3744      IF (DABS(B1-A1).GT.SMALL) ERLARG = ERLARG + ERRO12 00037280
3745      IF (EXTRAP) GO TO 100                  00037290
3746      C
3747      C      TEST WHETHER THE INTERVAL TO BE BISECTED NEXT IS THE 00037300
3748      C      SMALLEST INTERVAL                      00037310
3749      C
3750      IF (DABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200 00037320
3751      EXTRAP = .TRUE.                         00037330
3752      NRMAX = 2                            00037340
3753      100     IF (IERRO.EQ.3 .OR. ERLARG.LE.ERTEST) GO TO 140 00037350
3754      C
3755      C      THE SMALLEST INTERVAL HAS THE LARGEST ERROR. 00037360
3756      C      BEFORE BISECTING DECREASE THE SUM OF THE ERRORS 00037370
3757      C      OVER THE LARGER INTERVALS(ERLARG) AND PERFORM 00037380
3758      C      EXTRAPOLATION                      00037390
3759      C
3760      ID = NRMAX                         00037400
3761      DO 120 K=ID,JUPBND                  00037410
3762      MAXERR = IORD(NRMAX)                00037420
3763      ERRMAX = ELIST(MAXERR)              00037430
3764      IF (DABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200 00037440
3765      NRMAX = NRMAX + 1                  00037450
3766      120     CONTINUE                      00037460
3767      C
3768      C      PERFORM EXTRAPOLATION          00037470
3769      C
3770      140     NUMRL2 = NUMRL2 + 1          00037480
3771      RLIST2(NUMRL2) = AREA             00037490
3772      CALL D01AJY(NUMRL2, RLIST2, RESEPS, ABSEPS, RES3LA, NRES) 00037500

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3773      KTMIN = KTMIN + 1                                00037690
3774      IF (KTMIN.GT.5 .AND. ABSERR.LT.0.1D-02*ERRSUM) IER = 5 00037700
3775      IF (ABSEPS.GE.ABSERR) GO TO 160                00037710
3776      KTMIN = 0                                     00037720
3777      ABSERR = ABSEPS                            00037730
3778      RESULT = RESEPS                           00037740
3779      CORREC = ERLARG                           00037750
3780      ERTEST = DMAX1(EPSABS,EPSREL*DABS(RESEPS)) 00037760
3781      IF (ABSERR.LE.ERTEST) GO TO 220            00037770
3782      C
3783      C      PREPARE BISECTION OF THE SMALLEST INTERVAL 00037780
3784      C
3785      160   IF (NUMRL2.EQ.1) NOEXT = .TRUE.          00037810
3786      IF (IER.EQ.5) GO TO 220                    00037820
3787      MAXERR = IORD(1)                           00037830
3788      ERRMAX = ELIST(MAXERR)                     00037840
3789      NRMAX = 1                                 00037850
3790      EXTRAP = .FALSE.                         00037860
3791      SMALL = SMALL*0.5D+00                   00037870
3792      ERLARG = ERRSUM                          00037880
3793      GO TO 200                                00037890
3794      180   SMALL = DABS(B-A)*0.375D+00        00037900
3795      ERLARG = ERRSUM                          00037910
3796      ERTEST = ERRBND                         00037920
3797      RLIST2(2) = AREA                         00037930
3798      200 CONTINUE                            00037940
3799      C
3800      C      SET FINAL RESULT AND ERROR ESTIMATE 00037950
3801      C
3802      C
3803      220   IF (ABSERR.EQ.OFLOW) GO TO 280       00037990
3804      IF (IER+IERR0.EQ.0) GO TO 260           00038000
3805      IF (IERR0.EQ.3) ABSERR = ABSERR + CORREC 00038010
3806      IF (IER.EQ.0) IER = 3                  00038020
3807      IF (RESULT.NE.0.D+00.AND. AREA. NE.0.D+00) GO TO 240 00038030
3808      IF (ABSERR.GT.ERRSUM) GO TO 280         00038040
3809      IF (AREA.EQ.0.D+00) GO TO 320          00038050
3810      GO TO 260                                00038060
3811      240   IF (ABSERR/DABS(RESULT).GT.ERRSUM/DABS(AREA)) GO TO 280 00038070
3812      C
3813      C      TEST ON DIVERGENCY                 00038080
3814      C
3815      260   IF (KSGN.EQ.-1 .AND. DMAX1(DABS(RESULT),DABS(AREA)).LE.DEFABS* 00038110
3816      *0.1D-01) GO TO 320                      00038120
3817      IF (0.1D-01.GT.(RESULT/AREA) .OR. (RESULT/AREA).GT.0.1D+03.OR. 00038130
3818      * ERRSUM.GT.DABS(AREA)) IER = 6          00038140
3819      GO TO 320                                00038150
3820      C
3821      C      COMPUTE GLOBAL INTEGRAL SUM        00038160
3822      C
3823      280   RESULT = 0.D+00                     00038170
3824      DO 300 K=1,LAST                         00038180
3825      RESULT = RESULT + RLIST(K)             00038190
3826      300 CONTINUE                            00038200
3827      ABSERR = ERRSUM                         00038210
3828      320   IF (IER.GT.2) IER = IER - 1        00038220
3829      IORD(1) = 4*LAST1                       00038230
3830      RETURN                                  00038240
3831      END                                     00038250
3832      C
3833      C
3834      SUBROUTINE D01AJX(LIMIT, LAST, MAXERR, ERMAX, ELIST, IORD, LIORD, 00038260
3835      * NRMAX)                                00038270
3836      C      SUBROUTINE D01AJX, PART OF PEM (VERSION 82360). 00038280
3837      C
3838      C      MARK 8 RELEASE. NAG COPYRIGHT 1979 00038290
3839      C      BASED ON QUADPACK ROUTINE ORDER 00038300
3840      C      *****
3841      C
3842      C      PURPOSE                               00038310
3843      C      THIS ROUTINE MAINTAINS THE DESCENDING ORDERING 00038320
3844      C      IN THE LIST OF THE LOCAL ERROR ESTIMATES 00038330
3845      C      RESULTING FROM THE INTERVAL SUBDIVISION 00038340
3846      C      PROCESS. AT EACH CALL TWO ERROR ESTIMATES 00038350
3847      C      ARE INSERTED USING THE SEQUENTIAL SEARCH 00038360
3848      C      METHOD . TOP-DOWN FOR THE LARGEST ERROR 00038370
3849      C      ESTIMATE, BOTTOM-UP FOR THE SMALLEST ERROR 00038380

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3850      C          ESTIMATE.                                00038460
3851      C          CALL D01AJX                            00038470
3852      C          CALL D01AJX                            00038480
3853      C          (LIMIT,LAST,MAXERR,ERMAX,E LIST,IORD,LIORD,NRMAX) 00038490
3854      C          (LIMIT,LAST,MAXERR,ERMAX,E LIST,IORD,LIORD,NRMAX) 00038500
3855      C          00038510
3856      C          PARAMETERS (MEANING AT OUTPUT)           00038520
3857      C          LIMIT - MAXIMUM NUMBER OF ERROR ESTIMATES THE LIST 00038530
3858      C          CAN CONTAIN                           00038540
3859      C          00038550
3860      C          LAST - NUMBER OF ERROR ESTIMATES CURRENTLY 00038560
3861      C          IN THE LIST. E LIST(LAST) CONTAINS        00038570
3862      C          THE SMALLEST ERROR ESTIMATE.            00038580
3863      C          00038590
3864      C          MAXERR - MAXERR POINTS TO THE NRMAX-TH LARGEST ERROR 00038600
3865      C          ESTIMATE CURRENTLY IN THE LIST.           00038610
3866      C          00038620
3867      C          ERMAX - NRMAX-TH LARGEST ERROR ESTIMATE    00038630
3868      C          ERMAX = E LIST(MAXERR)                   00038640
3869      C          00038650
3870      C          E LIST - ARRAY OF DIMENSION LAST CONTAINING 00038660
3871      C          THE ERROR ESTIMATES.                  00038670
3872      C          00038680
3873      C          IORD - ARRAY CONTAINING POINTERS TO E LIST SO 00038690
3874      C          THAT IORD(1) POINTS TO THE LARGEST           00038700
3875      C          ERROR ESTIMATE,...,IORD(LAST) TO THE       00038710
3876      C          SMALLEST ERROR ESTIMATE.             00038720
3877      C          00038730
3878      C          LIORD - DIMENSION OF IORD                 00038740
3879      C          00038750
3880      C          NRMAX - MAXERR = IORD(NRMAX)              00038760
3881      C          00038770
3882      C          *****
3883      C          00038780
3884      C          .. SCALAR ARGUMENTS ..                      00038800
3885      C          DOUBLE PRECISION ERMAX                  00038810
3886      C          INTEGER LAST, LIMIT, LIORD, MAXERR, NRMAX   00038820
3887      C          .. ARRAY ARGUMENTS ..                      00038830
3888      C          DOUBLE PRECISION E LIST(LAST)               00038840
3889      C          INTEGER IORD(LIORD)                    00038850
3890      C          ..
3891      C          .. SCALARS IN COMMON ..                  00038860
3892      C          INTEGER JUPBND                     00038870
3893      C          ..
3894      C          .. LOCAL SCALARS ..                      00038880
3895      C          DOUBLE PRECISION ERRMAX, ERRMIN        00038890
3896      C          INTEGER I, IBEG, IDO, ISUCC, J, JBND, K     00038910
3897      C          ..
3898      C          COMMON /AD01AJ/ JUPBND                  00038920
3899      C          00038930
3900      C          ..
3901      C          CHECK WHETHER THE LIST CONTAINS MORE THAN 00038940
3902      C          TWO ERROR ESTIMATES.                00038950
3903      C          00038960
3904      C          IF (LAST.GT.2) GO TO 20                 00038970
3905      C          IORD(1) = 1                         00038980
3906      C          IORD(2) = 2                         00038990
3907      C          GO TO 180                         00039000
3908      C          ..
3909      C          THIS PART OF THE ROUTINE IS ONLY EXECUTED 00039010
3910      C          IF, DUE TO A DIFFICULT INTEGRAND, SUBDIVISION 00039020
3911      C          INCREASED THE ERROR ESTIMATE. IN THE NORMAL CASE 00039030
3912      C          THE INSERT PROCEDURE SHOULD START AFTER THE 00039040
3913      C          NRMAX-TH LARGEST ERROR ESTIMATE.        00039050
3914      C          20 ERRMAX = E LIST(MAXERR)            00039060
3915      C          IF (NRMAX.EQ.1) GO TO 60             00039070
3916      C          IDO = NRMAX - 1                     00039080
3917      C          DO 40 I=1,IDO                   00039090
3918      C          ISUCC = IORD(NRMAX-1)            00039100
3919      C          IF (ERRMAX.LE.E LIST(ISUCC)) GO TO 60 00039110
3920      C          IORD(NRMAX) = ISUCC            00039120
3921      C          NRMAX = NRMAX - 1             00039130
3922      C          40 CONTINUE                   00039140
3923      C          ..
3924      C          COMPUTE THE NUMBER OF ELEMENTS IN THE LIST TO 00039150
3925      C          BE MAINTAINED IN DESCENDING ORDER. THIS NUMBER 00039160
3926      C          DEPENDS ON THE NUMBER OF SUBDIVISIONS STILL 00039170

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3927      C      ALLOWED          00039230
3928      C
3929      60 JUPBND = LAST          00039240
3930      IF (LAST.GT.(LIMIT/2+2)) JUPBND = LIMIT + 3 - LAST 00039250
3931      ERRMIN = ELIST(LAST)    00039260
3932      C
3933      C      INSERT ERRMAX BY TRAVERSING THE LIST TOP-DOWN 00039270
3934      C      STARTING COMPARISON FROM THE ELEMENT          00039280
3935      C      ELIST(IORD(NRMAX+1)) 00039290
3936      C
3937      JBND = JUPBND - 1        00039300
3938      IBEG = NRMAX + 1        00039310
3939      IF (IBEG.GT.JBND) GO TO 100 00039320
3940      DO 80 I=IBEG,JBND       00039330
3941      ISUCC = IORD(I)         00039340
3942      IF (ERRMAX.GE.ELIST(ISUCC)) GO TO 120 00039350
3943      IORD(I-1) = ISUCC     00039360
3944      80 CONTINUE            00039370
3945      100 IORD(JBND) = MAXERR 00039380
3946      IORD(JUPBND) = LAST    00039390
3947      GO TO 180              00039400
3948      C
3949      C      INSERT ERRMIN BY TRAVERSING THE LIST BOTTOM-UP 00039410
3950      C
3951      120 IORD(I-1) = MAXERR 00039420
3952      K = JBND              00039430
3953      DO 140 J=I,JBND       00039440
3954      ISUCC = IORD(K)         00039450
3955      IF (ERRMIN.LT.ELIST(ISUCC)) GO TO 160 00039460
3956      IORD(K+1) = ISUCC     00039470
3957      K = K - 1              00039480
3958      140 CONTINUE            00039490
3959      IORD(I) = LAST        00039500
3960      GO TO 180              00039510
3961      160 IORD(K+1) = LAST   00039520
3962      C
3963      C      SET MAXERR AND ERMAX 00039530
3964      C
3965      180 MAXERR = IORD(NRMAX) 00039540
3966      ERMAX = ELIST(MAXERR) 00039550
3967      RETURN                00039560
3968      END                    00039570
3969      C
3970      C
3971      SUBROUTINE D01AJY(N, EPSTAB, RESULT, ABSERR, RES3LA, NRES) 00039580
3972      C      SUBROUTINE D01AJY, PART OF PEM (VERSION 82360). 00039590
3973      C
3974      C      MARK 8 RELEASE. NAG COPYRIGHT 1979 00039600
3975      C      BASED ON QUADPACK ROUTINE EPSALG 00039610
3976      C      *****
3977      C
3978      C      PURPOSE          00039620
3979      C      THE ROUTINE TRANSFORMS A GIVEN SEQUENCE OF 00039630
3980      C      APPROXIMATIONS, BY MEANS OF THE EPSILON 00039640
3981      C      ALGORITHM OF P. WYNNE. 00039650
3982      C
3983      C      AN ESTIMATE OF THE ABSOLUTE ERROR IS ALSO GIVEN. 00039660
3984      C      THE CONDENSED EPSILON TABLE IS COMPUTED. ONLY THOSE 00039670
3985      C      ELEMENTS NEEDED FOR THE COMPUTATION OF THE 00039680
3986      C      NEXT DIAGONAL ARE PRESERVED. 00039690
3987      C
3988      C      CALLING SEQUENCE 00039700
3989      C      CALL D01AJY (N,EPSTAB,RESULT,ABSERR,RES3LA,NRES) 00039710
3990      C
3991      C      PARAMETERS 00039720
3992      C      N      - EPSTAB(N) CONTAINS THE NEW ELEMENT IN THE 00039730
3993      C      FIRST COLUMN OF THE EPSILON TABLE. 00039740
3994      C
3995      C      EPSTAB - ONE DIMENSIONAL ARRAY CONTAINING THE 00039750
3996      C      ELEMENTS OF THE TWO LOWER DIAGONALS OF 00039760
3997      C      THE TRIANGULAR EPSILON TABLE. 00039770
3998      C      THE ELEMENTS ARE NUMBERED STARTING AT THE 00039780
3999      C      RIGHT-HAND CORNER OF THE TRIANGLE. 00039790
4000      C      THE DIMENSION SHOULD BE AT LEAST N+2. 00039800
4001      C
4002      C      RESULT - RESULTING APPROXIMATION TO THE INTEGRAL 00039810
4003      C

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4004      C      ABSERR - ESTIMATE OF THE ABSOLUTE ERROR COMPUTED FROM      00040000
4005      C      RESULT AND THE 3 PREVIOUS /RESULTS/                  00040010
4006      C      RES3LA - ARRAY CONTAINING THE LAST 3 /RESULTS/          00040020
4007      C      NRES   - NUMBER OF CALLS TO THE ROUTINE                00040030
4008      C      (SHOULD BE ZERO AT FIRST CALL)                      00040040
4009      C
4010      C
4011      C
4012      C *****SCALAR ARGUMENTS ..                                     00040050
4013      C .. SCALAR ARGUMENTS ..                                     00040060
4014      C DOUBLE PRECISION ABSERR, RESULT                         00040070
4015      C INTEGER N, NRES                                         00040080
4016      C .. ARRAY ARGUMENTS ..                                     00040090
4017      C DOUBLE PRECISION EPSTAB(52), RES3LA(3)                 00040100
4018      C ..
4019      C .. LOCAL SCALARS ..                                     00040110
4020      C DOUBLE PRECISION DELTA1, DELTA2, DELTA3, E0, E1, E1ABS, E2, E3, 00040120
4021      C * EPMACH,EPSINF, ERR1, ERR2, ERR3, ERROR, OFLOW, RES, SS, TOL1, 00040130
4022      C * TOL2,TOL3                                         00040140
4023      C INTEGER I, IB2, IB, IE, INO, K1, K2, K3, LIMEXP, NEWLM, NUM 00040150
4024      C .. FUNCTION REFERENCES ..                               00040160
4025      C DOUBLE PRECISION X02AAF, X02ACF                         00040170
4026      C ..
4027      C
4028      C MACHINE DEPENDENT CONSTANTS                           00040180
4029      C -----
4030      C /LIMEXP/ IS THE MAXIMUM NUMBER OF ELEMENTS THE EPSILON 00040190
4031      C TABLE CAN CONTAIN. IF THIS NUMBER IS REACHED, THE UPPER 00040200
4032      C DIAGONAL OF THE EPSILON TABLE IS DELETED.           00040210
4033      C
4034      C DATA LIMEXP /50/
4035      C EPMACH = X02AAF(1.0D0)                                00040220
4036      C OFLOW = X02ACF(1.0D0)                                00040230
4037      C
4038      C LIST OF MAJOR VARIABLES                            00040240
4039      C -----
4040      C E0      - THE 4 ELEMENTS ON WHICH THE                  00040250
4041      C E1      COMPUTATION OF A NEW ELEMENT IN               00040260
4042      C E2      THE EPSILON TABLE IS BASED                   00040270
4043      C E3      E0
4044      C           E3   E1   NEW                           00040280
4045      C           E2
4046      C NEWLM - NUMBER OF ELEMENTS TO BE COMPUTED IN THE NEW 00040290
4047      C DIAGONAL                                         00040300
4048      C ERROR   - ERROR = ABS(E1-E0)+ABS(E2-E1)+ABS(NEW-E2) 00040310
4049      C RESULT  - THE ELEMENT IN THE NEW DIAGONAL WITH LEAST 00040320
4050      C ERROR                                         00040330
4051      C
4052      C NRES = NRES + 1                                     00040340
4053      C ABSERR = OFLOW                                    00040350
4054      C RESULT = EPSTAB(N)                                00040360
4055      C IF (N.LT.3) GO TO 200                            00040370
4056      C EPSTAB(N+2) = EPSTAB(N)                          00040380
4057      C NEWLM = (N-1)/2                                  00040390
4058      C EPSTAB(N) = OFLOW                             00040400
4059      C NUM = N                                       00040410
4060      C K1 = N                                       00040420
4061      C DO 80 I=1,NEWLM                                00040430
4062      C     K2 = K1 - 1                                 00040440
4063      C     K3 = K1 - 2                                 00040450
4064      C     RES = EPSTAB(K1+2)                         00040460
4065      C     E0 = EPSTAB(K3)                           00040470
4066      C     E1 = EPSTAB(K2)                           00040480
4067      C     E2 = RES                                 00040490
4068      C     E1ABS = DABS(E1)                           00040500
4069      C     DELTA2 = E2 - E1                           00040510
4070      C     ERR2 = DABS(DELTA2)                         00040520
4071      C     TOL2 = DMAX1(DABS(E2),E1ABS)*EPMACH        00040530
4072      C     DELTA3 = E1 - E0                           00040540
4073      C     ERR3 = DABS(DELTA3)                         00040550
4074      C     TOL3 = DMAX1(E1ABS,DABS(E0))*EPMACH        00040560
4075      C     IF (ERR2.GT.TOL2 .OR. ERR3.GT.TOL3) GO TO 20 00040570
4076      C
4077      C     IF E0, E1 AND E2 ARE EQUAL TO WITHIN MACHINE 00040580
4078      C     ACCURACY, CONVERGENCE IS ASSUMED            00040590
4079      C     RESULT = E2                                 00040600
4080      C     ABSERR = ABS(E1-E0)+ABS(E2-E1)             00040610

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4081      C          00040770
4082          RESULT = RES          00040780
4083          ABSERR = ERR2 + ERR3 00040790
4084          GO TO 200          00040800
4085      20          E3 = EPSTAB(K1) 00040810
4086          EPSTAB(K1) = E1          00040820
4087          DELTA1 = E1 - E3          00040830
4088          ERR1 = DABS(DELTA1) 00040840
4089          TOL1 = DMAX1(E1ABS,DABS(E3))*EPMACH 00040850
4090      C          00040860
4091      C          IF TWO ELEMENTS ARE VERY CLOSE TO EACH OTHER, OMIT 00040870
4092      C          A PART OF THE TABLE BY ADJUSTING THE VALUE OF N 00040880
4093      C          00040890
4094          IF (ERR1.LT.TOL1 .OR. ERR2.LT.TOL2 .OR. ERR3.LT.TOL3) GOTO 40 00040900
4095          SS = 0.1D+01/DELTA1 + 0.1D+01/DELTA2 - 0.1D+01/DELTA3 00040910
4096          EPSINF = DABS(SS*E1) 00040920
4097      C          00040930
4098      C          TEST TO DETECT IRREGULAR BEHAVIOUR IN THE TABLE, AND 00040940
4099      C          EVENTUALLY OMIT A PART OF THE TABLE ADJUSTING THE VALUE 00040950
4100      C          OF N 00040960
4101      C          00040970
4102          IF (EPSINF.GT.0.1D-03) GO TO 60 00040980
4103      40          N = I + I - 1 00040990
4104          GO TO 100 00041000
4105      C          00041010
4106      C          COMPUTE A NEW ELEMENT AND EVENTUALLY ADJUST 00041020
4107      C          THE VALUE OF RESULT 00041030
4108      C          00041040
4109      60          RES = E1 + 0.1D+01/SS 00041050
4110          EPSTAB(K1) = RES 00041060
4111          K1 = K1 - 2 00041070
4112          ERROR = ERR2 + DABS(RES-E2) + ERR3 00041080
4113          IF (ERROR.GT.ABSERR) GO TO 80 00041090
4114          ABSERR = ERROR 00041100
4115          RESULT = RES 00041110
4116          80 CONTINUE 00041120
4117      C          00041130
4118      C          SHIFT THE TABLE 00041140
4119      C          00041150
4120      100         IF (N.EQ.LIMEXP) N = 2*(LIMEXP/2) - 1 00041160
4121          IB = 1 00041170
4122          IF ((NUM/2)*2.EQ.NUM) IB = 2 00041180
4123          IE = NEWELM + 1 00041190
4124          DO 120 I=1,IE 00041200
4125          IB2 = IB + 2 00041210
4126          EPSTAB(IB) = EPSTAB(IB2) 00041220
4127          IB = IB2 00041230
4128          120 CONTINUE 00041240
4129          IF (NUM.EQ.N) GO TO 160 00041250
4130          IND = NUM - N + 1 00041260
4131          DO 140 I=1,N 00041270
4132          EPSTAB(I) = EPSTAB(IND) 00041280
4133          IND = IND + 1 00041290
4134          140 CONTINUE 00041300
4135          160 IF (NRES.GE.4) GO TO 180 00041310
4136          RES3LA(NRES) = RESULT 00041320
4137          ABSERR = OFLOW 00041330
4138          GO TO 200 00041340
4139      C          00041350
4140      C          COMPUTE ERROR ESTIMATE 00041360
4141      C          00041370
4142      180         ABSERR = DABS(RESULT-RES3LA(3)) + DABS(RESULT-RES3LA(2)) + 00041380
4143          *DABS(RESULT-RES3LA(1)) 00041390
4144          RES3LA(1) = RES3LA(2) 00041400
4145          RES3LA(2) = RES3LA(3) 00041410
4146          RES3LA(3) = RESULT 00041420
4147          200 ABSERR = DMAX1(ABSERR,5.0D+00*EPMACH*DABS(RESULT)) 00041430
4148          RETURN 00041440
4149          END 00041450
4150      C          00041460
4151      C          00041470
4152      C          SUBROUTINE D01AJZ(F, A, B, RESULT, ABSERR, RESABS, RESASC) 00041480
4153      C          SUBROUTINE D01AJZ, PART OF PEM (VERSION 82360). 00041490
4154      C          00041500
4155      C          MARK 8 RELEASE. NAG COPYRIGHT 1979 00041510
4156      C          BASED ON QUADPACK ROUTINE QUARUL 00041520
4157      C          ***** 00041530

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4158 C 00041540
4159 C PURPOSE 00041550
4160 C TO COMPUTE I = INTEGRAL OF F OVER (A,B), WITH ERROR 00041560
4161 C ESTIMATE 00041570
4162 C J = INTEGRAL OF ABS(F) OVER (A,B) 00041580
4163 C 00041590
4164 C CALLING SEQUENCE 00041600
4165 C CALL D01AJZ (F,A,B,RESULT,ABSERR,RESABS,RESASC) 00041610
4166 C 00041620
4167 C PARAMETERS 00041630
4168 C F - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND 00041640
4169 C FUNCTION F(X). THE ACTUAL NAME FOR F NEEDS 00041650
4170 C TO BE DECLARED E X T E R N A L IN THE 00041660
4171 C CALLING PROGRAM 00041670
4172 C 00041680
4173 C A - LOWER LIMIT OF INTEGRATION 00041690
4174 C 00041700
4175 C B - UPPER LIMIT OF INTEGRATION 00041710
4176 C 00041720
4177 C RESULT - APPROXIMATION TO THE INTEGRAL I. 00041730
4178 C RESULT IS CALCULATED BY APPLYING 00041740
4179 C THE 21-POINT GAUSS-KRONROD RULE 00041750
4180 C (RESK), OBTAINED BY OPTIMAL 00041760
4181 C ADDITION OF ABSCISSAE TO THE 00041770
4182 C 10-POINT GAUSS RULE (RESG). 00041780
4183 C 00041790
4184 C ABSERR - ESTIMATE OF THE MODULUS OF THE 00041800
4185 C ABSOLUTE ERROR, WHICH SHOULD NOT 00041810
4186 C EXCEED ABS(I-RESULT) 00041820
4187 C RESABS - APPROXIMATION TO THE INTEGRAL J 00041830
4188 C 00041840
4189 C RESASC - APPROXIMATION TO THE INTEGRAL OF 00041850
4190 C ABS(F-I/(B-A)) OVER (A,B) 00041860
4191 C 00041870
4192 C **** 00041880
4193 C .. SCALAR ARGUMENTS .. 00041890
4194 C DOUBLE PRECISION A, ABSERR, B, RESABS, RESASC, RESULT 00041900
4195 C .. FUNCTION ARGUMENTS .. 00041910
4196 C DOUBLE PRECISION F 00041920
4197 C .. 00041930
4198 C .. LOCAL SCALARS .. 00041940
4199 C DOUBLE PRECISION ABSC, CENTRE, DHLGTH, EPMACH, FC, FSUM, FVALI, 00041950
4200 C * FVAL2,HLGTH, RESG, RESK, RESKH, UFLOW 00041960
4201 C INTEGER J 00041970
4202 C .. LOCAL ARRAYS .. 00041980
4203 C DOUBLE PRECISION FV1(10), FV2(10), WG(10), XGK(11), XGK(11) 00041990
4204 C .. FUNCTION REFERENCES .. 00042000
4205 C DOUBLE PRECISION X02AAF, X02ABF 00042010
4206 C .. 00042020
4207 C .. 00042030
4208 C THE ABSCISSAE AND WEIGHTS ARE GIVEN FOR THE 00042040
4209 C INTERVAL (-1,1) . BECAUSE OF SYMMETRY ONLY THE 00042050
4210 C POSITIVE ABSCISSAE AND THEIR CORRESPONDING 00042060
4211 C WEIGHTS ARE GIVEN. 00042070
4212 C XGK - ABSCISSAE OF THE 21-POINT GAUSS-KRONROD RULE 00042080
4213 C XGK(2), XGK(4), .... ABSCISSAE OF THE 10-POINT 00042090
4214 C GAUSS RULE 00042100
4215 C XGK(1), XGK(3), .... ABSCISSAE WHICH 00042110
4216 C ARE OPTIMALLY ADDED TO THE 10-POINT 00042120
4217 C GAUSS RULE 00042130
4218 C WG - WEIGHTS OF THE 21-POINT GAUSS-KRONROD RULE 00042140
4219 C WG - WEIGHTS OF THE 10-POINT GAUSS RULE, 00042150
4220 C CORRESPONDING TO THE ABSCISSAE XGK(2), 00042160
4221 C XGK(4), ... WG(1), WG(3), ... ARE SET 00042170
4222 C TO ZERO. 00042180
4223 C 00042190
4224 C DATA XGK(1), XGK(2), XGK(3), XGK(4), XGK(5), XGK(6), XGK(7), XGK(8) 00042200
4225 C *, XGK(9), XGK(10), XGK(11) /0.99565716302580807355272807D+00, 00042210
4226 C *0.9739065285171717200779640121D+00, 00042220
4227 C *0.9301574913557082260012071801D+00, 00042230
4228 C *0.8650633666889845107320966884D+00, 00042240
4229 C *0.7808177265864168970637175783D+00, 00042250
4230 C *0.6794095682990244062343273651D+00, 00042260
4231 C *0.5627571346686046833390000993D+00, 00042270
4232 C *0.4333953941292471907992659432D+00, 00042280
4233 C *0.2943928627014601981311266031D+00, 00042290
4234 C *0.1488743389816312108848260011D+00, 0.0D0/ 00042300

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4235      DATA WGK(1), WGK(2), WGK(3), WGK(4), WGK(5), WGK(6), WGK(7),WGK(8)00042310
4236      *, WGK(9), WGK(10), WGK(11) /0.1169463886737187427806439606D-01, 00042320
4237      *0.3255816230796472747881897246D-01, 00042330
4238      *0.5475589657435199603138130024D-01, 00042340
4239      *0.7503967481091995276704314092D-01, 00042350
4240      *0.9312545458369760553506546508D-01, 00042360
4241      *0.1093871588022976418992105903D+00, 00042370
4242      *0.1234919762620658510779581098D+00, 00042380
4243      *0.1347092173114733259280540018D+00, 00042390
4244      *0.1427759385770600807970942731D+00, 00042400
4245      *0.1477391049013384913748415160D+00, 00042410
4246      *0.1494455540029169056649364684D+00/
4247      DATA WG(1), WG(2), WG(3), WG(4), WG(5), WG(6), WG(7), WG(8),WG(9),00042430
4248      * WG(10) /0.000,0.6667134430868813759356880989D-01,0.000, 00042440
4249      *0.1494513491505805931457763397D+00,0.000, 00042450
4250      *0.2190863625159820439955349342D+00,0.000, 00042460
4251      *0.2692667193099963550912269216D+00,0.000, 00042470
4252      *0.2955242247147528701738929947D+00/ 00042480
4253      EPMACH = X02AAF(1.000) 00042490
4254      UFLOW = X02ABF(1.000) 00042500
4255      C 00042510
4256      C      LIST OF MAJOR VARIABLES 00042520
4257      C      -----
4258      C      CENTRE - MID POINT OF THE INTERVAL 00042530
4259      C      HLGTH - HALF LENGTH OF THE INTERVAL 00042540
4260      C      ABSC - ABSISSA 00042550
4261      C      FVAL* - FUNCTION VALUE 00042560
4262      C      RESG - 10-POINT GAUSS FORMULA 00042570
4263      C      RESK - 21-POINT GAUSS-KRONROD FORMULA 00042580
4264      C      RESKH - APPROXIMATION TO MEAN VALUE OF F OVER 00042590
4265      C      (A,B), I.E. TO I/(B-A) 00042600
4266      C 00042610
4267      C      CENTRE = 0.5D+00*(A+B) 00042620
4268      C      HLGTH = 0.5D+00*(B-A) 00042630
4269      C      DHLGTH = DABS(HLGTH) 00042640
4270      C 00042650
4271      C      COMPUTE THE 21-POINT GAUSS-KRONROD APPROXIMATION TO 00042660
4272      C      THE INTEGRAL, AND ESTIMATE THE ABSOLUTE ERROR 00042670
4273      C 00042680
4274      C      RESG = 0.0D+00 00042690
4275      C      FC = F(CENTRE) 00042700
4276      C      RESK = WGK(11)*FC 00042710
4277      C      RESABS = DABS(RESK) 00042720
4278      DO 20 J=1,10 00042730
4279      ABSC = HLGTH*XGK(J) 00042740
4280      FVAL1 = F(CENTRE-ABSC) 00042750
4281      FVAL2 = F(CENTRE+ABSC) 00042760
4282      FV1(J) = FVAL1 00042770
4283      FV2(J) = FVAL2 00042780
4284      FSUM = FVAL1 + FVAL2 00042790
4285      RESG = RESG + WGK(J)*FSUM 00042800
4286      RESK = RESK + WGK(J)*FSUM 00042810
4287      RESABS = RESABS + WGK(J)*(DABS(FVAL1)+DABS(FVAL2)) 00042820
4288      20 CONTINUE 00042830
4289      RESKH = RESK*0.5D+00 00042840
4290      RESASC = WGK(11)*DABS(FC-RESKH) 00042850
4291      DO 40 J=1,10 00042860
4292      RESASC = RESASC + WGK(J)*(DABS(FV1(J)-RESKH)+DABS(FV2(J)-RESKH)) 00042870
4293      * ) 00042880
4294      40 CONTINUE 00042890
4295      RESULT = RESK*HLGTH 00042900
4296      RESABS = RESABS*DHLGTH 00042910
4297      RESASC = RESASC*DHLGTH 00042920
4298      ABSERR = DABS((RESK-RESG)*HLGTH) 00042930
4299      IF (RESASC.NE.0.D+00) ABSERR = RESASC*DMIN1(0.1D+01,(0.2D+03* 00042940
4300      *ABSERR/RESASC)*X1.5D0) 00042950
4301      IF (RESABS.GT.UFLOW/(0.5D+02*EPMACH)) ABSERR = DMAX1(EPMACH*RESABS*00042960
4302      *0.5D+02,ABSERR) 00042970
4303      RETURN 00042980
4304      END 00042990
4305      C 00043000
4306      C      INTEGER FUNCTION P01AAF(IFAIL, ERROR, SRNAME) 00043010
4307      C      FUNCTION P01AAF, PART OF PEM (VERSION 82360). 00043020
4308      C 00043030
4309      C 00043040
4310      C      MARK 1 RELEASE. NAG COPYRIGHT 1971 00043050
4311      C      MARK 3 REVISED 00043060
4312      C 00043070

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4389 C DATA Z/Z0010000000000000/ 00043790
4390 C X02ABF = Z 00043800
4391 C RETURN 00043810
4392 C END 00043820
4393 C 00043830
4394 C 00043840
4395 C DOUBLE PRECISION FUNCTION X02ACF(X) 00043850
4396 C FUNCTION X02ACF, PART OF PEM (VERSION 82360). 00043860
4397 C 00043870
4398 C NAG COPYRIGHT 1975 00043880
4399 C MARK 4.5 RELEASE 00043890
4400 C DOUBLE PRECISION X 00043900
4401 C * RMAX * 00043910
4402 C 00043920
4403 C IBM DOUBLE PRECISION VERSION 00043930
4404 C 00043940
4405 C RETURNS THE VALUE OF THE LARGEST POSITIVE REAL FLOATING- 00043950
4406 C POINT NUMBER REPRESENTABLE ON THE COMPUTER 00043960
4407 C FOR ICL 1900 00043970
4408 C X02ACF = (2.0 - 2.0**(-36.0))*2.0**254.0 00043980
4409 C FOR IBM 360/370 00043990
4410 C X02ACF = (1.0D0-16.0D0*(-14.0D0))*16.0D0*63.0D0 00044000
4411 C DOUBLE PRECISION Z 00044010
4412 C DIMENSION ZZ(2)
4413 C EQUIVALENCE (ZZ(1),Z)
4414 C DATA ZZ /037777777777.07777777777777/
4415 C DATA Z/Z7FFFFFFFFFFFFF/ 00044020
4416 C X02ACF = Z 00044030
4417 C RETURN 00044040
4418 C END 00044050
4419 C 00044060
4420 C 00044070
4421 C SUBROUTINE X04AAF(I,NERR) 00044080
4422 C SUBROUTINE X04AAF, PART OF PEM (VERSION 82360). 00044090
4423 C 00044100
4424 C MARK 7 RELEASE. NAG COPYRIGHT 1978 00044110
4425 C MARK 7C REVISED IER-190 (MAY 1979) 00044120
4426 C IF I = 0, SETS NERR TO CURRENT ERROR MESSAGE UNIT NUMBER 00044130
4427 C (STORED IN NERR1).
4428 C IF I = 1, CHANGES CURRENT ERROR MESSAGE UNIT NUMBER TO 00044140
4429 C VALUE SPECIFIED BY NERR. 00044150
4430 C 00044160
4431 C 00044170
4432 C *** NOTE ***
4433 C THIS ROUTINE ASSUMES THAT THE VALUE OF NERR1 IS SAVED 00044180
4434 C BETWEEN CALLS. IN SOME IMPLEMENTATIONS IT MAY BE 00044190
4435 C NECESSARY TO STORE NERR1 IN A LABELLED COMMON 00044200
4436 C BLOCK /AX04AA/ TO ACHIEVE THIS. 00044210
4437 C 00044220
4438 C .. SCALAR ARGUMENTS .. 00044230
4439 C INTEGER I, NERR 00044240
4440 C .. 00044250
4441 C .. LOCAL SCALARS .. 00044260
4442 C INTEGER NERR1 00044280
4443 C .. 00044290
4444 C DATA NERR1 /6/ 00044300
4445 C IF (I.EQ.0) NERR = NERR1 00044310
4446 C IF (I.EQ.1) NERR1 = NERR 00044320
4447 C RETURN 00044330
4448 C END 00044340
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3BRKPT PRINTS

**TECHNICAL REPORT DATA**  
*(Please read instructions on the reverse before completing)*

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15. SUPPLEMENTARY NOTES		
16. ABSTRACT  The Pollution Episodic Model (PEM) is an urban-scale model designed to predict short-term average ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants at multiple receptors. The two pollutants may be non-reactive, or chemically-coupled through a first-order chemical transformation. Up to 300 isolated point sources and 50 distributed area sources may be considered in the calculations. Concentration and deposition flux estimates are made using the mean meteorological data for an hour. Up to a maximum of 24 hourly scenarios of meteorology may be included in an averaging period.		
The concentration algorithms used in PEM are specially developed to account for the effects of dry deposition, sedimentation, and first-order chemical transformation. The Gaussian plume-type algorithms for point sources are derived from analytical solutions of a gradient-transfer model. In the limit, when deposition and settling velocities of the pollutants and the chemical transformation rate are zero, these expressions reduce to the familiar Gaussian plume diffusion algorithms. The concentration algorithms for area sources in PEM are derived from an innovative approach based on mass balance considerations. These algorithms are simple, efficient, and accurate. The computer program of the Texas Episodic Model is used as a framework for the development of the PEM program.		
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