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POLLUTION EPISODIC MODEL USER'S GUIDE

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POLLUTION EPISODIC MODEL USER'S GUIDE

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ACKNOWLEDGEMENTS

This report was prepared for the Office of Research and Development, Environmental Sciences Research Laboratory of the U. S. Environmental Protection Agency to support the needs of EPA's Office of Air Quality Planning and Standards in urban particulate modeling. This work was accomplished under interagency agreements among the U. S. Department of Energy, the National Oceanic and Atmospheric Administration, and the EPA. The authors are grateful to Dr. Jack Shreffler of ESRL for the opportunity to do this work, and for his interest and patience. The authors also express their appreciation to the following members of the Atmospheric Turbulence and Diffusion Division: Director Bruce B. Hicks for his understanding and support, Dr. Ray Hosker for useful suggestions and discussions during the course of this work, and Mrs. Mary Rogers for her expert technical typing and patient revisions. Special thanks are due to Bernadette Kirk, Nancy Price, and Louise Taylor, who worked as programmers for this project at various times and assisted in the development and testing of the concentration algorithms for PEM.

Several figures and tables shown in this report are reproduced from the Users' Guide to Texas Episodic Model with permission from the Texas Air Control Board. The library routine D01AJF used for numerical integration in PEM has been released by the Computer Sciences Division of the Oak Ridge National Laboratory for inclusion in the program listing. The Numerical Algorithms Group holds the copyright to this routine and its document. The latter is reproduced in this report from the NAG FORTRAN Mini-Manual.

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.

This User's Guide to PEM was prepared by NOAA's Atmospheric Turbulence and Diffusion Division in partial fulfillment of Interagency Agreement No. AD-13-F-1-707-0 with the U.S. Environmental Protection Agency. Details of the development and testing of the concentration algorithms used in PEM for point and area sources are given in another report prepared under this Interagency Agreement. This work, covering the period September 1981 to March 1983, was completed as of April 30, 1983.

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, $\sigma_y(x)$ 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 SO_2 to $SO_4^=$.

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) <u>Control parameters</u>

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 ($0 < x \leq x_m$),

$$C_1 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{21}}{L_z} \tag{1a}$$

$$C_2 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{22}}{L_z} \tag{1b}$$

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

$$C_1 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{41}}{L} \tag{2a}$$

$$C_2 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{42}}{L} \tag{2b}$$

$$L_y = \sqrt{2\pi}\ \sigma_y\ ,\ L_z = \sqrt{2\pi}\ \sigma_z \tag{3}$$

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

$$H_c = 2\,(1.5 - \frac{V}{U})\,d \qquad (4)$$

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.

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2.2.3 Dispersion Parameters

The Gaussian dispersion parameters, σ_y and σ_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:

$$\sigma_z(x) = a\ x^b \tag{5a}$$

$$\sigma_y(x) = c\ x^d \tag{5b}$$

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 σ_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 capaicty 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 (Δ) between wind direction azimuth and the azimuth from the source to the receptor. If Δ exceeds the maximum crosswind angle of the plume (Δ_{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	Δ_{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 (Δx) 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 Δx 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_o) are assumed to be located at the center of the square; contributions of this area source are determined at the receptor (R_o) 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

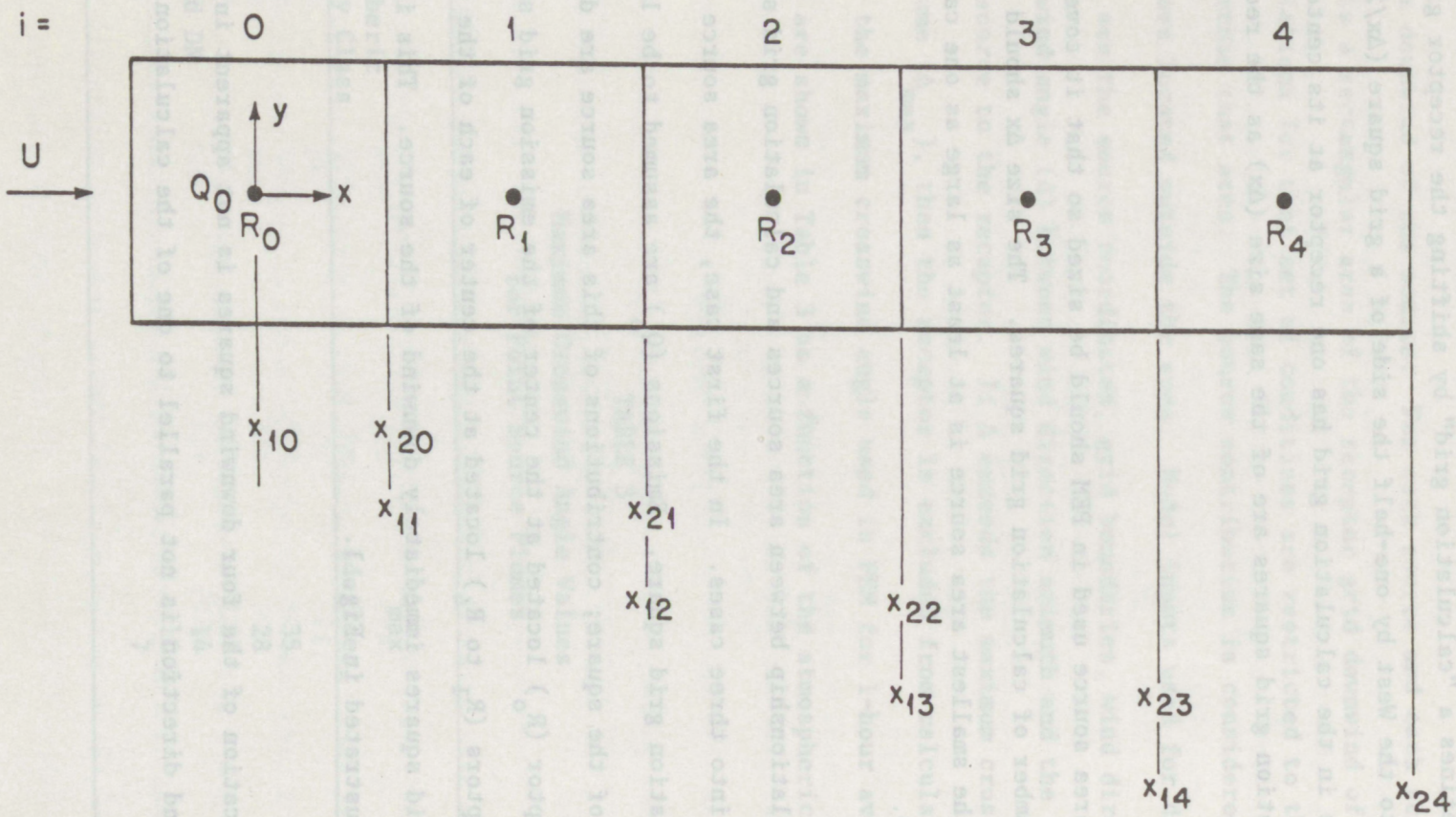

Figure 1. Schematic diagram showing a single grid square with emissions and four downwind calculation grid squares with receptors, and the distances used in area-source algorithms. These distances are measured downwind from the source Q_o.

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

ξ 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 ξ

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

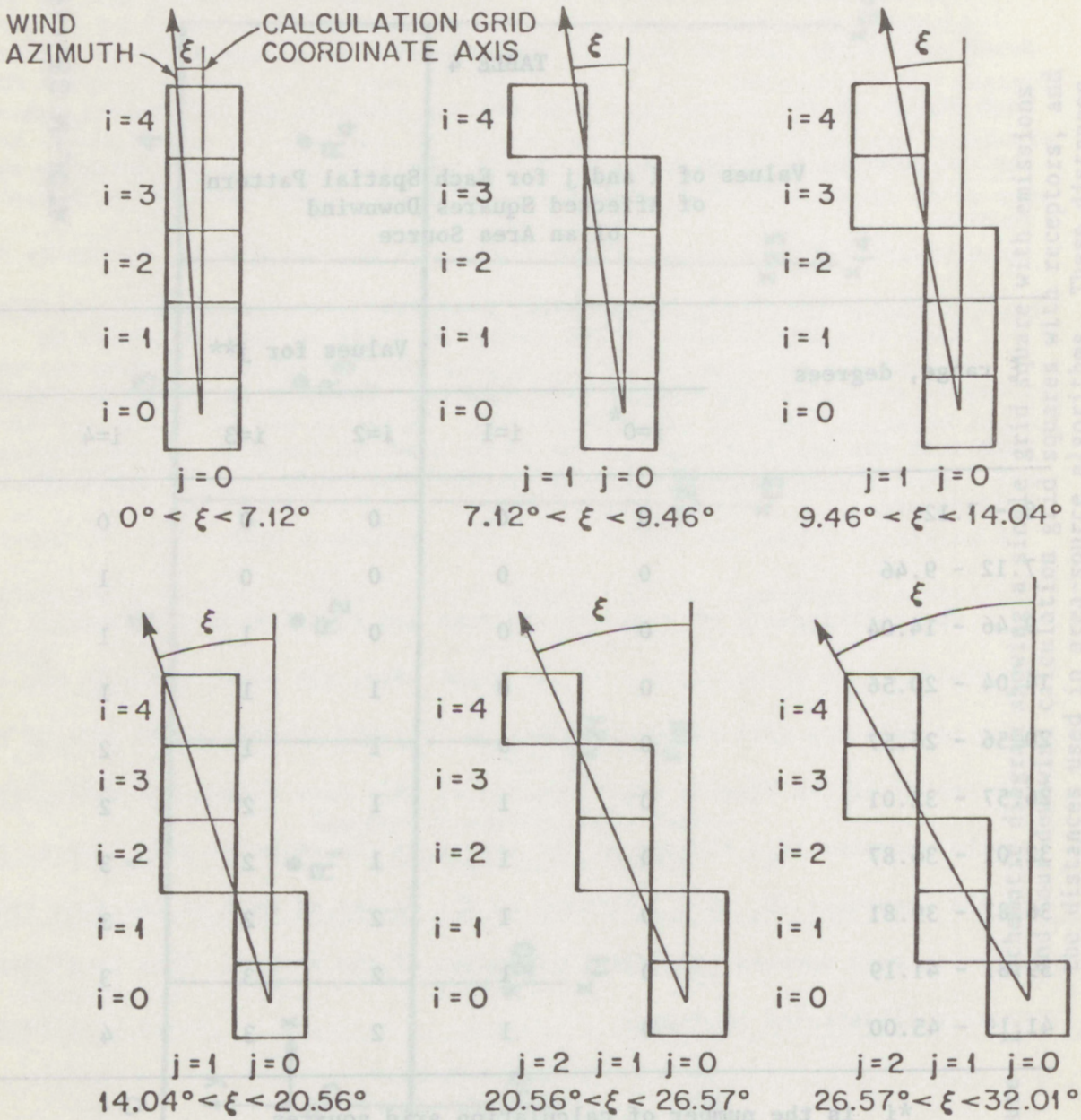

Figure 2. Spatial patterns of affected calculation grid squares downwind of an area source.

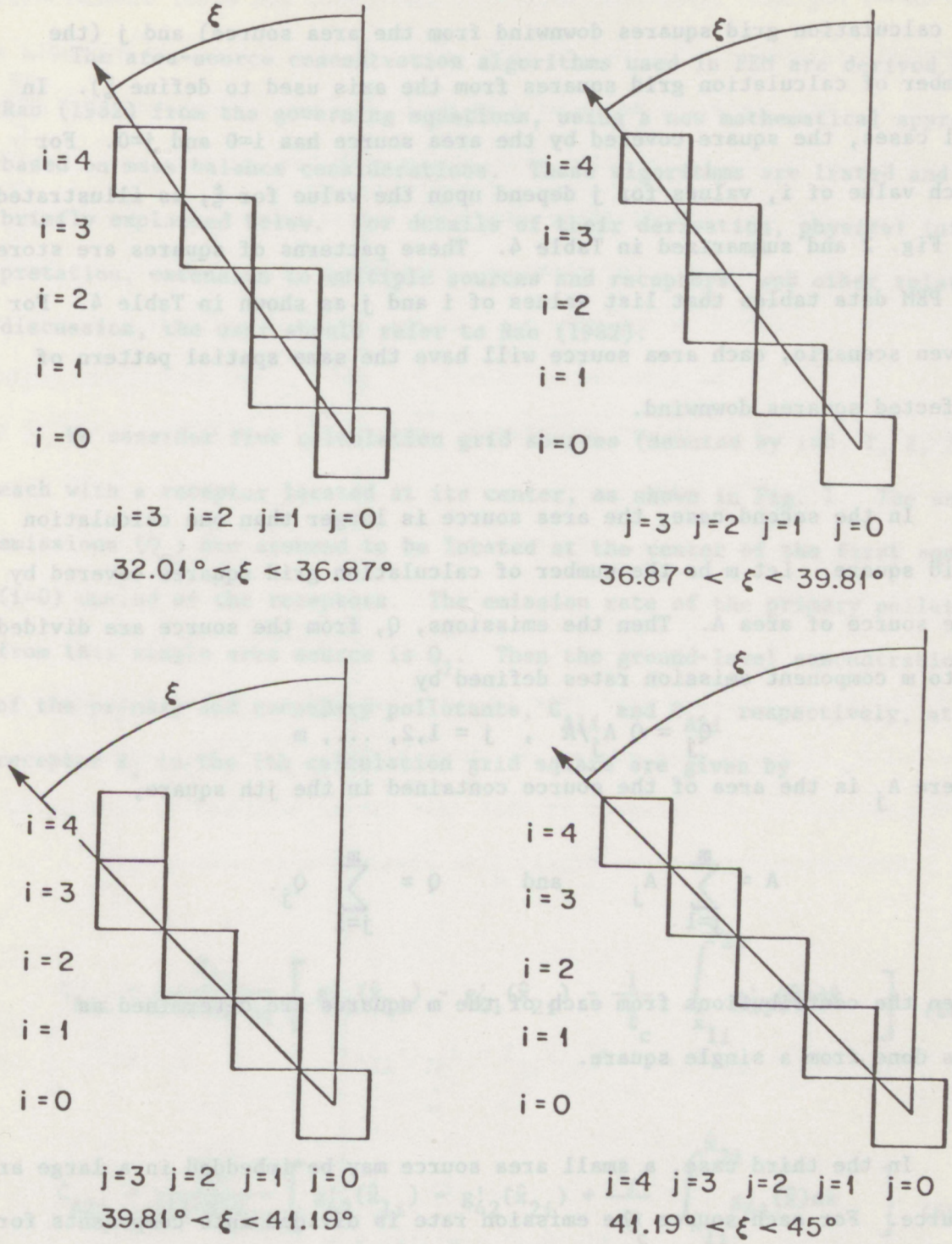

Figure 2. Continued

value of ξ, 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 ξ). 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 ξ, 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

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

where A_j is the area of the source contained in the jth square,

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

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 ith calculation grid square are given by

$$C_{A1i} = \frac{Q_1}{2(1-b)V_{d1}} \left[g'_{41}(\hat{x}_{1i}) - g'_{41}(\hat{x}_{2i}) - \frac{1}{\hat{\tau}_c} \int_{\hat{x}_{1i}}^{\hat{x}_{2i}} g'_{41}(\hat{x})d\hat{x} \right] \quad (6a)$$

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

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_{1i} and x_{2i} are distances measured from Q_o to the upwind and downwind edges, respectively, of the calculation grid square with the ith receptor (see Fig. 1); $\hat{x}_{1i}$ and $\hat{x}_{2i}$ are the corresponding dimensionless values; τ_c is characteristic time scale of the first-order chemical transformation, and $\hat{\tau}_c$ is its dimensionless value as defined in Appendix A; γ 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,

$$\sigma_z(x) = a\, x^b \tag{7}$$

for area sources.

Now let us consider five area sources, located upwind of a single receptor R_o in i=0th 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:

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

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

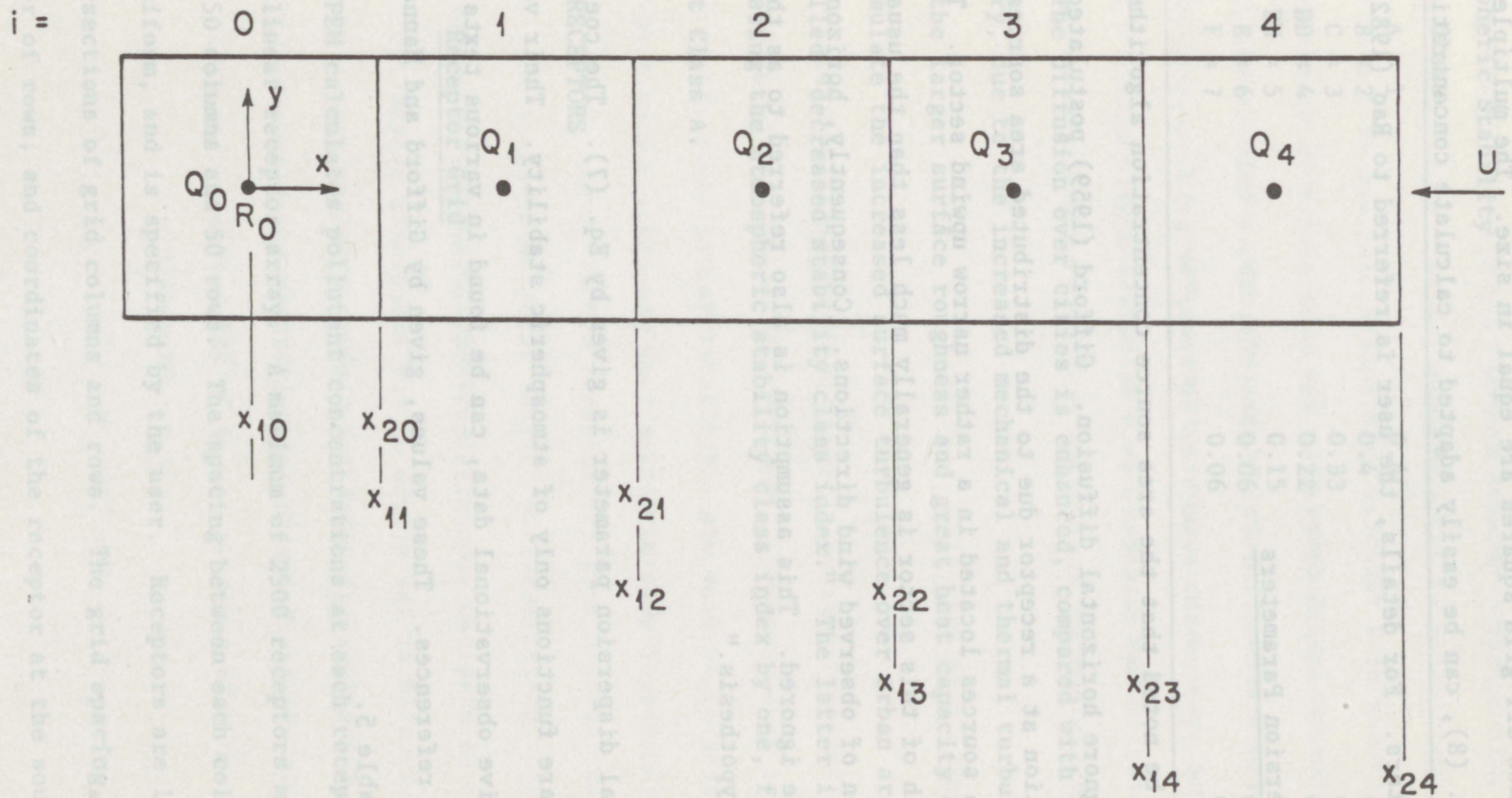

Figure 3. Schematic diagram showing a single grid square with receptor and four upwind grid squares with emissions, and the distances used in area-source algorithms. These distances are measured upwind from the receptor R_o.

Here x_{1i} and x_{2i} are the distances measured from the receptor R_o to the downwind and upwind edges, respectively, of the ith 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° 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

$$E = 90° - W$$

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

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

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 σ_y and σ_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

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

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

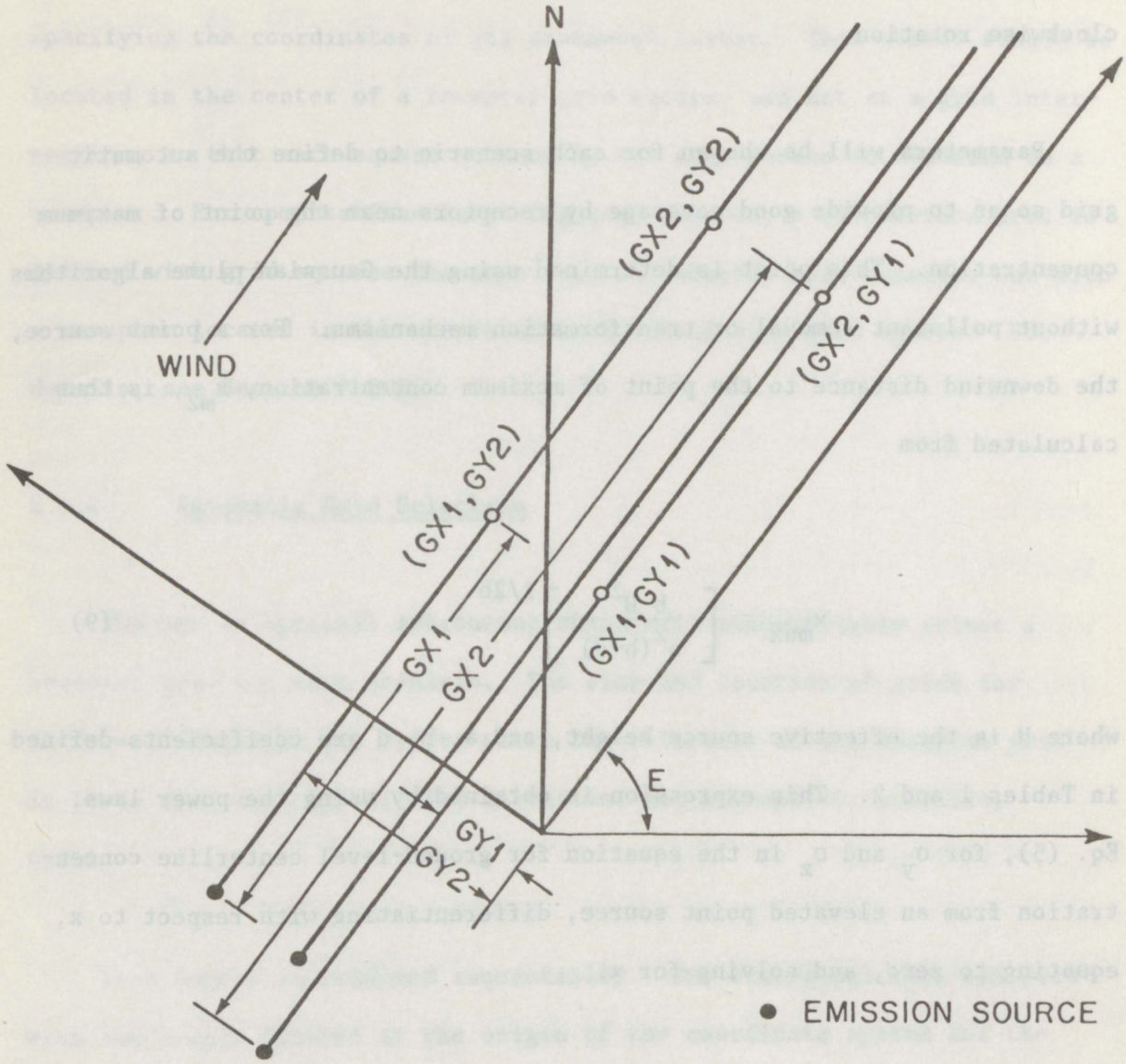

Figure 4. Points used for automatic selection of receptor grid by AUTGRD subroutine.

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 sytem. 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.

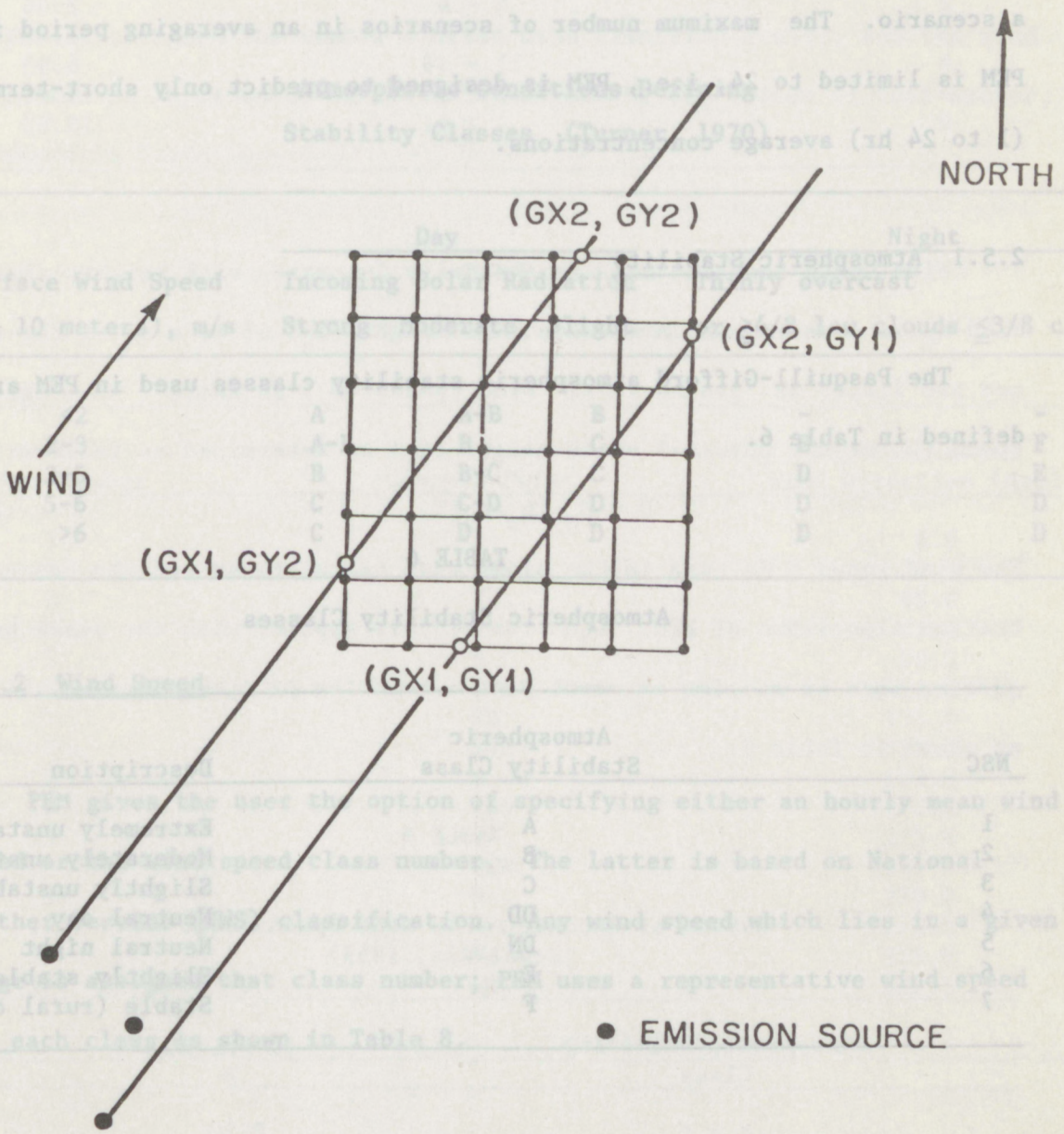

Figure 5. Example of a receptor grid selected by AUTGRD subroutine.

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: Incoming Solar Radiation Strong	Day: Moderate	Day: Slight	Night: Thinly overcast or ≥4/8 low clouds	Night: ≤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:

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

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 paramters 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

reproduced from TEM Users' Guide with permission from Texas Air Control Board (TACB).

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 σ_y to account for the greater horizontal plume meander due to fluctuations in wind direction. This is not done in PEM, since its σ_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 souce 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

```
                 ¦ MAIN
                 ¦
                 ¦
                 ¦----- INMOD
                 ¦
¦----------+ Loop on scenarios
¦          ¦
¦          ¦----- INMOD
¦          ¦
¦          ¦----- AUTGRD ----- RISE
¦          ¦
¦          ¦
¦    ¦-----+ Loop on area sources
¦    ¦     ¦
¦    ¦     ¦----- PSG4P ----- DO1AJF ----- FUN2
¦    ¦     ¦
¦    ¦     ¦----- DO1AJF ----- FUN3 ----- ARGCHK
¦    ¦-----+
¦          ¦
¦          ¦
¦    ¦-----+ Loop on point sources
¦    ¦     ¦
¦    ¦     ¦----- RISE
¦    ¦     ¦
¦    ¦     ¦----- QZCAL -----¦ RISE
¦    ¦     ¦                 ¦ EXPO
¦    ¦     ¦                 ¦ ARGCHK
¦    ¦     ¦                 ¦ PSG4P ----- DO1AJF ----- FUN2
¦    ¦     ¦                 ¦ DO1AJF ----- FUN1 ----- ARGCHK
¦    ¦     ¦                                           EXPO
¦    ¦     ¦
¦    ¦-----+
¦          ¦
¦          ¦----- WORST
¦          ¦
¦          ¦----- WOROUT
¦          ¦
¦          ¦----- OUTMOD -----¦ WOROUT
¦          ¦                 ¦ ARRAY
¦          ¦                 ¦ SCENMX
¦          ¦
¦----------+
           ¦
           ¦----- MAXOUT
           ¦
```

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 DO1AJF. 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/momentum 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

$$Xcal = A + BX$$

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.

HMIX Mixing height

The distance in meters from the ground to the bottom of a layer of stable air.

The default value is HMIX=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 $\mu g/m^3$; 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.

<u>At the end of the run</u>:

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), NCSOPT 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 τ_c is nondimensionalized by $\sqrt{2}\,\sigma_z/U$. The horizontal crosswind distance y is nondimensionalized by $\sqrt{2}\,\sigma_y$. Thus, we define

$$\hat{V}_{d1} = V_{d1}/U \quad , \quad \hat{V}_{d2} = V_{d2}/U$$

$$\hat{W}_1 = W_1/U \quad , \quad \hat{W}_2 = W_2/U$$

$$\hat{V}_{11} = \hat{V}_{d1} - \hat{W}_1/2 \quad , \quad \hat{V}_{12} = \hat{V}_{d2} - \hat{W}_2/2$$

$$\hat{V}_{13} = \hat{V}_{11} - (\hat{W}_1 - \hat{W}_2)/2 \qquad \text{(A-1)}$$

$$\hat{V}_{21} = \hat{V}_{d1} - \hat{W}_1 \quad , \quad \hat{V}_{22} = \hat{V}_{d2} - \hat{W}_2$$

$$\hat{x} = x/\sqrt{2}\,\sigma_z \quad , \quad \hat{z} = z/\sqrt{2}\,\sigma_z$$

$$\hat{H} = H/\sqrt{2}\,\sigma_z \quad , \quad \hat{L} = L/\sqrt{2}\,\sigma_z$$

$$\hat{\tau}_c = \tau_c U/\sqrt{2}\,\sigma_z \quad , \quad \hat{y} = y/\sqrt{2}\,\sigma_y$$

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
σ_y , σ_z	= Gaussian dispersion parameters in y and z directions
τ_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:

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

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

where $$\beta_1^2 = -2\,\hat{W}_1\,\hat{x}\,\hat{H} + \hat{W}_1^2\,\hat{x}^2$$

$$\alpha_1 = 4\sqrt{\pi}\,\hat{V}_{11}\,\hat{x}\;e^{\xi_1^2}\,\mathrm{erfc}\,\xi_1 \tag{A-4}$$

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

$$g'_{22}(\hat{x},0) = e^{-\beta_2^2}\Big[(Q_2/Q_1 + \gamma)\;e^{-\hat{H}^2}\cdot(2 - \alpha_2)$$

$$-\gamma\,\exp(-\hat{H}^2 - \hat{x}/\hat{\tau}_c)\cdot(2 - \alpha_3)$$

$$-\gamma\,4\sqrt{\pi}\,(\hat{V}_{21} - \hat{V}_{22})\,\hat{x}\cdot F_1(\hat{x},0)\Big] \tag{A-5}$$

where $$\beta_2^2 = -2\,\hat{W}_2\,\hat{x}\,\hat{H} + \hat{W}_2^2\,\hat{x}^2$$

$$\alpha_2 = 4\sqrt{\pi}\,\hat{V}_{12}\,\hat{x}\;e^{\xi_2^2}\,\mathrm{erfc}\,\xi_2$$

$$\alpha_3 = 4\sqrt{\pi}\,\hat{V}_{13}\,\hat{x}\;e^{\xi_3^2}\,\mathrm{erfc}\,\xi_3$$

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

and

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

$$\left[1 - \sqrt{\pi}\,(\xi_4 - \hat{H}/\sqrt{t})\;e^{\xi_4^2}\,\mathrm{erfc}\,\xi_4\right]$$

$$\left[1 - \sqrt{\pi}\,\xi_5\;e^{\xi_5^2}\;\mathrm{erfc}\,\xi_5\right]\,dt \tag{A-7}$$

where

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

$$\xi_5 = 2\,\hat{V}_{12}\,\hat{x}\,\sqrt{1-t} \tag{A-8}$$

In Eq. (A-5), γ 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 $\hat{V}_{21} \neq 0$,

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

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 $\hat{V}_{21} = 0$,

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

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 $\hat{V}_{22} \neq 0$,

$$g'_{42}(\hat{x}) = e^{-\beta_2^2} \Bigg[(Q_2/Q_1 + \gamma) \left\{ (\hat{V}_{12}/\hat{V}_{22})\, e^{\xi_2^2} \operatorname{erfc} \xi_2 - (\hat{W}_2/2\hat{V}_{22})\, e^{\beta_2^2} \operatorname{erfc} \beta_2 \right\} - \gamma\, e^{-\hat{x}/\hat{\tau}_c} \left\{ (\hat{V}_{13}/\hat{V}_{21})\, e^{\xi_3^2} \operatorname{erfc} \xi_3 - (\hat{W}_2/2\,\hat{V}_{21})\, e^{\beta_2^2} \operatorname{erfc} \beta_2 \right\} - \gamma\, 4\sqrt{\pi}\, (\hat{V}_{21} - \hat{V}_{22})\, \hat{x} \cdot F_2(\hat{x}) \Bigg] \tag{A-11}$$

where $\xi_2 = 2\,\hat{V}_{12}\,\hat{x}$, $\beta_2 = \hat{W}_2\,\hat{x}$

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

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

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

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

<u>For $\hat{V}_{21} \neq 0$ and $\hat{V}_{22} = 0$,</u>

$$g'_{42}(\hat{x}) = e^{-\xi_2^2} \left[(Q_2/Q_1 + \gamma) \left\{ (1 + 2\,\xi_2^2)\, e^{\xi_2^2} \operatorname{erfc} \xi_2 - 2\,\xi_2/\sqrt{\pi} \right\} \right.$$

$$- \gamma\, e^{-\hat{x}/\hat{\tau}_c} \left\{ (\hat{V}_{13}/\hat{V}_{21})\, e^{\xi_3^2} \operatorname{erfc} \xi_3 - (\hat{W}_2/2\hat{V}_{21})\, e^{\xi_2^2} \operatorname{erfc} \xi_2 \right\}$$

$$\left. - \gamma\, 4\sqrt{\pi}\ \hat{V}_{21}\, \hat{x} \cdot F_2(\hat{x}) \right] \qquad \text{(A-15)}$$

where $\xi_2 = 2\,\hat{V}_{12}\,\hat{x} = \hat{V}_{d2}\,\hat{x} = \hat{W}_2\,\hat{x} = \beta_2$

$\xi_3 = 2\,\hat{V}_{13}\,\hat{x}$

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

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

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

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

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

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

$$+ \gamma\, 4\sqrt{\pi}\, \hat{V}_{22}\, \hat{x} \cdot F_2(\hat{x}) \Bigg] \tag{A-17}$$

where $\xi_2 = 2\,\hat{V}_{12}\,\hat{x}\,, \quad \xi_3 = 2\,\hat{V}_{13}\,\hat{x} = \hat{W}_2\,\hat{x} = \beta_2\,,$

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

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

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

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

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 Report (in press), U.S. Environmental Protection Agency, Research Triangle Park, NC; NOAA Tech. Memo. ERL ARL-124; 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,

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

and

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

where

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

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

For stable atmosphere, with a buoyancy-dominated plume,

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

and

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

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,

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

and

$$\Delta h_{MAX} = 6RV/U \tag{B-8}$$

For stable atmosphere, with a momentum-dominated plume,

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

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

The variables used in the above equations are defined below:

$$F = gVR^2\ (T-T_A)\ /T \tag{B-10}$$

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

g	= acceleration due to gravity, 9.8 m/s^2
Δh	= plume rise, m
Δh_{MAX}	= maximum plume rise, m
R	= inside radius of stack exit, m
T	= plume temperature at stack exit, °K
T_A	= ambient temperature, °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

$$D_1(\hat{x},\hat{y}) = V_{d1} \cdot C_1(\hat{x},\hat{y},0) \qquad \text{(C-1)}$$

$$D_2(\hat{x},\hat{y}) = V_{d2} \cdot C_2(\hat{x},\hat{y},0) \qquad \text{(C-2)}$$

D gives the amount of pollutant deposited per unit time per unit surface area, and is usually calculated as kg/km^2-hr, while seasonal estimates are expressed as kg/km^2-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 kg/km^2-hr when V_d is given in cm/s and C in g/m^3, the right-hand side of the equations should be multiplied by 36000. To obtain D in $\mu g/m^2$-hr when V_d is given in cm/s and C in $\mu g/m^3$, 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 $\mu g/m^2$-hr; however, if these values are too large to be clearly printed in a map format, then the program converts them into kg/km^2-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 ($d < 0.1$ μm), 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 ($d = 0.1 \sim 50$ μm), $0 < W < V_d$; deposition is enhanced here beyond that due to gravitational settling, primarily because of increased turbulent transfer resulting from surface roughness. For larger particles ($d > 50$ μm), 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 Report (in press), U. S. Environmental Protection Agency, Research Triangle Park, NC; NOAA Tech. Memo. ERL ARL-124; 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 ϵ–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] PIESSENS, R., DE DONCKER, E., ÜBERHUBER, 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 $\geq$ 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 $<$ 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:

$|I-\text{RESULT}| \leq tol$

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 $|I-\text{RESULT}| \leq \text{ABSERR} \leq tol$.

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

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     .. LOCAL ARRAYS ..
      REAL W(800)
      INTEGER IW(102)
C     .. FUNCTION REFERENCES ..
      REAL X01AAF
C     .. SUBROUTINE REFERENCES ..
C     D01AJF
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, 1HA, 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, 42HABSERR - 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 = , I4/)
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
ABSERR - 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
CONTROL CARDS
  1  TITLE          PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE
  2  OPTIONS            1    1    1    1    0    2    0    0    1    0    1    1    1
  3  GRID                   0.        0.        25        25        .04        0.        0.
  4  POLLUTANTS         2    1        1.0       0.0       0.1       0.0       1.0       1.5
  5  SCALING               1.0       1.0        0.        0.        0.        0.
  6  LABELS         GAS 1                                   GAS 2
SCENARIO CARDS
                     4    3    9                             15.0        1.      1000.
AREA SOURCE CARDS
                          .38       .02       120.       0.5       0.05
                  BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY
POINT SOURCE CARDS
                          .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

PEM (VERSION 82360)

POLLUTION EPISODIC MODEL

INCLUDING

DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION

OF POLLUTANTS

```
                    POLLUTION EPISODIC MODEL

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

     AVERAGING TIME OPTION: ATOPT=1

          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 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: NSTDWN=0

        0  ALGORITHM IS IN EFFECT
        1  ALGORITHM IS NOT USED

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

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

```
                                    POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM 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            A=     0.0    B=     0.0
     CALIBRATION IDENTIFICATION:
     DEPOSITION VELOCITY (CM/S):                      VD1=   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: XKT=  1.000 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 SCENARIC PARAMETERS: PEM EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

WIND DIRECTIONS

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

WIND SPEED CLASSES

CLASS INDEX	SPEED (M/S)	CLASS INTERVAL(KT)
1	1.50	0-3
2	2.46	4-6
3	4.47	7-10
4	6.93	11-16
5	9.61	17-21
6	12.52	OVER 21

STABILITY CLASSES

CLASS INDEX	CLASS
1	A
2	B
3	C
4	DD (DAY)
5	DN (NIGHT)
6	E
7	F

SCENARIC 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	DD	3	4.470	9	180.00	15.00	1.000	1000.0

POLLUTION EPISODIC MODEL

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

AREA SOURCE NUMBER	COORDINATES X(KM)	COORDINATES Y(KM)	LENGTH OF SIDE (M)	POLLUTANT-1 EMISSION RATE INPUT (G/S)	POLLUTANT-1 EMISSION RATE SCALED	POLLUTANT-2 EMISSION RATE INPUT (G/S)	POLLUTANT-2 EMISSION RATE 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	0.500	0.050	0.050

POLLUTION EPISODIC MODEL

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

POINT SOURCE NUMBER	LABEL	COORDINATES X(KM)	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	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	3.000	0.500	32.400

SUMS OF THE POINT SOURCE EMISSION RATES 2.000 G/S 0.200 G/S

POLLUTION EPISODIC MODEL

OUTPUT: PEM EXAMPLE 1 CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

SCENARIO 1 POINT 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 POL-1 (G/S)	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	0.20	0.0	1.00	0.10	15.00	1.000	5.000	305.55	BUOYANCY DOWNWASH	4.747	17.33
2	0.68	0.04	1.00	0.10	10.00	3.000	0.500	305.55	BUOYANCY 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 1 5 15 27 33 27 15 5 1 0 0 0													0.96
0.92	0 1 4 12 22 27 22 12 4 1 0 0 0 1 5 15 28 35 28 15 5 1 0 0 0													0.92
0.88	0 1 4 12 23 29 23 12 4 1 0 0 0 1 5 15 30 38 30 15 5 1 0 0 0													0.88
0.84	0 1 4 12 24 31 24 12 4 1 0 0 0 1 4 15 31 41 31 15 4 1 0 0 0													0.84
0.80	0 1 3 12 25 33 25 12 3 1 0 0 0 0 3 14 33 44 33 14 3 0 0 0 0													0.80
0.76	0 0 3 11 26 35 26 11 3 0 0 0 0 0 3 14 35 48 35 14 3 0 0 0 0													0.76
0.72	0 0 2 11 27 37 27 11 2 0 0 0 0 0 2 13 37 52 37 13 2 0 0 0 0													0.72
0.68	0 0 2 10 28 40 28 10 2 0 0 0 0 0 2 12 39 57 39 12 2 0 0 0 0													0.68
0.64	0 0 1 9 29 43 29 9 1 0 0 0 0 0 1 11 41 63 41 11 1 0 0 0 0													0.64
0.60	0 0 1 8 30 47 30 8 1 0 0 0 0 0 1 10 43 70 43 10 1 0 0 0 0													0.60
0.56	0 0 1 7 31 51 31 7 1 0 0 0 0 0 0 8 44 78 44 8 0 0 0 0 0													0.56
0.52	0 0 0 6 31 55 31 6 0 0 0 0 0 0 0 6 46 89 46 6 0 0 0 0 0													0.52
0.48	0 0 0 4 31 60 31 4 0 0 0 0 0 0 0 5 47 101 47 5 0 0 0 0 0													0.48
0.44	0 0 0 3 30 65 30 3 0 0 0 0 0 0 0 3 46 117 46 3 0 0 0 0 0													0.44
0.40	0 0 0 2 28 70 28 2 0 0 0 0 0 0 0 2 44 135 44 2 0 0 0 0 0													0.40
0.36	0 0 0 1 25 75 25 1 0 0 0 0 0 0 0 0 40 158 40 0 0 0 0 0 0													0.36
0.32	0 0 0 0 20 78 20 0 0 0 0 0 0 0 0 0 32 186 32 0 0 0 0 0 0													0.32
0.28	0 0 0 0 13 78 13 0 0 0 9 9 9 0 0 0 21 218 21 0 0 0 0 0 0													0.28
0.24	0 0 0 0 7 71 7 0 0 0 21 21 21 0 0 0 10 250 9 0 0 0 0 0 0													0.24
0.20	0 0 0 0 2 56 2 0 0 0 38 38 38 0 0 0 0 269 0 0 0 0 0 0 0													0.20
0.16	0 0 0 0 0 30 0 0 0 0 62 62 62 0 0 0 0 230 0 0 0 0 0 0 0													0.16
0.12	0 0 0 0 0 7 0 0 0 0 252 252 252 0 0 0 0 83 0 0 0 0 0 0 0													0.12
0.08	0 0 0 0 0 0 0 0 0 0 234 234 234 0 0 0 0 0 0 0 0 0 0 0 0													0.08
0.04	0 0 0 0 0 0 0 0 0 0 201 201 201 0 0 0 0 0 0 0 0 0 0 0 0													0.04
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	0.08	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 KILOMETER 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	0	0	1	1	1	0	0	0	0	0	0	0	0.96
0.92	0	0	0	1	1	1	0	0	0	0	0	0	0	0.92
0.88	0	0	0	1	1	1	0	0	0	0	0	0	0	0.88
0.84	0	0	0	1	1	1	0	0	0	0	0	0	0	0.84
0.80	0	0	0	1	1	1	0	0	0	0	0	0	0	0.80
0.76	0	0	0	1	1	1	0	0	0	0	0	0	0	0.76
0.72	0	0	0	1	1	1	0	0	0	0	0	0	0	0.72
0.68	0	0	0	1	1	1	0	0	0	0	0	0	0	0.68
0.64	0	0	0	1	2	1	0	0	0	0	0	0	0	0.64
0.60	0	0	0	1	2	1	0	0	0	0	0	0	0	0.60
0.56	0	0	0	1	2	1	0	0	0	0	0	0	0	0.56
0.52	0	0	0	1	2	1	0	0	0	0	0	0	0	0.52
0.48	0	0	0	1	2	1	0	0	0	0	0	0	0	0.48
0.44	0	0	0	1	2	1	0	0	0	0	0	0	0	0.44
0.40	0	0	0	1	3	1	0	0	0	0	0	0	0	0.40
0.36	0	0	0	1	3	1	0	0	0	0	0	0	0	0.36
0.32	0	0	0	1	3	1	0	0	0	0	0	0	0	0.32
0.28	0	0	0	0	3	0	0	0	0	0	0	0	0	0.28
0.24	0	0	0	0	3	0	0	0	0	1	1	1	0	0.24
0.20	0	0	0	0	2	0	0	0	0	1	1	1	0	0.20
0.16	0	0	0	0	0	1	0	0	0	2	2	2	0	0.16
0.12	0	0	0	0	0	0	0	0	0	9	9	9	0	0.12
0.08	0	0	0	0	0	0	0	0	0	8	8	8	0	0.08
0.04	0	0	0	0	0	0	0	0	0	7	7	7	0	0.04
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=DD, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 1 HR. POLLUTANT-2: GAS 2
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 0	1 1	2 3	2 1	1 0	0 0	0 0	1 2	3 4	3 2	1 0	0 0	0	0.96
0.92	0 0	0 1	2 3	2 1	0 0	0 0	0 0	1 2	3 4	3 2	1 0	0 0	0	0.92
0.88	0 0	0 1	3 3	3 1	0 0	0 0	0 0	1 2	3 4	3 2	1 0	0 0	0	0.88
0.84	0 0	0 1	3 3	3 1	0 0	0 0	0 0	0 2	4 5	4 2	0 0	0 0	0	0.84
0.80	0 0	0 1	3 4	3 1	0 0	0 0	0 0	0 2	4 5	4 2	0 0	0 0	0	0.80
0.76	0 0	0 1	3 4	3 1	0 0	0 0	0 0	0 2	4 5	4 2	0 0	0 0	0	0.76
0.72	0 0	0 1	3 4	3 1	0 0	0 0	0 0	0 1	4 6	4 1	0 0	0 0	0	0.72
0.68	0 0	0 1	3 4	3 1	0 0	0 0	0 0	0 1	4 6	4 1	0 0	0 0	0	0.68
0.64	0 0	0 1	3 5	3 1	0 0	0 0	0 0	0 1	5 7	5 1	0 0	0 0	0	0.64
0.60	0 0	0 1	3 5	3 1	0 0	0 0	0 0	0 1	5 8	5 1	0 0	0 0	0	0.60
0.56	0 0	0 1	3 5	3 1	0 0	0 0	0 0	0 1	5 9	5 1	0 0	0 0	0	0.56
0.52	0 0	0 1	3 4	3 1	0 0	0 0	0 0	0 1	5 10	5 1	0 0	0 0	0	0.52
0.48	0 0	0 0	3 6	3 0	0 0	0 0	0 0	0 1	5 11	5 1	0 0	0 0	0	0.48
0.44	0 0	0 0	3 7	3 0	0 0	0 0	0 0	0 0	5 13	5 0	0 0	0 0	0	0.44
0.40	0 0	0 0	3 7	3 0	0 0	0 0	0 0	0 0	5 15	5 0	0 0	0 0	0	0.40
0.36	0 0	0 0	3 8	3 0	0 0	0 0	0 0	0 0	4 17	4 0	0 0	0 0	0	0.36
0.32	0 0	0 0	2 8	2 0	0 0	0 0	0 0	0 0	3 20	3 0	0 0	0 0	0	0.32
0.28	0 0	0 0	1 8	1 0	0 0	1 1	1 0	0 0	2 23	2 0	0 0	0 0	0	0.28
0.24	0 0	0 0	1 7	1 0	0 0	2 2	2 0	0 0	1 27	1 0	0 0	0 0	0	0.24
0.20	0 0	0 0	0 6	0 0	0 0	4 4	4 0	0 0	0 28	0 0	0 0	0 0	0	0.20
0.16	0 0	0 0	0 3	0 0	0 0	6 6	6 0	0 0	0 24	0 0	0 0	0 0	0	0.16
0.12	0 0	0 0	0 1	0 0	0 0	25 25	25 0	0 0	0 9	0 0	0 0	0 0	0	0.12
0.08	0 0	0 0	0 0	0 0	0 0	24 24	24 0	0 0	0 0	0 0	0 0	0 0	0	0.08
0.04	0 0	0 0	0 0	0 0	0 0	20 20	20 0	0 0	0 0	0 0	0 0	0 0	0	0.04
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	0.08	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. POLLUTANT-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 1	2 6	11 13	11 6	2 1	0 0	0	0.96
0.92	0 0	2 5	9 11	9 5	2 0	0 0	0 0	2 6	12 14	12 6	2 0	0 0	0	0.92
0.88	0 0	2 5	9 11	9 5	2 0	0 0	0 0	2 6	12 15	12 6	2 0	0 0	0	0.88
0.84	0 0	1 5	10 12	10 5	1 0	0 0	0 0	2 6	13 17	13 6	2 0	0 0	0	0.84
0.80	0 0	1 5	10 13	10 5	1 0	0 0	0 0	1 6	13 18	13 6	1 0	0 0	0	0.80
0.76	0 0	1 4	10 14	10 4	1 0	0 0	0 0	1 6	14 19	14 6	1 0	0 0	0	0.76
0.72	0 0	1 4	11 15	11 4	1 0	0 0	0 0	1 5	15 21	15 5	1 0	0 0	0	0.72
0.68	0 0	1 4	11 16	11 4	1 0	0 0	0 0	1 5	16 23	16 5	1 0	0 0	0	0.68
0.64	0 0	1 4	12 17	12 4	1 0	0 0	0 0	0 4	16 25	16 4	0 0	0 0	0	0.64
0.60	0 0	0 3	12 18	12 3	0 0	0 0	0 0	0 4	17 28	17 4	0 0	0 0	0	0.60
0.56	0 0	0 3	12 20	12 3	0 0	0 0	0 0	0 3	18 31	18 3	0 0	0 0	0	0.56
0.52	0 0	0 2	12 21	12 2	0 0	0 0	0 0	0 3	18 35	18 3	0 0	0 0	0	0.52
0.48	0 0	0 2	12 23	12 2	0 0	0 0	0 0	0 2	18 40	18 2	0 0	0 0	0	0.48
0.44	0 0	0 1	12 25	12 1	0 0	0 0	0 0	0 1	18 46	18 1	0 0	0 0	0	0.44
0.40	0 0	0 1	11 27	11 1	0 0	0 0	0 0	0 1	17 53	17 1	0 0	0 0	0	0.40
0.36	0 0	0 0	9 29	9 0	0 0	0 0	0 0	0 0	15 61	15 0	0 0	0 0	0	0.36
0.32	0 0	0 0	7 30	7 0	0 0	0 0	0 0	0 0	12 72	12 0	0 0	0 0	0	0.32
0.28	0 0	0 0	5 29	5 0	0 0	4 4	4 0	0 0	8 84	8 0	0 0	0 0	0	0.28
0.24	0 0	0 0	3 27	3 0	0 0	9 9	9 0	0 0	4 96	4 0	0 0	0 0	0	0.24
0.20	0 0	0 0	1 21	1 0	0 0	15 15	15 0	0 0	0 102	0 0	0 0	0 0	0	0.20
0.16	0 0	0 0	0 11	0 0	0 0	23 23	23 0	0 0	0 86	0 0	0 0	0 0	0	0.16
0.12	0 0	0 0	0 2	0 0	0 0	91 91	91 0	0 0	0 31	0 0	0 0	0 0	0	0.12
0.08	0 0	0 0	0 0	0 0	0 0	85 85	85 0	0 0	0 0	0 0	0 0	0 0	0	0.08
0.04	0 0	0 0	0 0	0 0	0 0	73 73	73 0	0 0	0 0	0 0	0 0	0 0	0	0.04
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	0.08	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: PEM 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				POLLUTANT-2: GAS 2			
SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES X(KM)	Y(KM)	CONCENTRATION UNCALIBRATED	CALIBRATED	COORDINATES X(KM)	Y(KM)	CONCENTRATION UNCALIBRATED	CALIBRATED
1	1	0.68	0.20	268.5979	0.0	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:

		POLLUTANT-1: GAS 1				POLLUTANT-2: GAS 2			
SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	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

IHC002I STOP 0

TABLE 13

INPUT DATA FOR EXAMPLE PROBLEM 2

```
                                    CARD IMAGES

CONTROL CARDS
  1  TITLE          PEM EXAMPLE 2  CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS
  2  OPTIONS            3    1    1    3    0    2    0    0    1    0    0    0    1
  3  GRID                   0.        0.        25        25       2.0        0.        0.
  4  POLLUTANTS         2    1       2.0       0.0       0.5       .25      20.0       1.5
  5  SCALING               1.0       1.0        0.        0.        0.        0.
  6  LABELS         GAS                                      PARTICLE

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
                            21.        1.      2000.       25.       .25
                            25.        1.      2000.       25.       .25
                            29.        1.      2000.       25.       .25
                    BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY

POINT SOURCE CARDS
                             2.        2.       10.      .10       20.       2.0       10.      32.4 STACK 1
                            14.        2.       30.      .30       10.       2.0       15.      100. STACK 2
                             2.       16.       30.      .30       35.       1.0       12.      125. STACK 3
                    BLANK CARD TO SIGNAL END OF POINT SOURCE INVENTORY
```

TABLE 14

OUTPUT LISTING FOR EXAMPLE PROBLEM 2

PEM (VERSION 82360)

POLLUTION EPISODIC MODEL

INCLUDING

DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION

OF POLLUTANTS

```
                    POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM 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 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= 3

    STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=0

       0  ALGORITHM IS IN EFFECT
       1  ALGORITHM IS NOT USED

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

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

POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS: PEM 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:	ASCALE= 1.000	ASCALE= 1.000
CALIBRATION COEFFICIENTS:	A= 0.0 B= 0.0	A= 0.0 B= 0.0
CALIBRATION IDENTIFICATION:		
DEPOSITION VELOCITY (CM/S):	VD1= 2.000	VD2= 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

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

WIND SPEED CLASSES

CLASS INDEX	SPEED (M/S)	CLASS INTERVAL(KT)
1	1.50	0-3
2	2.46	4-6
3	4.47	7-10
4	6.93	11-16
5	9.61	17-21
6	12.52	OVER 21

STABILITY CLASSES

CLASS INDEX	CLASS
1	A
2	B
3	C
4	DD (DAY)
5	DN (NIGHT)
6	E
7	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	CN	4	6.930	11	225.00	5.00	1.000	1000.0
2	CN	4	6.930	11	225.00	5.00	1.000	1000.0
3	CN	4	6.930	11	225.00	5.00	1.000	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 X(KM)	COORDINATES Y(KM)	LENGTH OF SIDE (M)	POLLUTANT-1 EMISSION RATE INPUT (G/S)	POLLUTANT-1 EMISSION RATE SCALED	POLLUTANT-2 EMISSION RATE INPUT (G/S)	POLLUTANT-2 EMISSION RATE 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	LABEL	COORDINATES X(KM)	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	2.000	10.000	32.400
2	STACK 2	14.00	2.00	30.00	0.30	10.00	2.000	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 70.00 G/S 0.70 G/S

PEM OUTPUT: SECTION 1 OF 1, SCENARIO 3 PEM 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-1: GAS
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	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	48.00
46.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	46.00
44.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	44.00
42.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	42.00
40.00	0	0	0	0	0	0	0	0	0	0	0	0	1	2	1	0	0	0	0	0	0	0	0	0	0	40.00
38.00	0	0	0	0	0	0	0	0	0	0	0	1	2	1	0	0	0	0	0	0	0	0	0	0	1	38.00
36.00	0	0	0	0	0	0	0	0	0	0	1	2	1	0	0	0	0	0	0	0	0	0	0	1	1	36.00
34.00	0	0	0	0	0	0	0	0	0	1	3	1	0	0	0	0	0	0	0	0	0	0	1	1	1	34.00
32.00	0	0	0	0	0	0	0	0	2	3	1	0	0	0	0	0	0	0	0	0	0	1	1	1	0	32.00
30.00	0	0	0	0	0	0	0	2	4	2	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	30.00
28.00	0	0	0	0	0	0	1	5	2	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	28.00
26.00	0	0	0	0	0	1	7	1	0	0	0	0	0	1	0	0	0	0	1	2	1	0	0	0	0	26.00
24.00	0	0	0	0	1	10	1	0	0	0	0	0	1	0	0	0	0	1	2	1	0	0	0	0	0	24.00
22.00	0	0	0	0	16	1	0	0	0	0	0	1	0	0	0	0	1	2	1	0	0	0	0	0	0	22.00
20.00	0	0	0	28	0	0	0	0	0	0	1	0	0	0	0	2	3	1	0	0	0	0	0	0	0	20.00
18.00	0	0	60	0	0	0	0	0	1	1	0	0	0	0	2	4	2	0	0	0	0	0	0	0	0	18.00
16.00	0	0	0	0	0	0	0	1	1	1	0	0	0	2	5	2	0	0	0	0	0	0	0	0	0	16.00
14.00	0	0	0	0	0	0	0	2	1	0	0	0	2	6	2	0	0	0	0	0	0	0	0	0	0	14.00
12.00	0	0	0	0	0	1	3	0	0	0	0	1	8	2	0	0	0	0	0	0	0	0	0	0	0	12.00
10.00	0	0	0	0	1	5	1	0	0	0	1	12	1	0	0	4	0	4	0	4	0	0	0	0	0	10.00
8.00	0	0	0	1	8	1	0	0	0	0	17	1	0	0	5	0	5	0	5	0	0	0	0	0	0	8.00
6.00	0	0	2	15	1	0	0	0	0	30	0	0	0	7	0	7	0	7	0	0	0	0	0	0	0	6.00
4.00	0	10	43	2	0	0	0	0	55	0	0	0	14	0	14	0	14	0	0	0	0	0	0	0	0	4.00
2.00	0	10	10	0	0	0	0	0	0	0	0	65	0	65	0	65	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		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=DN, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME= 3 HR. POLLUTANT-1: GAS
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 0 0 0 0 0 0 0 0 0 0 0 0													48.00
46.00	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													46.00
44.00	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													44.00
42.00	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													42.00
40.00	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													40.00
38.00	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													38.00
36.00	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													36.00
34.00	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													34.00
32.00	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													32.00
30.00	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													30.00
28.00	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													28.00
26.00	0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0													26.00
24.00	0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0													24.00
22.00	0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0													22.00
20.00	0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0													20.00
18.00	0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0													18.00
16.00	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													16.00
14.00	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													14.00
12.00	0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0													12.00
10.00	0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0													10.00
8.00	0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0													8.00
6.00	0 0 0 1 0 0 0 0 0 2 0 0 0 1 0 1 0 1 0 0 0 0 0 0 0													6.00
4.00	0 1 3 0 0 0 0 0 4 0 0 0 1 0 1 0 1 0 0 0 0 0 0 0 0													4.00
2.00	0 1 1 0 0 0 0 0 0 0 0 5 0 5 0 5 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	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=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 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 6	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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	48.00
46.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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	46.00
44.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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	44.00
42.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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	42.00
40.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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	40.00
38.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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 1	38.00
36.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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 1 1 1	36.00
34.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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	1 1 1	34.00
32.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 1 1	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	1 1 1 0	32.00
30.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	1 1 1 0	30.00
28.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	1 1 1 0	28.00
26.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	1 1 1 0	26.00
24.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 2 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	1 1 1 0	24.00
22.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 2 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	1 2 1 0	22.00
20.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 2 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	1 2 1 0	20.00
18.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 2 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	1 2 1 0	18.00
16.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 2 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	1 2 1 0	16.00
14.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	2 1 0 0	14.00
12.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	2 0 0 0	12.00
10.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	3 0 0 0	10.00
8.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	3 0 0 0	8.00
6.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	3 0 0 0	6.00
4.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	3 0 0 0	4.00
2.00	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	3 0 0 0	2.00
0.0	0 0 0 0	0 0 0 0	0 0 0 0	0 0 0 0	0 1 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	3 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=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	0	0	0	0	1	5	10	13	10	5	2	1	0	0	0	48.00
46.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1	4	10	13	10	5	2	1	2	0	0	0	46.00
44.00	0	0	0	0	0	0	0	0	0	0	0	0	1	4	10	14	10	5	2	1	2	3	4	0	1	44.00
42.00	0	0	0	0	0	0	0	0	0	0	0	0	3	10	15	10	4	1	1	2	4	4	4	3	3	42.00
40.00	0	0	0	0	0	0	0	0	0	0	0	3	10	15	10	4	1	1	2	4	4	4	3	4	9	40.00
38.00	0	0	0	0	0	0	0	0	0	0	2	10	16	10	3	1	1	2	4	4	4	3	4	9	16	38.00
36.00	0	0	0	0	0	0	0	0	0	1	10	17	10	3	0	1	2	4	5	4	2	3	8	16	20	36.00
34.00	0	0	0	0	0	0	0	0	1	9	18	10	2	0	0	2	4	5	4	2	2	8	16	20	16	34.00
32.00	0	0	0	0	0	0	0	0	8	20	9	1	0	0	2	4	5	4	2	2	7	17	22	16	8	32.00
30.00	0	0	0	0	0	0	0	7	21	8	1	0	0	1	4	5	4	2	1	6	17	23	17	7	2	30.00
28.00	0	0	0	0	0	0	5	23	7	0	0	0	1	4	6	4	2	1	5	17	24	17	7	2	0	28.00
26.00	0	0	0	0	0	3	25	5	0	0	0	1	4	6	4	1	1	4	17	25	17	6	1	0	0	26.00
24.00	0	0	0	0	1	28	3	0	0	0	1	4	6	4	1	0	3	17	27	17	5	1	0	0	0	24.00
22.00	0	0	0	0	31	1	0	0	0	1	4	7	4	1	0	2	16	28	17	4	1	0	0	0	0	22.00
20.00	0	0	0	37	0	0	0	0	0	4	7	4	1	0	1	15	30	16	3	0	0	0	0	0	0	20.00
18.00	0	0	44	0	0	0	0	0	3	8	4	1	0	1	14	33	15	2	0	0	0	0	0	0	0	18.00
16.00	0	0	0	0	0	0	0	3	9	3	0	0	0	12	35	14	1	0	0	0	0	0	0	0	0	16.00
14.00	0	0	0	0	0	0	2	10	3	0	0	0	9	38	12	1	0	0	0	0	0	0	0	0	0	14.00
12.00	0	0	0	0	0	2	11	2	0	0	0	5	41	9	0	0	0	0	0	0	0	0	0	0	0	12.00
10.00	0	0	0	0	1	13	2	0	0	0	2	45	5	0	0	1	0	1	0	1	0	0	0	0	0	10.00
8.00	0	0	0	0	15	1	0	0	0	0	49	2	0	0	2	0	2	0	2	0	0	0	0	0	0	8.00
6.00	0	0	1	18	0	0	0	0	0	55	0	0	0	2	0	2	0	2	0	0	0	0	0	0	0	6.00
4.00	0	2	28	1	0	0	0	0	53	0	0	0	3	0	3	0	3	0	0	0	0	0	0	0	0	4.00
2.00	0	2	2	0	0	0	0	0	0	0	0	13	0	13	0	13	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		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:

		POLLUTANT-1: GAS				POLLUTANT-2: PARTICLE			
SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES X(KM)	COORDINATES Y(KM)	CONCENTRATION UNCALIBRATED	CONCENTRATION CALIBRATED	COORDINATES X(KM)	COORDINATES Y(KM)	CONCENTRATION UNCALIBRATED	CONCENTRATION CALIBRATED
1	1	30.00	2.00	65.0452	0.0	18.00	6.00	3.0750	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:

		POLLUTANT-1: GAS				POLLUTANT-2: PARTICLE			
SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES X(KM)	Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED	CALIBRATED	COORDINATES X(KM)	Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED	CALIBRATED
1	1	30.00	2.00	4683.2500	0.0	18.00	6.00	55.3507	0.0
IHC0021 STOP	0								

TABLE 15

INPUT DATA FOR EXAMPLE PROBLEM 3

```
                                        CARD IMAGES
CONTROL CARDS
  1  TITLE          PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION
  2  OPTIONS          3    0    0    6    0    2    0    0    1    1    0    1    0
  3  GRID                0.0       0.0       25        25       4.0       0.0       0.0
  4  POLLUTANTS       2    1       1.0       0.0       2.0       1.0      10.0       1.5
  5  SCALING             1.0       1.0       0.0       0.0       0.0       0.0
  6  LABELS         GAS                                  PARTICLE

SCENARIC CARDS
                     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

AREA SOURCE CARDS
                        6.0      18.0    20000.     250.0       2.5
                  BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY

POINT SOURCE CARDS
                       16.0       8.0      10.0       0.0      10.0      0.50       1.0      60.0STACK AR
                        4.0      48.0      12.5       0.0      15.0      0.75       2.0      70.0STACK AS
                       48.0      28.0      20.0       0.0      30.0      1.00       3.0      80.0STACK 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: NWSOPT=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= 4.000 KM
SOUTHWEST CORNER XRSWC= 0.0 KM W
YRSWC= 0.0 KM S

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

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                                POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM 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:              ASCALE=    1.000                    ASCALE=    1.000
    CALIBRATION COEFFICIENTS:             A=     0.0    B=      0.0          A=     0.0    B=      0.0
    CALIBRATION IDENTIFICATION:
    DEPOSITION VELOCITY (CM/S):              VD1=    1.000                     VD2=    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: PEM EXAMPLE 3 CHEMICAL TRANSFORMATION GAS TO PARTICLE 6-HR AVG CONCENTRATION

WIND DIRECTIONS

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

WIND SPEED CLASSES

CLASS INDEX	SPEED (M/S)	CLASS INTERVAL(KT)
1	1.50	0-3
2	2.46	4-6
3	4.47	7-10
4	6.93	11-16
5	9.61	17-21
6	12.52	OVER 21

STABILITY CLASSES

CLASS INDEX	CLASS
1	A
2	B
3	C
4	DD (DAY)
5	DN (NIGHT)
6	E
7	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	F		2.000		270.00	5.00	1.000	200.0
2	F		2.500		270.00	3.00	1.000	200.0
3	F		2.000		270.00	1.00	1.000	175.0
4	F		2.500		270.00	-1.00	1.000	175.0
5	F		2.000		270.00	-3.00	1.000	150.0
6	F		2.500		270.00	-5.00	1.000	150.0

POLLUTION EPISODIC MODEL

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

AREA SOURCE NUMBER	COORDINATES X(KM)	COORDINATES Y(KM)	LENGTH OF SIDE (M)	POLLUTANT-1 EMISSION RATE INPUT (G/S)	POLLUTANT-1 EMISSION RATE SCALED	POLLUTANT-2 EMISSION RATE INPUT (G/S)	POLLUTANT-2 EMISSION RATE SCALED
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 SOURCE NUMBER	LABEL	COORDINATES X(KM)	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: 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)	Y(KM)	EMISSION RATES POL-1 (G/S)	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	2.000	18.97
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	BUOYANCY	2.259	29.88
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	BUOYANCY	2.781	50.00

POLLUTION EPISODIC MODEL

OUTPUT: PEM 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)	Y(KM)	EMISSION RATES POL-1 (G/S)	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	2.823	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: PEM 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 POL-1 (G/S)	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	2.000	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	SOURCE COORDINATES X(KM)	Y(KM)	EMISSION RATES POL-1 (G/S)	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	18.55
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	BUOYANCY	2.823	29.12
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	BUOYANCY	3.476	48.91

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: HMIX= 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 POL-1 (G/S)	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	2.000	19.29
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	BUOYANCY	2.259	30.32
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	BUOYANCY	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: HMIX= 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 POL-1 (G/S)	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	18.69
2	4.00	48.00	12.50	0.0	15.00	0.750	2.000	343.15	BUOYANCY	2.823	29.31
3	48.00	28.00	20.00	0.0	30.00	1.000	3.000	353.15	BUOYANCY	3.476	49.12

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. POLLUTANT-1: GAS
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	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	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	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	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	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	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	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	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	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	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	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	0	0	0	0	0	0	0	0	0	0	0	0	52.00
48.00	0	0	145	49	24	13	8	6	4	3	2	2	1	1	1	1	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	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	0	0	0	0	0	0	0	0	0	0	0	0	40.00
36.00	0	0	60	69	72	75	76	16	7	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	36.00
32.00	0	0	60	69	72	75	76	16	7	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	32.00
28.00	0	0	60	69	72	75	76	16	7	4	1	0	0	96	54	31	20	14	10	7	5	4	3	3	2	28.00
24.00	0	0	60	69	72	75	76	16	7	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	24.00
20.00	0	0	60	69	72	75	76	16	7	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20.00
16.00	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	16.00
12.00	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	12.00
8.00	0	0	0	0	0	143	40	18	9	6	4	3	2	1	1	1	1	1	0	0	0	0	0	0	0	8.00
4.00	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	4.00
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	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. POLLUTANT-1: GAS
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	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	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	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	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	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	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	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	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	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	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	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	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	0	0	0	0	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	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	0	0	0	0	0	0	0	0	0	0	0	0	40.00
36.00	0	0	2	2	3	3	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	36.00
32.00	0	0	2	2	3	3	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	32.00
28.00	0	0	2	2	3	3	3	1	0	0	0	0	0	3	2	1	1	0	0	0	0	0	0	0	0	28.00
24.00	0	0	2	2	3	3	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	24.00
20.00	0	0	2	2	3	3	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20.00
16.00	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	16.00
12.00	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	12.00
8.00	0	0	0	0	0	5	1	1	0	0	0	0	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	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	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. POLLUTANT-2: PARTICLE
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	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	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	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	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	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	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	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	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	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	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	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	0	0	0	0	0	0	0	0	0	0	0	0	52.00
48.00	0	0	12	7	4	2	2	1	1	0	0	0	0	0	0	0	0	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	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	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	0	0	0	0	0	0	0	0	0	0	0	0	36.00
32.00	0	0	1	3	4	5	6	5	3	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	32.00
28.00	0	0	1	3	4	5	6	5	3	2	1	0	0	9	9	7	5	4	3	2	2	1	1	1	0	28.00
24.00	0	0	1	3	4	5	6	5	3	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	24.00
20.00	0	0	1	3	4	5	6	5	3	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20.00
16.00	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	16.00
12.00	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	12.00
8.00	0	0	0	0	0	10	4	2	1	1	0	0	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	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	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. POLLUTANT-2: PARTICLE
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	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	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	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	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	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	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	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	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	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	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	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	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	3	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	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	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	0	0	0	0	0	0	0	0	0	0	0	36.00
32.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0	0	0	0	0	0	0	0	0	0	0	0	32.00
28.00	0	0	86	185	271	346	415	329	229	144	68	0	0	627	631	505	387	293	221	167	126	95	62	43	31	28.00
24.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0	0	0	0	0	0	0	0	0	0	0	0	24.00
20.00	0	0	86	185	271	346	415	329	229	144	68	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20.00
16.00	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	16.00
12.00	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	12.00
8.00	0	0	0	0	0	734	318	164	91	52	31	18	11	7	4	2	1	1	0	0	0	0	0	0	0	8.00
4.00	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	4.00
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	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 MICROGRAMS PER CUBIC METER - CALIBRATION, POLLUTANT-1:
CALIBRATION, POLLUTANT-2:

		POLLUTANT-1: GAS				POLLUTANT-2: PARTICLE			
SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES X(KM)	Y(KM)	CONCENTRATION UNCALIBRATED	CALIBRATED	COORDINATES X(KM)	Y(KM)	CONCENTRATION UNCALIBRATED	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				POLLUTANT-2: PARTICLE			
SCENARIO NUMBER	WIND DIRECTION SUB-SCENARIO	COORDINATES X(KM)	Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED	CALIBRATED	COORDINATES X(KM)	Y(KM)	SURFACE DEPOSITION FLUX UNCALIBRATED	CALIBRATED
1	1	8.00	48.00	5213.8828	0.0	8.00	48.00	847.4036	0.0

IHC0021 STOP 0

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:

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

```
C                                                                       00000010
C                                                                       00000020
C                                                                       00000030
C                 *** PEM   (VERSION  82360) ***                        00000040
C                                                                       00000050
C                                                                       00000060
C                    POLLUTION EPISODIC MODEL                           00000070
C                          INCLUDING                                    00000080
C     DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION            00000090
C                        OF POLLUTANTS                                  00000100
C                                                                       00000110
C                                                                       00000120
C *** PEM PROGRAM DEVELOPMENT : --- DECEMBER 1982                       00000130
C                                                                       00000140
C     K. SHANKAR RAO AND MARTHA M. STEVENS                              00000150
C     ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL)            00000160
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION (NOAA)            00000170
C     U.S. DEPARTMENT OF COMMERCE                                       00000180
C     P.O. BOX - E                                                      00000190
C     OAK RIDGE, TENN 37830                                             00000200
C                                                                       00000210
C     PHONE: (615) 576-1238  OR  1241                                   00000220
C              FTS: 626-1238  OR  1241                                  00000230
C                                                                       00000240
C     ( THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT               00000250
C     BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE               00000260
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION )                 00000270
C                                                                       00000280
C                                                                       00000290
C *** EXTENDED ABSTRACT : PEM (VERSION 82360).                          00000300
C                                                                       00000310
C        PEM IS AN URBAN SCALE (UPTO 60 KM DISTANCES) AIR QUALITY       00000320
C     DISPERSION-DEPOSITION MODEL CAPABLE OF PREDICTING SHORT-TERM      00000330
C     (1 TO 24-HOUR) AVERAGE SURFACE CONCENTRATIONS AND DEPOSITION      00000340
C     FLUXES OF ONE OR TWO GASEOUS OR PARTICULATE POLLUTANTS AT         00000350
C     UP TO A MAXIMUM OF 50X50 GROUND-LEVEL RECEPTORS.  PREDICTIONS ARE 00000360
C     BASED ON STEADY-STATE GAUSSIAN PLUME HYPOTHESIS, BRIGGS' PLUME    00000370
C     RISE FORMULATIONS, AND PASQUILL-GIFFORD (PG) STABILITY CLASS-     00000380
C     IFICATION AND DISPERSION PARAMETER CURVES.  UP TO 300 INDIVIDUAL  00000390
C     POINT SOURCES AND UP TO 50 AREA SOURCES MAY BE INCLUDED IN THE    00000400
C     INPUTS TO THE MODEL.  CALCULATIONS ARE PERFORMED FOR EACH HOUR    00000410
C     USING THE SPECIFIED HOURLY METEOROLOGICAL DATA. UP TO 24 DIFFERENT00000420
C     SETS OF HOURLY METEOROLOGICAL DATA MAY BE SPECIFIED AS INPUT FOR  00000430
C     THE DETERMINATION OF AIR QUALITY FOR 24 DISTINCT WEATHER          00000440
C     SCENARIOS.  POLLUTANT CONCENTRATIONS AND DEPOSITION FLUXES FOR A  00000450
C     2 TO 24 AVERAGING PERIOD ARE CALCULATED BY AVERAGING THE CORRES-  00000460
C     PONDING VALUES CALCULATED FOR EACH HOUR IN THE PERIOD.            00000470
C                                                                       00000480
C        PEM IS BASED ON THE TEXAS EPISODIC MODEL (TEM, VERSION 8)      00000490
C     DEVELOPED BY THE TEXAS AIR CONTROL BOARD (1979).  TEM USES THE    00000500
C     GAUSSIAN PLUME CONCENTRATION ALGORITHMS DEVELOPED FOR NON-REACTIVE00000510
C     POLLUTANTS AND A PERFECTLY REFLECTING LOWER BOUNDARY.  CHEMICAL   00000520
C     AND PHYSICAL DEPLETION PROCESSES ARE THEREFORE IGNORED, EXCEPT FOR00000530
C     AN OPTION WHICH ALLOWS A SIMPLE EXPONENTIAL DECAY OF POLLUTANT    00000540
C     WITH TRAVEL TIME.  THIS METHOD REQUIRES AN ACCURATE ESTIMATE OF   00000550
C     THE POLLUTANT'S HALF-LIFE.                                        00000560
C                                                                       00000570
C        IN CONTRAST, PEM EXPLICITLY ACCOUNTS FOR THE DRY DEPOSITION,   00000580
C     GRAVITATIONAL SETTLING, AND A FIRST-ORDER CHEMICAL TRANSFORMATION 00000590
C     OR DECAY OF GASEOUS OR PARTICULATE POLLUTANTS (OF ANY SIZE) IN    00000600
C     THE CONCENTRATION ALGORITHMS.  THESE ALGORITHMS, BASED ON EXACT   00000610
C     SOLUTIONS OF A GRADIENT-TRANSFER ('K-THEORY') MODEL, WERE GIVEN BY00000620
C     RAO (1981, 1982) AS ANALYTICAL EXTENSIONS OF THE WIDELY-USED      00000630
C     GAUSSIAN PLUME DISPERSION ALGORITHMS UNDER VARIOUS ATMOSPHERIC    00000640
C     STABILITY AND MIXING CONDITIONS.  THUS, PEM TREATS DEPOSITION,    00000650
C     SEDIMENTATION, AND CHEMICAL TRANSFORMATION IN A PHYSICALLY REAL-  00000660
C     ISTIC AND STRAIGHTFORWARD MANNER, AND IT IS SUBJECT TO THE SAME   00000670
C     BASIC ASSUMPTIONS AND LIMITATIONS ASSOCIATED WITH ALL GAUSSIAN-   00000680
C     PLUME TYPE MODELS.  FOR FURTHER DETAILS REGARDING THE GRADIENT-   00000690
C     TRANSFER MODEL FORMULATIONS, ANALYTICAL SOLUTIONS, PARAMETERI-    00000700
C     ZATIONS, AND THE DEVELOPMENT OF THE ALGORITHMS FOR PEM, THE USER  00000710
C     SHOULD CONSULT THE REPORTS BY RAO (1981, 1982).                   00000720
C                                                                       00000730
C        BASED ON THE NUMBER OF POLLUTANTS (NPOL=1 OR 2) AND THE CHEMI- 00000740
C     CAL TRANSFORMATION/DECAY OPTION PARAMETER (ICT=0 OR 1) SPECIFIED  00000750
C     IN THE INPUT TO THE MODEL, PEM PROGRAM DOES ONE OF THE FOLLOWING: 00000760
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C                                                                       00000770
C     (1) IF NPOL=1 AND ICT=0 OR 1, SURFACE CONCENTRATIONS AND DEPOSI-  00000780
C         TION FLUXES OF ONE GASEOUS OR PARTICULATE POLLUTANT, WITH THE 00000790
C         GIVEN DEPOSITION AND SETTLING VELOCITIES, VD1 AND W1 RESPECTI- 00000800
C         VELY, ARE CALCULATED.  IF ICT=1, THEN CHEMICAL DECAY OF POLLU- 00000810
C         TANT IS ALSO CONSIDERED IF THE DECAY RATE XKT > 0. IS GIVEN   00000820
C         IN PERCENT PER HOUR.                                          00000830
C                                                                       00000840
C     (2) IF NPOL=2 AND ICT=0, SURFACE CONCENTRATIONS AND DEPOSITION    00000850
C         FLUXES OF TWO DIFFERENT AND UNCOUPLED GASEOUS OR PARTICULATE  00000860
C         POLLUTANT SPECIES WITH THE GIVEN DEPOSITION AND SETTLING VELOC-00000870
C         ITIES VD1 AND W1 (FOR SPECIES-1) AND VD2 AND W2 (FOR SPECIES-2)00000880
C         RESPECTIVELY, ARE CALCULATED.  EMISSION RATES FOR BOTH SPECIES 00000890
C         MAY BE DIFFERENT.  CHEMICAL DECAY IS NOT CONSIDERED FOR EITHER 00000900
C         SPECIES EVEN IF A VALUE OF XKT > 0. IS SPECIFIED.             00000910
C                                                                       00000920
C     (3) IF NPOL=2 AND ICT=1, THE TWO GASEOUS OR PARTICULATE POLLUTANT 00000930
C         SPECIES ARE COUPLED THROUGH A FIRST-ORDER CHEMICAL TRANSFORMA- 00000940
C         TION.  THE SURFACE CONCENTRATIONS AND DEPOSITION FLUXES OF BOTH00000950
C         THE PRIMARY POLLUTANT (SPECIES-1 OR REACTANT) AS WELL AS THE  00000960
C         SECONDARY POLLUTANT (SPECIES-2 OR REACTION PRODUCT) ARE CALCU- 00000970
C         LATED.  THE CHEMICAL TRANSFORMATION RATE (XKT > 0.) SHOULD BE 00000980
C         GIVEN.  BOTH SPECIES MAY BE GIVEN NON-EQUAL DEPOSITION AND SET-00000990
C         TLING VELOCITIES.  A NON-ZERO DIRECT EMISSION RATE FOR THE    00001000
C         SECONDARY POLLUTANT FROM  THE POINT AND/OR AREA SOURCES MAY   00001010
C         ALSO BE SPECIFIED AS INPUT FOR THIS CASE.                     00001020
C                                                                       00001030
C         FOR FURTHER DETAILS REGARDING THE USE OF THE PEM AND ITS I/O  00001040
C     OPTIONS, INPUT PARAMETERS AND UNITS, AND EXAMPLE PROBLEMS, THE    00001050
C     USER SHOULD CONSULT THE PEM USER'S GUIDE BY RAO AND STEVENS (1982)00001060
C                                                                       00001070
C                              *** REFERENCES ***                       00001080
C                                                                       00001090
C     (1) STAFF OF THE TEXAS AIR CONTROL BOARD, 1979: USER'S GUIDE :    00001100
C         TEXAS EPISODIC MODEL.  TEXAS AIR CONTROL BOARD, PERMITS       00001110
C         SECTION, AUSTIN, TEXAS 78723, 215 PP.                         00001120
C                                                                       00001130
C     (2) RAO, K. S., 1981: ANALYTICAL SOLUTIONS OF A GRADIENT-TRANSFER 00001140
C         MODEL FOR PLUME DEPOSITION AND SEDIMENTATION.  EPA-          ,00001150
C         U.S.E.P.A., RESEARCH TRIANGLE PARK, NC;                       00001160
C         NOAA TECH. MEMO. ERL/ARL-109, NOAA-ATDL, OAK RIDGE, TN 37830, 00001170
C         75 PP.  ATDL CONTRIBUTION FILE NO. 81/14.                     00001180
C                                                                       00001190
C     (3) RAO, K. S., 1982: GAUSSIAN PLUME CONCENTRATION ALGORITHMS WITH00001200
C         DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION.       00001210
C         EPA-          , RESEARCH TRIANGLE PARK, NC;                   00001220
C         NOAA TECH. MEMO. ERL/ARL-    , NOAA-ATDL, OAK RIDGE, TN 37830. 00001230
C         ATDL CONTRIBUTION FILE NO. 82/27.                             00001240
C                                                                       00001250
C     (4) RAO, K. S., AND M. M. STEVENS, 1982:  POLLUTION EPISODIC      00001260
C         MODEL:  USER'S GUIDE.  EPA-                , RESEARCH         00001270
C         TRIANGLE PARK, NC.                                            00001280
C         NOAA TECH. MEMO. ERL/ARL-    , NOAA-ATDL, OAK RIDGE, TN 37830. 00001290
C         ATDL CONTRIBUTION FILE NO. 82/28.                             00001300
C                                                                       00001310
C                                                                       00001320
C                                                                       00001330
C *** PEM (VERSION 82360) : FORTRAN LISTING.                            00001340
C                                                                       00001350
C                                                                       00001360
C                                                                       00001370
C                                                                       00001380
C                                                                       00001390
C *** COMMON BLOCKS, DIMENSIONS, AND DATA STATEMENTS.                   00001400
C                                                                       00001410
C                                                                       00001420
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00001430
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00001440
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00001450
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00001460
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00001470
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),     00001480
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,              00001490
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00001500
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                00001510
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,        00001520
     * NSTDWN,INTER,NPRINT                                              00001530
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```
C
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC
      COMMON/PARM1A/GAMMA
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT
      COMMON/PARM2A/AA,BA
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2
      COMMON/PARM4/V11,V21,V12,V22,V13
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42
      COMMON/PARM7/QZC1,QZC2
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C
      COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
      EXTERNAL FUN3
      REAL*8 FUN3
      REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR,T1A,T2A
      DIMENSION IW(102)
      DIMENSION PRL(2,2),DWL(4),ANGLIM(7)
      DIMENSION ITABLE(5,10),EPSLIM(10)
      DIMENSION AAR(6),BAR(6),CX1(7),DX1(7),CX2(7),DX2(7)
      DIMENSION XA1(5),XA2(5),XA2C(5),RCA1(5),RCA2(5)
      DIMENSION RCA2CT(5,50),QA2QA1(50),TERMB2(5)
C
      DATA PRL/4HMOME,4HNTUM,4HBUOY,4HANCY/
      DATA DWL/4H    ,4H    ,4HDOWN,4HWASH/
      DATA EPSLIM/.12427,.16511,.24504,.35884,.46373,
     1            .55868,.64350,.69482,.71890,.78540/
      DATA ITABLE/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,
     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/
      DATA ANGLIM/0.610865,0.488692,0.366519,0.244346,
     1 0.244346,0.183260,0.122173/
      DATA CX1/.495,.310,.197,.122,.122,.0934,.0625/
      DATA DX1/.873,.897,.908,.916,.916,.912,.911/
      DATA CX2/.606,.523,.285,.193,.193,.141,.080/
      DATA DX2/.851,.840,.867,.865,.865,.868,.884/
      DATA AAR/.4,.4,.33,.22,.15,.06/
      DATA BAR/.91,.91,.86,.80,.75,.71/
C
C
C
C *** DEFINE PROGRAM CONSTANTS.
C
      PI=3.14159
      SQPI=SQRT(PI)
      SQRT2=SQRT(2.)
      A1B=1000./(SQRT2*SQPI)
      A1C=2.*SQPI
      AI=0.
      BI=1.
      EPSABS=1.0E-4
      EPSREL=1.0E-4
      LW=800
      NIW=102
C     EXPMAX=174.
      EXPMAX= 87.
      EXPMIN=50.
      ETAMAX=SQRT(EXPMAX)
C
      WRITE (IWR,5432)
 5432 FORMAT ('1',///////46X,'PEM   (VERSION  82360)'/////
     1 45X,'POLLUTION EPISODIC MODEL'/////
     2 52X,'INCLUDING'//
     3 30X,'DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION'//
     4 50X,'OF POLLUTANTS'/)
C
      INDEX=0
C
C  CALL INPUT MODULE TO READ ALL WEATHER AND SOURCE INFORMATION,
C     DEPOSITION AND SEDIMENTATION VELOCITIES OF POLLUTANT SPECIES,
C     AND CHEMICAL DECAY OR TRANFORMATION RATE.
C
C     ************
      CALL INMOD
C     ************
C
      VD136=VD1*36.
```

```
      VD236=VD2*36.
C
C
C *** DETERMINE VALUE OF PARAMETER ISPEC.
C     ISPEC IS AN INTERNAL ROUTING PARAMETER USED IN PEM
C     TO DETERMINE THE APPROPRIATE CONCENTRATION ALGORITHMS
C     TO BE USED FOR A GIVEN PROBLEM.
C     VALUE OF ISPEC  IS BASED ON NUMBER OF POLLUTANTS,
C     AND CHEMICAL TRANSFORMATION OPTION PARAMETER.
C
      IF(NPOL.EQ.2) GO TO 41
C     ONLY ONE POLLUTANT SPECIES.  CHEMICAL DECAY CAN BE CONSIDERED
C     BY SETTING ICT = 1 AND XKT > 0.
      ISPEC=1
      GO TO 43
C
C     TWO POLLUTANT SPECIES.
   41 IF(ICT.EQ.1) GO TO 42
C     NO CHEMICAL COUPLING. THE TWO SPECIES ARE INDEPENDENT
C     OF EACH OTHER.  CHEMICAL DECAY IS NOT CONSIDERED FOR
C     EITHER SPECIES.
      ISPEC=2
      GO TO 43
C
C     CHEMICAL COUPLING EXISTS BETWEEN SPECIES-1 (REACTANT)
C     AND SPECIES-2 (PRODUCT).
   42 ISPEC=3
   43 CONTINUE
C
C
C
C *** DEFINE TIME-AVERAGING MULTIPLIER CONSTANTS.
C
      IF(NTOPT.EQ.1) STCONV = 1.
      IF(NTOPT.EQ.2) STCONV= 0.04166667
      IF(NTOPT.EQ.3) STCONV= 1.0/FLOAT(NSCEN)
C
      INDEX=1
C
C  CALL INPUT MODULE TO BRING IN WEATHER DATA FOR ONE SCENARIO
C    (NUMBER OF SCENARIO = ISCEN).
C
C     ************
  100 CALL INMOD
C     ************
C
C  CALCULATE WIND VECTOR (WVEC) FOR SCENARIO. IFLAG IS USED BELOW
C    (STMT. 275) TO DETERMINE METHOD OF RESTRICTING THE AREA OF THE
C    RECEPTOR GRID AFFECTED BY EACH SOURCE.
C
  175 IF(NWDOPT.EQ.1) GO TO 200
      DO 180 IWD=1,16
      DETA=ABS(WD(ISCEN)-SECTAN(IWD))
      IF(DETA.LE.0.19634954) GO TO 185
  180 CONTINUE
  185 GO TO 205
  200 WD(ISCEN)=SECTAN(IWD)
  205 IF(IWD.LT.8.OR.IWD.GT.10) GO TO 210
      IFLAG=1
      GO TO 241
  210 IF(IWD.NE.11) GO TO 215
      IFLAG=2
      GO TO 241
  215 IF(IWD.LT.12.OR.IWD.GT.14) GO TO 220
      IFLAG=3
      GO TO 241
  220 IF(IWD.NE.15) GO TO 225
      IFLAG=4
      GO TO 241
  225 IF(IWD.LT.16.AND.IWD.GT.2) GO TO 230
      IFLAG=5
      GO TO 241
  230 IF(IWD.NE.3) GO TO 235
      IFLAG=6
      GO TO 241
  235 IF(IWD.LT.4.OR.IWD.GT.6) GO TO 240
      IFLAG=7
```

```
      GO TO 241
240   IFLAG=8
241   WVEC= WD(ISCEN) + 3.14159265
      IF(WVEC.GT.6.2831853) WVEC=WVEC - 6.2831853
      WDV=4.712388981-WD(ISCEN)
      IF(WDV.LT.0.)WDV=WDV+6.283185307
      WDPANG=WDV+ANGLIM(ISC)
      WDMANG=WDV-ANGLIM(ISC)
C
C  CALL AUTGRD TO CALCULATE RECEPTOR GRID PARAMETERS AUTOMATICALLY.
C     ************
      IF(IGRID.EQ.1) CALL AUTGRD
C     ************
C
C *** INITIALIZATION.
C
C  INITIALIZE CONCENTRATION AND SURFACE DEPOSITION FLUX ARRAYS
      IF(NTOPT.GT.1.AND.ISCEN.GT.1) GO TO 4
      DO 2 I=1,LX
      DO 2 J=1,LY
      CONC(I,J,1)=0.
      SDF(I,J,1)=0.
      IF(ISPEC.EQ.1.AND.NCSOPT.EQ.0) GO TO 2
      CONC(I,J,2)=0.
      SDF(I,J,2)=0.
    2 CONTINUE
C
C
C
    4 VGRID= 1./GRID
      GRIDSQ= GRID*GRID
      ELX= LX
      ELY= LY
      XB1= XSWC + 0.5*GRID
      XB2= XSWC + (ELX-0.5)*GRID
      YB1= YSWC + 0.5*GRID
      YB2= YSWC + (ELY-0.5)*GRID
C
C  IF NO AREA SOURCES, SKIP AREA SOURCE CALCULATIONS.
      IF(NAS.LT.1) GO TO 245
C
C
C
C***  A R E A   S O U R C E   C A L C U L A T I O N S  ***
C
C     IWV HELPS DETERMINE THE PATTERN OF GRID SQUARES AFFECTED BY EACH
C     AREA SOURCE.  PATTERN DEPENDS ONLY ON WIND DIRECTION.
C     EPS IS THE ANGLE BETWEEN THE WIND VECTOR AND THE NEAREST
C     COORDINATE AXIS.
C
      IWV= 1 + WVEC/0.78540
      GO TO (2411,2412,2413,2414,2415,2416,2417,2418),IWV
2411  ITABX=1
      ISIGNX=1
      ISIGNY=1
      EPS= WVEC
      GO TO 2419
2412  ITABX=0
      ISIGNX=1
      ISIGNY=1
      EPS= 1.5708 - WVEC
      GO TO 2419
2413  ITABX=0
      ISIGNX=1
      ISIGNY=-1
      EPS= WVEC - 1.57080
      GO TO 2419
2414  ITABX=1
      ISIGNX=1
      ISIGNY=-1
      EPS= 3.1416 - WVEC
      GO TO 2419
2415  ITABX=1
      ISIGNX=-1
      ISIGNY=-1
      EPS= WVEC - 3.1416
      GO TO 2419
```

```
 2416  ITABX=0
       ISIGNX=-1
       ISIGNY=-1
       EPS= 4.7124 - WVEC
       GO TO 2419
 2417  ITABX=0
       ISIGNX=-1
       ISIGNY=1
       EPS= WVEC - 4.7124
       GO TO 2419
 2418  ITABX=1
       ISIGNX=-1
       ISIGNY=1
       EPS= 6.2832 - WVEC
 2419  IF(ITABX.EQ.0) GO TO 2420
       ITABY=0
       INCRX=0
       INCRY=1
       GO TO 2421
 2420  ITABY=1
       INCRX=1
       INCRY=0
 2421  DO 2422 L=1,10
       IF(EPS.GT.EPSLIM(L)) GO TO 2422
       IEPS=L
       GO TO 2423
 2422  CONTINUE
       IEPS=10
C
C      REDUCE STABILITY CLASS BY 1 (EXCEPT FOR ISC=1) TO SIMULATE
C      SURFACE TURBULENCE IN URBAN CONDITIONS.
C
 2423  IA= ISC-1
       IF(IA.EQ.0) IA=1
       AA= AAR(IA)
       BA= BAR(IA)
       BA1=2.*(1.-BA)
       DXA=1000.*GRID/COS(EPS)
       UPL=WS(ISCEN)
       UINV=1./UPL
       UINV1=UINV/100.
C
C      DEFINE NONDIMENSIONAL DEPOSITION AND SEDIMENTATION PARAMETERS.
C
C      ISPEC = 1 OR 2 OR 3
       BAVD1=0.01*VD1*BA1
       VDC1=VD1*UINV1
       WC1=W1*UINV1
       V11=VDC1-0.5*WC1
       V21=VDC1-WC1
       IF(V21.EQ.0.) GO TO 44
       R11=V11/V21
       R21=0.5*WC1/V21
    44 IF(ISPEC.EQ.1) GO TO 46
C
C      ISPEC = 2 OR 3
       BAVD2=0.01*VD2*BA1
       VDC2=VD2*UINV1
       WC2=W2*UINV1
       V12=VDC2-0.5*WC2
       V22=VDC2-WC2
       IF(V22.EQ.0.) GO TO 45
       R12=V12/V22
       R22=0.5*WC2/V22
    45 IF(ISPEC.EQ.2) GO TO 47
C
C      ISPEC = 3
       V13=V11-0.5*(WC1-WC2)
       IF(V21.EQ.0.) GO TO 46
       R13=V13/V21
       R23=0.5*WC2/V21
C
C      ISPEC = 1 OR 3
    46 UTAUC=TAUC*UPL
    47 CONTINUE
C
C
```

```
C     CALCULATE RELATIVE CONCENTRATIONS AT A RECEPTOR LOCATED AT THE
C     CENTER OF THE CALCULATION GRID SQUARE CONTAINING THE AREA SOURCE
C     EMISSIONS, AND AT THE CENTER OF EACH OF THE FOUR GRID SQUARES
C     IMMEDIATELY DOWNWIND OF THE SOURCE.
C
C     FIRST DEFINE DOWNWIND DISTANCES TO THE LEADING AND TRAILING EDGES,
C     AND MID-POINTS OF THE FIVE CALCULATION GRID SQUARES.
      XA1(1)=0.0
      XA2(1)=0.5*DXA
C
      DO 102 I=1,5
      SZ2=AA*(XA2(I)**BA)
      IF(SZ2.GT.5000.) SZ2=5000.
      XA2C(I)=XA2(I)/(SQRT2*SZ2)
C
      IF(I.EQ.5) GO TO 102
      XA1(I+1)=XA2(I)
      XA2(I+1)=XA1(I+1)+DXA
  102 CONTINUE
C
      K=1
      IF(ISPEC.NE.3) GO TO 104
C
C     START LOOP ON ALL AREA SOURCES IF ISPEC = 3
      DO 114 K=1,NAS
      IF(EA(K,1).EQ.0.) EA(K,1)=1.E-6
      QA2QA1(K)=EA(K,2)/EA(K,1)
      IF(K.EQ.1) GO TO 103
      IF(QA2QA1(K).EQ.QA2QA1(K-1)) GO TO 112
  103 Q2Q1=QA2QA1(K)
      G42PX1=Q2Q1
C
  104 G41PX1=1.
      IF(ISPEC.EQ.2) G42PX1=1.
C
C     START LOOP ON FIVE CALCULATION GRID SQUARES WITH RECEPTORS.
      DO 111 I=1,5
      X1A=XA1(I)
      X2A=XA2(I)
      X2CA=XA2C(I)
C
C     ISPEC = 1 OR 2 OR 3
      D31=2.*V11*X2CA
      D11=WC1*X2CA
      D21=D11*D11
      R31=1.+2.*D21
      R41=2.*D11/SQPI
      IF(ISPEC.EQ.1) GO TO 107
C
C     ISPEC = 2 OR 3
      D32=2.*V12*X2CA
      D12=WC2*X2CA
      D22=D12*D12
      R32=1.+2.*D22
      R42=2.*D12/SQPI
      IF(ISPEC.EQ.2) GO TO 107
C
C     ISPEC = 3
      D33=2.*V13*X2CA
      D6=4.*SQPI*(V21-V22)*X2CA
C
  107 IF(ICT.EQ.0) XCT=0.
      IF(ICT.EQ.1) XCT=X2A/UTAUC
      EXCT=EXP(-XCT)
      IF(ISPEC.EQ.3) GO TO 108
C
C     ISPEC = 1 OR 2
C     ************
      CALL PSG4P(G41PX2,G42PX2)
C     ************
      IF(ICT.EQ.1) GO TO 108
C     ISPEC = 1 WITH ICT = 0 OR ISPEC = 2
      RCA1(I)=(G41PX1-G41PX2)/BAVD1
      IF(RCA1(I).LT.0.) RCA1(I)=0.0
      G41PX1=G41PX2
      IF(ISPEC.EQ.1) GO TO 111
C     ISPEC = 2
```

```
      RCA2(I)=(G42PX1-G42PX2)/BAVD2
      IF(RCA2(I).LT.0.) RCA2(I)=0.0
      G42PX1=G42PX2
      GO TO 111
C
C     ISPEC = 1 WITH ICT = 1 OR ISPEC = 3
  108 IF(K.GT.1) GO TO 109
      T1A=X1A/UTAUC
      T2A=X2A/UTAUC
C     COMPUTE INTEGRAL FUNC=F3(T1A,T2A); FUN3 IS THE INTEGRAND FUNCTION.
C     ************
      CALL D01AJF(FUN3,T1A,T2A,EPSABS,EPSREL,RESULT,
     1  ABSERR,WORK,LW,IW,NIW,IFAIL)
C     ************
      FUNC=RESULT
      TERMB1=FUNC
      IF(ISPEC.EQ.1) GO TO 106
      TERMB2(I)=GAMMA*FUNC*VDC1/VDC2
      IF(ISPEC.EQ.3) GO TO 109
C
C     ISPEC = 1 WITH ICT = 1
  106 RCA1(I)=((G41PX1-G41PX2)/VDC1-TERMB1)/BA1
      IF(RCA1(I).LT.0.) RCA1(I)=0.0
      RCA1(I)=RCA1(I)*UINV
      G41PX1=G41PX2
      GO TO 111
C
C     ISPEC = 3
C     ************
  109 CALL PSG4P(G41PX2,G42PX2)
C     ************
      IF(K.GT.1) GO TO 110
      TERMA1=(G41PX1-G41PX2)/VDC1
      DUM1=(TERMA1-TERMB1)/BA1
      IF(DUM1.LT.0.) DUM1=0.0
      RCA1(I)=DUM1*UINV
      G41PX1=G41PX2
  110 TERMA2=(G42PX1-G42PX2)/VDC2
      DUM2=(TERMA2+TERMB2(I))/BA1
      IF(DUM2.LT.0.) DUM2=0.0
      RCA2CT(I,K)=DUM2*UINV
      G42PX1=G42PX2
C
  111 CONTINUE
C     END LOOP ON I=1,5 CALCULATION GRID SQUARES.
      GO TO 114
C
  112 DO 113 I=1,5
      RCA2CT(I,K)=RCA2CT(I,K-1)
  113 CONTINUE
C
  114 CONTINUE
C     END LOOP ON K=1,NAS AREA SOURCES IF ISPEC = 3
C
C
C  LOOP THROUGH ALL AREA SOURCES.  EMISSIONS FROM EACH AREA SOURCE
C    ARE APPORTIONED AMONG THE RECEPTOR GRID SQUARES WHOLLY OR
C    PARTIALLY COVERED BY THE SOURCE.  EACH AFFECTED RECEPTOR GRID
C    SQUARE IS TREATED AS A SOURCE.
C
C     START LOOP ON K=1,NAS AREA SOURCES.
      DO 2429 K=1,NAS
      AREA= SIZE(K)*SIZE(K)
      AX1= XA(K)
      AX2= AX1 + SIZE(K)
      NX1= (AX1-XSWC)*VGRID + 5.
      NX2= (AX2-XSWC)*VGRID + 5.
      IF(NX1.GT.LX+8.OR.NX2.LT.1) GO TO 2429
      IF(NX1.GE.1) GO TO 32
      NX1= 1
      AX1= XSWC - 4.*GRID
   32 IF(NX2.LE.LX+8) GO TO 34
      NX2= LX+8
      AX2= XSWC + (ELX + 4.)*GRID
   34 X1= XSWC + (FLOAT(NX1)-5.)*GRID
      X2= XSWC + (FLOAT(NX2)-4.)*GRID
      AY1= YA(K)
```

```
      AY2= AY1 + SIZE(K)
      NY1= (AY1-YSWC)*VGRID + 5.
      NY2= (AY2-YSWC)*VGRID + 5.
      IF(NY1.GT.LY+8.OR.NY2.LT.1) GO TO 2429
      IF(NY1.GE.1) GO TO 36
      NY1= 1
      AY1= YSWC - 4.*GRID
   36 IF(NY2.LE.LY+8) GO TO 38
      NY2= LY+8
      AY2= YSWC + (ELY + 4.)*GRID
   38 Y1= YSWC + (FLOAT(NY1)-5.)*GRID
      Y2= YSWC + (FLOAT(NY2)-4.)*GRID
C
C     START LOOP ON IX=NX1,NX2 COLUMNS OF THE RECEPTOR GRID.
      DO 2428 IX=NX1,NX2
      IF(NX1.NE.NX2) GO TO 10
      DXQ= AX2-AX1
      GO TO 13
   10 IF(IX.NE.NX1) GO TO 11
      DXQ= GRID+X1-AX1
      GO TO 13
   11 IF(IX.NE.NX2) GO TO 12
      DXQ= GRID+AX2-X2
      GO TO 13
   12 DXQ=GRID
C
C     START LOOP ON JY=NY1,NY2 ROWS OF THE RECEPTOR GRID.
   13 DO 2427 JY=NY1,NY2
      IF(NY1.NE.NY2) GO TO 20
      DY= AY2-AY1
      GO TO 23
   20 IF(JY.NE.NY1) GO TO 21
      DY= GRID+Y1-AY1
      GO TO 23
   21 IF(JY.NE.NY2) GO TO 22
      DY= GRID+AY2-Y2
      GO TO 23
   22 DY=GRID
   23 SPLIT= DXQ*DY/(AREA*GRIDSQ)
C
C  LOOP FOR THE FIVE RECEPTORS AFFECTED BY EACH RECEPTOR GRID SQUARE
C    CONTAINING EMISSIONS.  THE RECEPTORS IN THE FOUR DOWNWIND SQUARES
C    AND IN THE SOURCE SQUARE ITSELF ARE AFFECTED.
C
      DO 2426 L=1,5
      NX= IX + ISIGNX*(ITABLE(L,IEPS)*ITABX + (L-1)*INCRX) - 4
      IF(NX.LT.1.OR.NX.GT.LX) GO TO 2426
      NY= JY + ISIGNY*(ITABLE(L,IEPS)*ITABY + (L-1)*INCRY) - 4
      IF(NY.LT.1.OR.NY.GT.LY) GO TO 2426
C
C     CALCULATE GROUND-LEVEL CONCENTRATIONS CONC (MICROGRAMS PER CUBIC
C     METER) AND SURFACE DEPOSITION FLUXES (MICROGRAMS PER SQUARE
C     METER PER HOUR) OF POLLUTANTS AT RECEPTOR IN COLUMN NX, ROW NY
C     OF THE RECEPTOR GRID DUE TO AREA SOURCE K.
C
C     ISPEC = 1 OR 2 OR 3
      CINC1=RCA1(L)*EA(K,1)*SPLIT*STCONV
      CONC(NX,NY,1)=CONC(NX,NY,1)+CINC1
      SDF(NX,NY,1)=SDF(NX,NY,1)+VD136*CINC1
      IF(ISPEC.EQ.1) GO TO 2426
      IF(ISPEC.EQ.3) GO TO 2425
C
C     ISPEC = 2
      CINC2=RCA2(L)*EA(K,2)*SPLIT*STCONV
      CONC(NX,NY,2)=CONC(NX,NY,2)+CINC2
      SDF(NX,NY,2)=SDF(NX,NY,2)+VD236*CINC2
      GO TO 2426
C
C     ISPEC = 3
 2425 CINC2=RCA2CT(L,K)*EA(K,1)*SPLIT*STCONV
      CONC(NX,NY,2)=CONC(NX,NY,2)+CINC2
      SDF(NX,NY,2)=SDF(NX,NY,2)+VD236*CINC2
C
 2426 CONTINUE
C     END LOOP ON L=1,5 CALCULATION GRID SQUARES WITH RECEPTORS.
C
 2427 CONTINUE
```

```
693    C      END LOOP ON JY=NY1,NY2 ROWS OF THE RECEPTOR GRID.                00006920
694    C                                                                       00006930
695    2428   CONTINUE                                                        00006940
696    C      END LOOP ON IX=NX1,NX2 COLUMNS OF THE RECEPTOR GRID.            00006950
697    C                                                                       00006960
698    2429   CONTINUE                                                        00006970
699    C      END LOOP ON K=1,NAS AREA SOURCES.                               00006980
700    C                                                                       00006990
701    C                                                                       00007000
702    C                                                                       00007010
703    C *** POINT SOURCES.                                                   00007020
704    C                                                                       00007030
705    C  HPEN= MINIMUM EFFECTIVE SOURCE HEIGHT NECESSARY FOR PLUME TO        00007040
706    C     PENETRATE INVERSION.                                             00007050
707    245    HPEN= PEN(ISCEN)*HMIX(ISCEN)                                    00007060
708    C                                                                       00007070
709    C                                                                       00007080
710    C  IF NO POINT SOURCES, SKIP POINT SOURCE CALCULATIONS.                00007090
711           IF(NPS.LT.1) GO TO 603                                           00007100
712    C                                                                       00007110
713    C                                                                       00007120
714    C                                                                       00007130
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  ***            00007140
716    C                                                                       00007150
717    C  LOOP THROUGH ALL POINT SOURCES.                                     00007160
718           DO 600 I=1,NPS                                                   00007170
719           IF((NWDOPT.GT.1.AND.IWDOPT.GT.1).OR.NTOPT.EQ.2) GO TO 246        00007180
720           IF(NPRINT.EQ.0) GO TO 246                                        00007190
721           IF((I-1)/50*50.NE.I-1) GO TO 246                                 00007200
722           WRITE(IWR,1005) TT,ISCEN,HMIX(ISCEN),HPEN                        00007210
723           WRITE(IWR,1007)                                                  00007220
724    246    IPS=I                                                            00007230
725           IF(HP(I).GE.HMIX(ISCEN)) GO TO 600                               00007240
726           IRISE=2                                                          00007250
727           IBUOY=1                                                          00007260
728           EFF= 2.45*VP(I)*DP(I)*DP(I)*(TP(I)-TA(ISCEN))/TP(I)              00007270
729           IF(EFF.LT.0.) EFF=1.0E-7                                         00007280
730    C                                                                       00007290
731    C  CALCULATE INVERSE WIND SPEED (UINV) AT THE PHYSICAL HEIGHT (HP(I))  00007300
732    C     OF POINT SOURCE I.  DO NOT CHANGE IF STACK HEIGHT IS LESS        00007310
733    C     THAN 10 METERS.                                                  00007320
734    C                                                                       00007330
735           UINV = 1./WS(ISCEN)                                              00007340
736           IF(HP(I).GT.10.) UINV = UINV*((10./HP(I))**P(ISC))               00007350
737           UPL=1./UINV                                                      00007360
738           UINV1=UINV/100.                                                  00007370
739    C      DEFINE EMISSION RATES (SOURCE STRENGTHS) OF POLLUTANT SPECIES,  00007380
740    C       AND NONDIMENSIONAL DEPOSITION AND SEDIMENTATION PARAMETERS.    00007390
741    C                                                                       00007400
742    C      ISPEC = 1 OR 2 OR 3                                              00007410
743           Q1=EP(I,1)                                                       00007420
744           VDC1=VD1*UINV1                                                   00007430
745           WC1=W1*UINV1                                                     00007440
746           V11=VDC1-0.5*WC1                                                 00007450
747           V21=VDC1-WC1                                                     00007460
748           IF(V21.EQ.0.) GO TO 48                                           00007470
749           R11=V11/V21                                                      00007480
750           R21=0.5*WC1/V21                                                  00007490
751    48     IF(ISPEC.EQ.1) GO TO 50                                          00007500
752    C                                                                       00007510
753    C                                                                       00007520
754    C      ISPEC = 2 OR 3                                                   00007530
755           Q2=EP(I,2)                                                       00007540
756           VDC2=VD2*UINV1                                                   00007550
757           WC2=W2*UINV1                                                     00007560
758           V12=VDC2-0.5*WC2                                                 00007570
759           V22=VDC2-WC2                                                     00007580
760           IF(V22.EQ.0.) GO TO 49                                           00007590
761           R12=V12/V22                                                      00007600
762           R22=0.5*WC2/V22                                                  00007610
763    49     IF(ISPEC.EQ.2) GO TO 51                                          00007620
764    C                                                                       00007630
765    C      ISPEC = 3                                                        00007640
766           IF(Q1.EQ.0.) Q1=1.E-6                                            00007650
767           Q2Q1=Q2/Q1                                                       00007660
768           V13=V11-0.5*(WC1-WC2)                                            00007670
769           IF(V21.EQ.0.) GO TO 50                                           00007680
```

```
      R13=V13/V21
      R23=0.5*WC2/V21
C
C     ISPEC = 1 OR 3
   50 UTAUC=TAUC*UPL
C
   51 KLID=0
C
C
C *** PEAK EFFECTIVE SOURCE HEIGHT CALCULATIONS.
C
      IF(ISC.LT.6) GO TO 247
C
C  DETERMINE WHETHER PLUME IS MOMENTUM-DOMINATED (IBUOY=0),
C                            OR BUOYANCY-DOMINATED (IBUOY=1).
C
C
C
C
      IF(ISC.EQ.6) BRIGC=115.28
      IF(ISC.EQ.7) BRIGC=87.14
      IF(VP(I).GT.BRIGC*(TP(I)-TA(ISCEN))*SQRT(TA(ISCEN))/TP(I)) IBUOY=0
      GO TO 249
  247 AF= 21.425
      BF= 0.75
      IF(EFF.LT.55.) GO TO 248
      AF= 38.710
      BF= 0.6
  248 IF(3.*VP(I)*DP(I).GT.AF*EFF**BF) IBUOY=0
  249 CONTINUE
C
C  CALL SUBROUTINE RISE WITH IRISE=2 TO GET PEAK EFFECTIVE SOURCE
C    HEIGHT, ESH(2).
C
C     ************
      CALL RISE
C     ************
      IRISE=1
      IF(NPRINT.EQ.0) GO TO 1250
      IF(NWDOPT.LE.1.OR.IWDOPT.LE.1) WRITE(IWR,1010)
     1 I,XP(I),YP(I),EP(I,1),EP(I,2),HP(I),DP(I),VP(I),TP(I),
     2 PRL(1,IBUOY+1),PRL(2,IBUOY+1),DWL(IDWN),DWL(IDWN+1),UPL,ESH(2)
C
C  CALCULATE DISTANCE AT WHICH PLUME REACHES MAXIMUM HEIGHT (PEAK).
C
 1250 IF(IBUOY.EQ.0) GO TO 252
      IF(ISC.LT.6) GO TO 250
      PEAK=0.00207148/(UINV*SQRT(DTDZ(ISC-5)*9.8/TA(ISCEN)))
      GO TO 253
  250 PEAK=0.001*XS
      GO TO 253
  252 PEAK= 0.
      IF(ISC.GE.6) GO TO 253
      IF(ABS(VP(I)).LT..000001) GO TO 253
      PEAK=(0.004*UINV*(DP(I)*(VP(I) + 3./UINV))**2)/VP(I)
C
C  IF MAXIMUM EFFECTIVE SOURCE HEIGHT EXCEEDS HPEN, PLUME ESCAPES
C    THE MIXING LAYER, AND SOURCE IS IGNORED.
C
  253 IF(ESH(2).GT.HPEN) GO TO 600
C
C  IF MAXIMUM EFFECTIVE SOURCE HEIGHT EXCEEDS MIXING HEIGHT BUT
C    NOT HPEN, PLUME DOES NOT ESCAPE THE MIXING LAYER, AND MAXIMUM
C    EFFECTIVE SOURCE HEIGHT IS SET EQUAL TO THE MIXING HEIGHT.
C
      IF(ESH(2).GT.HMIX(ISCEN)) ESH(2)=HMIX(ISCEN)
C
C
C  SET LIMITS (XMIN,XMAX,YMIN,YMAX) ON PORTION OF RECEPTOR GRID
C    EXAMINED FOR EACH SOURCE. THE EXTENT OF THIS PORTION DEPENDS
C    ON SOURCE LOCATION, GRID DIMENSIONS, AND WIND DIRECTION.
C
  275 XMAX= XB2
      XMIN= XB1
      YMAX= YB2
      YMIN= YB1
      IF(XP(I)+60.0.LT.XB2) XMAX= XP(I) + 60.
```

```
      IF(XP(I)-60.0.GT.XB1) XMIN= XP(I) - 60.
      IF(YP(I)+60.0.LT.YB2) YMAX= YP(I) + 60.
      IF(YP(I)-60.0.GT.YB1) YMIN= YP(I) - 60.
      GO TO (280,285,290,295,300,305,310,315),IFLAG
  280 IF(WDPANG.GT.3.14)GOTO282
      IF(WDMANG.LT.0)GOTO284
      YMIN=YP(I)
      XL1=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      GOTO320
  282 YMIN=YP(I)+(XB1-XP(I))*TAN(WDPANG)
      XMAX=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      GOTO320
  284 YMIN=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      XMIN=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      GOTO320
  285 XL1=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      YL1=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      GOTO320
  290 IF(WDPANG.GT.1.57.AND.WDMANG.LT.0.)GOTO292
      IF(WDPANG.GT.6.28.AND.WDMANG.LT.4.712)GOTO294
      XMIN=XP(I)
      YL1=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      YL2=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  292 YMIN=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      XMIN=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      GOTO320
  294 XMIN=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      YMAX=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      GOTO320
  295 XL1=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      YL2=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  300 IF(WDPANG.GT.6.28)GOTO302
      IF(WDMANG.LT.3.14)GOTO304
      YMAX=YP(I)
      XL1=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      GOTO320
  302 YMAX=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      XMIN=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      GOTO320
  304 YMAX=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      XMAN=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      GOTO320
  305 YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      GOTO320
  310 IF(WDMANG.LT.1.57)GOTO312
      IF(WDPANG.GT.4.712)GOTO314
      XMAX=XP(I)
      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG)
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```
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  312 XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      GOTO320
  314 XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  315 XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      GOTO320
  320 IF(XMIN.GT.XB2.OR.XMAX.LT.XB1.OR.YMIN.GT.YB2.OR.YMAX.LT.YB1)
     1 GO TO 600
      IF(XMIN.LT.XB1) XMIN=XB1
      IF(XMAX.GT.XB2) XMAX=XB2
      IF(YMIN.LT.YB1) YMIN=YB1
      IF(YMAX.GT.YB2) YMAX=YB2
C
C  DETERMINE THE RANGE OF RECEPTOR GRID ROW AND COLUMN NUMBERS (LXMAX,
C    LXMIN,LYMAX,LYMIN) CORRESPONDING TO XMAX, ETC. ABOVE -
C
      LXMAX=(XMAX-XSWC)/GRID + 1.
      LXMIN= (XMIN-XSWC)/GRID + 1.
      LYMAX= (YMAX-YSWC)/GRID + 1.
      LYMIN= (YMIN-YSWC)/GRID + 1.
C
C     START LOOP ON ALL AFFECTED RECEPTORS.
      DO 500 IX=LXMIN,LXMAX
      XI=IX
      XG= XSWC + (XI-0.5)*GRID
      XD= XG - XP(I) + 0.00001
      XDSQ=XD*XD
      DO 500 JY=LYMIN,LYMAX
      YJ=JY
      YG= YSWC + (YJ-0.5)*GRID
      YD= YG - YP(I) + 0.00001
C  DSQ= SQUARE OF SOURCE-RECEPTOR DISTANCE. IF SOURCE-RECEPTOR DISTANCE
C    IS GREATER THAN 60 KM., RECEPTOR IS SKIPPED.
      DSQ= XDSQ + YD*YD
      IF(DSQ.GT.3600.) GO TO 500
      DELTA= ATAN(XD/YD)
      IF(DELTA.LT.0.) DELTA = DELTA + 3.1415927
      IF(XD.LT.0.) DELTA = DELTA + 3.1415927
      DELTA= ABS(DELTA - WVEC)
      IF(DELTA.GT.3.1415927) DELTA= ABS(6.2831853 - DELTA)
C  IF THE CROSSWIND ANGLE (DELTA) EXCEEDS A LIMITING VALUE WHICH
C    DEPENDS ON STABILITY CLASS (ANGLIM), THE RECEPTOR IS SKIPPED.
C      ANGLIM = 35,28,21,14,14,10.5,AND 7.0 DEGREES FOR 1-HOUR
C      FOR STABILITY CLASSES A, B, C, DD, DN, E, AND F RESPECTIVELY.
C
      IF(DELTA.GT.ANGLIM(ISC)) GO TO 500
C  DELTA IS THE ANGLE BETWEEN THE WIND VECTOR AND THE SOURCE-RECEPTOR
C    DIRECTION.  THE DOWNWIND DISTANCE USED IN THE GAUSSIAN PLUME
C    EQUATION IS=   DIST= SQRT(DSQ)*COS(DELTA).
      DIST=SQRT(DSQ)*COS(DELTA)
      IF(DIST.LT.0.002) GO TO 500
C
C
C *** DETERMINE PROBABILITY DENSITY OF CROSSWIND DISTRIBUTION
C    OF CONCENTRATIONS.
C
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      XM=DIST*1000.                                                     00010000
      IF(XM.GE.10000.) GO TO 323                                        00010010
      SIGY=CX1(ISC)*(XM**DX1(ISC))                                      00010020
      GO TO 324                                                         00010030
  323 SIGY=CX2(ISC)*(XM**DX2(ISC))                                      00010040
  324 YM=XM*TAN(DELTA)                                                  00010050
      DUMY=YM/SIGY                                                      00010060
      ARG=0.5*DUMY*DUMY                                                 00010070
      IF(ARG.GE.EXPMIN) GO TO 325                                       00010080
      EXPA=EXP(-ARG)                                                    00010090
      GO TO 326                                                         00010100
  325 EXPA=1.                                                           00010110
  326 PYC=(A1B/SIGY)*EXPA                                               00010120
C                                                                       00010130
C                                                                       00010140
C *** DETERMINE PROBABILITY DENSITIES OF VERTICAL DISTRIBUTIONS         00010150
C     OF  SPECIES-1 AND SPECIES-2 POLLUTANT CONCENTRATIONS.             00010160
C                                                                       00010170
      IF(DIST.GT.D47) GO TO 330                                         00010180
C **** NEAR-SOURCE REGION (DIST .LE. D47).                              00010190
C     CALCULATE QZC1 AND QZC2 FROM QZCAL (MODULE M=1).                  00010200
C     ************                                                      00010210
      CALL QZCAL                                                        00010220
C     ************                                                      00010230
      GO TO 350                                                         00010240
C                                                                       00010250
  330 IF(DIST.LT.D80) GO TO 331                                         00010260
C **** WELL-MIXED REGION (DIST .GE. D80).                               00010270
C     CALCULATE QZC1 AND QZC2 FROM QZCAL (MODULE M=2).                  00010280
C     ************                                                      00010290
      CALL QZCAL                                                        00010300
C     ************                                                      00010310
      GO TO 350                                                         00010320
C                                                                       00010330
  331 IF(KLID.EQ.1) GO TO 337                                           00010340
C     CALCULATE QZC1 AND QZC2 FOR POLLUTANT SPECIES                     00010350
C     AT DIST=D47 AND DIST=D80 FOR USE IN INTERPOLATION                 00010360
C     IN PLUME-TRAPPING REGION.                                         00010370
      DUMX=DIST                                                         00010380
      DIST=D47                                                          00010390
C     ************                                                      00010400
      CALL QZCAL                                                        00010410
C     ************                                                      00010420
      QZC11=QZC1                                                        00010430
      IF(ISPEC.EQ.1) GO TO 332                                          00010440
      QZC21=QZC2                                                        00010450
C                                                                       00010460
  332 DIST=D80                                                          00010470
C     ************                                                      00010480
      CALL QZCAL                                                        00010490
C     ************                                                      00010500
      QZC12=QZC1                                                        00010510
      IRC1=1                                                            00010520
      IF(QZC11.EQ.0.OR.QZC12.EQ.0.) IRC1=0                              00010530
      IF(ISPEC.EQ.1) GO TO 333                                          00010540
      QZC22=QZC2                                                        00010550
      IRC2=1                                                            00010560
      IF(QZC21.EQ.0.OR.QZC22.EQ.0.) IRC2=0                              00010570
C                                                                       00010580
  333 KLID=1                                                            00010590
      DIST=DUMX                                                         00010600
      IF(IRC1.EQ.0) GO TO 334                                           00010610
      DIFX1=ALOG(D80/D47)                                               00010620
      DIFC1=ALOG(QZC12/QZC11)                                           00010630
      GO TO 335                                                         00010640
  334 DIFC1=QZC12-QZC11                                                 00010650
  335 IF(ISPEC.EQ.1) GO TO 337                                          00010660
      IF(IRC2.EQ.0) GO TO 336                                           00010670
      DIFX2=ALOG(D80/D47)                                               00010680
      DIFC2=ALOG(QZC22/QZC21)                                           00010690
      GO TO 337                                                         00010700
  336 DIFC2=QZC22-QZC21                                                 00010710
C                                                                       00010720
C **** PLUME-TRAPPING REGION (D47 < DIST < D80).                        00010730
C     CALCULATE QZC1 AND QZC2 BY LINEAR INTERPOLATION                   00010740
C     (BETWEEN VALUES AT DIST=D47 AND DIST=D80) ON                      00010750
C     A LOG-LOG PLOT OF QZC VERSUS DOWNWIND DISTANCE.                   00010760
```

```
C     IF EITHER OF THE QZC VALUES AT D47 AND D80 ARE
C     ZERO, USE A LINEAR PLOT FOR INTERPOLATION.
  337 IF(IRC1.EQ.0) GO TO 338
      RATX1=ALOG(DIST/D47)/DIFX1
      QZC1L=ALOG(QZC11)+RATX1*DIFC1
      QZC1=EXP(QZC1L)
      GO TO 339
  338 RATX1=(DIST-D47)/D8047
      QZC1=QZC11+RATX1*DIFC1
  339 IF(ISPEC.EQ.1) GO TO 350
C
      IF(IRC2.EQ.0) GO TO 340
      RATX2=ALOG(DIST/D47)/DIFX2
      QZC2L=ALOG(QZC21)+RATX2*DIFC2
      QZC2=EXP(QZC2L)
      GO TO 350
  340 RATX2=(DIST-D47)/D8047
      QZC2=QZC21+RATX2*DIFC2
C
C
C
C     CALCULATE GROUND-LEVEL CONCENTRATIONS CONC (MICROGRAMS PER CUBIC
C     METER) AND SURFACE DEPOSITION FLUX SDF (MICROGRAMS PER SQUARE
C     METER PER HOUR) OF POLLUTANTS AT RECEPTOR IN COLUMN IX, ROW JY
C     OF THE RECEPTOR GRID DUE TO POINT SOURCE I.
C
C     ISPEC = 1 OR 2 OR 3
  350 C1=Q1*UINV*PYC*QZC1
      IF(NCSOPT.EQ.0) GO TO 355
      CALL WORST(IX,JY,C1)
      IF(NTOPT.GT.1) CONC(IX,JY,2)=CONC(IX,JY,2) + C1
  355 CINC1=C1*STCONV
      CONC(IX,JY,1)=CONC(IX,JY,1)+CINC1
      SDF(IX,JY,1)=SDF(IX,JY,1)+VD136*CINC1
      IF(ISPEC.EQ.1) GO TO 370
      IF(ISPEC.EQ.3) GO TO 360
C
C     ISPEC = 2
      C2=Q2*UINV*PYC*QZC2
      GO TO 365
C
C     ISPEC = 3
  360 C2=Q1*UINV*PYC*QZC2
C
  365 CINC2=C2*STCONV
      CONC(IX,JY,2)=CONC(IX,JY,2)+CINC2
      SDF(IX,JY,2)=SDF(IX,JY,2)+VD236*CINC2
  370 CONTINUE
C
  500 CONTINUE
C     END LOOP ON ALL AFFECTED RECEPTORS.
C
  600 CONTINUE
C     END LOOP ON ALL POINT SOURCES.
C
C
C
C *** PRINT OUTPUT.
C
C     OUTPUT AT END OF EACH SCENARIO OR SUB-SCENARIO
C
C     TIME AVERAGING:  NTOPT=2 OR 3
C       AT END OF EACH SCENARIO, CALL WOROUT TO PRINT OUTPUT FOR
C         NCSOPT OPTION.
C       IF LAST SCENARIO, CALL OUTMOD TO PRINT OUTPUT FOR NLIST, NTAPE,
C         AND NARRAY OPTIONS.  CALL MAXOUT TO PRINT OUTPUT FOR NMAX.
C         OTHERWISE, GO TO 100 FOR THE NEXT SCENARIO.
C
C     NO TIME AVERAGING: NTOPT=1
C       AT END OF EACH SCENARIO (OR SUB-SCENARIO WHEN NWDOPT.GT.1),
C         CALL OUTMOD TO PRINT OUTPUT FOR NCSOPT, NLIST, NTAPE,
C         AND NARRAY OPTIONS.
C       IF LAST SCENARIO (AND LAST SUB-SCENARIO WHEN NWDOPT.GT.1),
C         CALL MAXOUT TO PRINT OUTPUT FOR NMAX OPTION.
C         OTHERWISE, GO TO 100 FOR THE THE NEXT SCENARIO OR SUB-SCENARIO
C
  603 IF(NTOPT.EQ.1) GO TO 620
```

```
C
C     TIME AVERAGING: NTOPT=2 OR 3
C
      IF(NCSOPT.GT.0) CALL WOROUT
      IF(ISCEN.NE.NSCEN) GO TO 100
      CALL OUTMOD
      GO TO 999
C
C     NO TIME AVERAGING: NTOPT=1
C
  620 CALL OUTMOD
      IF(ISCEN.NE.NSCEN) GO TO 100
      IF(NWDOPT.LE.1) GO TO 999
      IF(IWDOPT.LT.4) GO TO 100
C
  999 IF(NMAX.GT.0) CALL MAXOUT
C
      STOP
C
C
 1005 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'OUTPUT:  ',20A4//
     14X,'SCENARIO',I2,4X,'POINT SOURCE PLUME RISE CALCULATIONS'/
     221X,'MIXING HEIGHT: HMIX=',F7.2,' M'/
     321X,'IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN ',F7.1,
     4' M, THE SOURCE IS IGNORED'/)
 1007 FORMAT(14X,'SOURCE',8X,'EMISSION RATES',61X,'WIND SPEED AT',4X,
     1 'MAXIMUM'/' POINT',6X,'COORDINATES',4X,'POL-1',6X,'POL-2',4X,
     2 'HEIGHT  DIAMETER  EXIT VEL  EXIT TEMP',6X,'DOMINANT',5X,
     3 'STACK HEIGHT',4X,'EFFECTIVE'/' SOURCE',3X,'X(KM)',4X,'Y(KM)',3X,
     4 '(G/S)',6X,'(G/S)',5X,'(M)',6X,'(M)',7X,'(M/S)',4X,'(DEG K)',6X,
     5 'INFLUENCE',8X,'(M/S)',6X,'SOURCE HEIGHT(M)'/)
 1010 FORMAT(1X,I4,2X,F8.2,1X,F8.2,2X,F8.2,2X,F8.2,2X,F7.2,3X,F6.3,3X,
     1 F8.3,3X,F7.2,2X,2A4,1X,2A4,3X,F7.3,8X,F8.2)
      END
C
C
      SUBROUTINE QZCAL
C                     SUBROUTINE QZCAL  (VERSION 82360), PART OF PEM.
C
C
C  SUBROUTINE QZCAL CALCULATES QZC1 AND QZC2,  REPRESENTING THE
C     PROBABLITY DENSITIES OF VERTICAL DISTRIBUTIONS OF CONCENTRATIONS
C     OF POLLUTANT SPECIES 1 AND 2, RESPECTIVELY, AT A GIVEN
C     DISTANCE DOWNWIND OF A POINT SOURCE.
C
C
C *** PEM  ALGORITHMS AND PROGRAM DEVELOPMENT: ---DECEMBER 1982
C
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C     BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION )
C
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC
      COMMON/PARM1A/GAMMA
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT
```

```
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2                                 00012310
      COMMON/PARM4/V11,V21,V12,V22,V13                                  00012320
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6                       00012330
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42              00012340
      COMMON/PARM7/QZC1,QZC2                                            00012350
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C                               00012360
      COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW                          00012370
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00012380
      EXTERNAL FUN1                                                     00012390
      REAL*8 FUN1                                                       00012400
      REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR                00012410
      DIMENSION IW(102)                                                 00012420
C                                                                       00012430
C                                                                       00012440
C                                                                       00012450
      IF(DIST.GE.PEAK) GO TO 5                                          00012460
C                                                                       00012470
C  CALL SUBROUTINE RISE FOR EFFECTIVE SOURCE HEIGHT AT DOWNWIND         00012480
C    DISTANCE = DIST, LESS THAN DISTANCE TO MAXIMUM HEIGHT (PEAK).      00012490
C     ***********                                                       00012500
      CALL RISE                                                         00012510
C     ************                                                      00012520
      HGT= ESH(1)                                                       00012530
      GO TO 6                                                           00012540
C                                                                       00012550
C  USE MAXIMUM EFFECTIVE SOURCE HEIGHT, SINCE DOWNWIND DISTANCE         00012560
C    EXCEEDS THE DISTANCE TO MAXIMUM HEIGHT.                            00012570
    5 HGT= ESH(2)                                                       00012580
    6 JD=2                                                              00012590
      IF(DIST.LT.0.5) JD=1                                              00012600
      IF(DIST.GT.5.0) JD=3                                              00012610
C                                                                       00012620
C                                                                       00012630
      HL=HMIX(ISCEN)                                                    00012640
      X=DIST                                                            00012650
      XM=X*1000.                                                        00012660
      SIGZ= AX(ISC,JD)*(XM**BX(ISC,JD))                                 00012670
      IF(SIGZ.GT.5000.) SIGZ=5000.                                      00012680
      SZ=SIGZ                                                           00012690
      C2=SQRT2*SZ                                                       00012700
      HC=HGT/C2                                                         00012710
      XC=XM/C2                                                          00012720
C                                                                       00012730
C     ISPEC = 1 OR 2 OR 3                                               00012740
      D31=2.*V11*XC                                                     00012750
      D11=WC1*XC                                                        00012760
      D21=D11*D11                                                       00012770
      R31=1.+2.*D21                                                     00012780
      R41=2.*D11/SQPI                                                   00012790
      IF(ISPEC.EQ.1) GO TO 9                                            00012800
C                                                                       00012810
C     ISPEC = 2 OR 3                                                    00012820
      D32=2.*V12*XC                                                     00012830
      D12=WC2*XC                                                        00012840
      D22=D12*D12                                                       00012850
      R32=1.+2.*D22                                                     00012860
      R42=2.*D12/SQPI                                                   00012870
      IF(ISPEC.EQ.2) GO TO 10                                           00012880
C                                                                       00012890
C     ISPEC = 3                                                         00012900
      D33=2.*V13*XC                                                     00012910
      D6=4.*SQPI*(V21-V22)*XC                                           00012920
C                                                                       00012930
    9 TCC=UTAUC/C2                                                      00012940
   10 IF(ICT.EQ.0) XCT=0.                                               00012950
      IF(ICT.EQ.1) XCT=XC/TCC                                           00012960
      EXCT=EXP(-XCT)                                                    00012970
C                                                                       00012980
      TERM1=0.                                                          00012990
      TERM2=0.                                                          00013000
      TERM3=0.                                                          00013010
C                                                                       00013020
      DUM1=D47+0.001                                                    00013030
      DUM2=D80-0.001                                                    00013040
      IF(X.LT.DUM1) GO TO 100                                           00013050
      IF(X.GT.DUM2) GO TO 200                                           00013060
C                                                                       00013070
```

```
 11 QZC1=0.0
    QZC2=0.0
    RETURN
C
C
C **** NEAR-SOURCE REGION (X .LE. D47).
C
100 M=1
    A1=A1B/SZ
    C3=HC*HC
    IF(C3.GE.EXPMIN) GO TO 11
    A2=1./EXP(C3)
C
C   ISPEC = 1 OR 2 OR 3
C   SPECIES-1 (PRIMARY) POLLUTANT: GAS OR PARTICLES.
    ETA1=HC+D31
    ETA1SQ=ETA1*ETA1
    IF(ETA1SQ.GT.EXPMAX) CALL ARGCHK(ETA1,ETA1SQ)
    B11=EXP(ETA1SQ)*ERFC(ETA1)
    ALPHA1=A1C*D31*B11
    SUM=2.-ALPHA1
    IF(SUM) 115,115,116
115 G21P=0.0
    GO TO 120
116 IF(WC1.EQ.0.) GO TO 117
    BETA1=-2.*D11*HC+D21
    CALL EXPO(-BETA1,EBT1)
    GO TO 118
117 EBT1=1.0
118 G21P=EXCT*EBT1*A2*SUM
120 QZC1=A1*G21P
    IF(ISPEC.EQ.1) RETURN
C
C
C   ISPEC = 2 OR 3
C   SPECIES-2 (SECONDARY) POLLUTANT: GAS OR PARTICLES.
    ETA2=HC+D32
    ETA2SQ=ETA2*ETA2
    IF(ETA2SQ.GT.EXPMAX) CALL ARGCHK(ETA2,ETA2SQ)
    B12=EXP(ETA2SQ)*ERFC(ETA2)
    ALPHA2=A1C*D32*B12
    SUM1=2.-ALPHA2
    IF(ISPEC.EQ.3) GO TO 145
C
C   ISPEC = 2
    IF(SUM1) 135,135,140
135 G22P=0.0
    QZC2=0.0
    RETURN
140 IF(WC2.EQ.0.) GO TO 141
    BETA2=-2.*D12*HC+D22
    CALL EXPO(-BETA2,EBT2)
    GO TO 142
141 EBT2=1.0
142 G22P=EBT2*A2*SUM1
    QZC2=A1*G22P
    RETURN
C
C   ISPEC = 3
145 TERM1=(Q2Q1+GAMMA)*A2*SUM1
C
    ETA3=HC+D33
    ETA3SQ=ETA3*ETA3
    IF(ETA3SQ.GT.EXPMAX) CALL ARGCHK(ETA3,ETA3SQ)
    B13=EXP(ETA3SQ)*ERFC(ETA3)
    ALPHA3=A1C*D33*B13
    TERM2=-GAMMA*EXCT*A2*(2.-ALPHA3)
C
    IF(V21.EQ.V22) GO TO 150
C   COMPUTE INTEGRAL FUNC=F1(XC,0.;HC); FUN1 IS THE INTEGRAND FUNCTION
    CALL D01AJF(FUN1,AI,BI,EPSABS,EPSREL,RESULT,
   1  ABSERR,WORK,LW,IW,NIW,IFAIL)
    RES=RESULT
    FUNC=RES/PI
    TERM3=-GAMMA*D6*FUNC
C
150 SUMT=TERM1+TERM2+TERM3
```

```
      IF(SUMT) 155,155,160
  155 G22P=0.0
      QZC2=0.0
      RETURN
  160 IF(WC2.EQ.0.) GO TO 161
      BETA2=-2.*D12*HC+D22
      CALL EXPO(-BETA2,EBT2)
      GO TO 162
  161 EBT2=1.0
  162 G22P=EBT2*SUMT
      QZC2=A1*G22P
      RETURN
C
C
C **** WELL-MIXED REGION (X .GE. D80).
C
C     IN THIS REGION, THE CONCENTRATION BELOW THE MIXING HEIGHT IS
C     UNIFORM REGARDLESS OF THE SOURCE OR RECEPTOR HEIGHTS BECAUSE
C     OF THOROUGH MIXING OF POLLUTANT BETWEEN THE GROUND AND THE
C     MIXING HEIGHT.
C
  200 M=2
      A1A=1000./HL
      CALL PSG4P(G41P,G42P)
      QZC1=A1A*G41P
      IF(ISPEC.EQ.1) RETURN
      QZC2=A1A*G42P
      RETURN
      END
C
C
      SUBROUTINE PSG4P(G41P,G42P)
C                          SUBROUTINE PSG4P (VERSION 82360), PART OF PEM.
C
C
C     THIS SUBROUTINE CALCULATES AND RETURNS VALUES OF G41P AND G42P.
C     THESE ARE NONDIMENSIONAL VERTICALLY-INTEGRATED PROBABILITY
C     DENSITY FUNCTIONS USED IN THE WELL-MIXED REGION CONCENTRATION
C     ALGORITHMS FOR SPECIES-1 AND SPECIES-2, RESPECTIVELY, DOWNWIND
C     OF A POINT SOURCE.  THESE FUNCTIONS ARE INDEPENDENT OF BOTH
C     SOURCE HEIGHT AND RECEPTOR HEIGHT.  THIS SUBROUTINE IS
C     USED BY BOTH POINT AND AREA SOURCES.  FOR AREA SOURCES,
C     G41P AND G42P REPRESENT SUSPENSION RATIOS OF POLLUTANTS.
C
C
C
C *** PEM ALGORITHMS AND PROGRAM DEVELOPMENT: --- DECEMBER 1982
C
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C
C     ( THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT
C     BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION )
C
C
C
      EXTERNAL FUN2
      REAL*8 FUN2
      REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR
      DIMENSION IW(102)
      COMMON/PARM1A/GAMMA
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT
      COMMON/PARM4/V11,V21,V12,V22,V13
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C
      COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
C
C     ISPEC = 1 OR 2 OR 3
```

```
C***** SPECIES-1 (PRIMARY) POLLUTANT: GAS OR PARTICLES.
C
      IF(D21.GT.EXPMAX) CALL ARGCHK(D11,D21)
      B11=EXP(D21)*ERFC(D11)
      IF(V21.EQ.0.) GO TO 201
      D31SQ=D31*D31
      IF(D31SQ.GT.EXPMAX) CALL ARGCHK(D31,D31SQ)
      SUM=R11*(EXP(D31SQ)*ERFC(D31))-R21*B11
      GO TO 202
  201 SUM=R31*B11-R41
  202 IF(SUM.LT.0.) SUM=0.0
      G41P=EXCT*EXP(-D21)*SUM
      IF(ISPEC.EQ.1) RETURN
C
C     ISPEC = 2 OR 3
C***** SPECIES-2 (SECONDARY) POLLUTANT: GAS OR PARTICLES.
C
      IF(D22.GT.EXPMAX) CALL ARGCHK(D12,D22)
      B12=EXP(D22)*ERFC(D12)
      IF(V22.EQ.0.) GO TO 203
      D32SQ=D32*D32
      IF(D32SQ.GT.EXPMAX) CALL ARGCHK(D32,D32SQ)
      SUM1=R12*(EXP(D32SQ)*ERFC(D32))-R22*B12
      GO TO 204
  203 SUM1=R32*B12-R42
  204 IF(ISPEC.EQ.3) GO TO 205
C
C     ISPEC = 2
      IF(SUM1.LT.0.) SUM1=0.0
      G42P=EXP(-D22)*SUM1
      RETURN
C
C     ISPEC = 3
  205 TERM1=(Q2Q1+GAMMA)*SUM1
C
      IF(V21.EQ.0.) GO TO 206
      D33SQ=D33*D33
      IF(D33SQ.GT.EXPMAX) CALL ARGCHK(D33,D33SQ)
      SUM2=R13*(EXP(D33SQ)*ERFC(D33))-R23*B12
      GO TO 207
  206 SUM2=R32*B12-R42
  207 TERM2=-GAMMA*EXCT*SUM2
C
      IF(V21.EQ.V22) GO TO 208
C     COMPUTE INTEGRAL FUNC=F2(XC); FUN2 IS THE INTEGRAND FUNCTION.
      CALL D01AJF(FUN2,AI,BI,EPSABS,EPSREL,RESULT,
     1  ABSERR,WORK,LW,IW,NIW,IFAIL)
      RES=RESULT
      FUNC=RES/(2.*PI)
      TERM3=-GAMMA*D6*FUNC
      GO TO 209
  208 TERM3=0.0
C
  209 SUMT=TERM1+TERM2+TERM3
      IF(SUMT.LT.0.) SUMT=0.0
      G42P=EXP(-D22)*SUMT
      RETURN
      END
C
C
      DOUBLE PRECISION FUNCTION FUN1(T)
      REAL*8 T,TERM1,TERM2,TERM3
C                    REAL*8 FUNCTION FUN1(VERSION 82360), PART OF PEM.
C
C
C     INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION IN SUBROUTINE
C     QZCAL (FOR POINT SOURCES) IS DEFINED HERE.
C
C
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982
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C     NOAA-ATDL, P.O. BOX-E
C     OAK RIDGE, TENN 37830
C
C
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2
```

```
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6                       00015380
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C                               00015390
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00015400
C                                                                       00015410
C                                                                       00015420
      SQT=SQRT(T)                                                       00015430
      SQ1T=SQRT(1.-T)                                                   00015440
      HC1=HC/SQT                                                        00015450
C                                                                       00015460
      ARG1= -(HC1*HC1)-(T*XCT)                                          00015470
      CALL EXPO(ARG1,EXP1)                                              00015480
      IF(EXP1.EQ.0.) GO TO 10                                           00015490
      TERM1= EXP1/(SQT*SQ1T)                                            00015500
C                                                                       00015510
      ETA4=HC1+D33*SQT                                                  00015520
      ETA4SQ=ETA4*ETA4                                                  00015530
      IF(ETA4SQ.GT.EXPMAX) CALL ARGCHK(ETA4,ETA4SQ)                     00015540
      TERM2A= EXP(ETA4SQ)*ERFC(ETA4)                                    00015550
      HC1SQ=HC1*HC1                                                     00015560
      IF(HC1SQ.GT.EXPMAX) CALL ARGCHK(HC1,HC1SQ)                        00015570
      TERM2= 1. -SQPI*(ETA4-HC1)*TERM2A                                 00015580
      IF(TERM2.LE.0.) GO TO 10                                          00015590
C                                                                       00015600
      ETA5=D32*SQ1T                                                     00015610
      ETA5SQ=ETA5*ETA5                                                  00015620
      IF(ETA5SQ.GT.EXPMAX) CALL ARGCHK(ETA5,ETA5SQ)                     00015630
      TERM3=1.-SQPI*ETA5*(EXP(ETA5SQ)*ERFC(ETA5))                       00015640
      IF(TERM3.LE.0.) GO TO 10                                          00015650
C                                                                       00015660
      FUN1=TERM1*TERM2*TERM3                                            00015670
      GO TO 11                                                          00015680
   10 FUN1=0.0                                                          00015690
   11 RETURN                                                            00015700
      END                                                               00015710
C                                                                       00015720
C                                                                       00015730
      DOUBLE PRECISION FUNCTION FUN2(T)                                 00015740
      REAL*8 T
C                    REAL*8 FUNCTION FUN2 (VERSION 82360), PART OF PEM. 00015750
C                                                                       00015760
C                                                                       00015770
C     INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION IN SUBROUTINE00015780
C     PSG4P (FOR POINT AND AREA SOURCES) IS DEFINED HERE.               00015790
C                                                                       00015800
C                                                                       00015810
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982             00015820
C     K. SHANKAR RAO                                                    00015830
C     NOAA-ATDL, P.O. BOX-E                                             00015840
C     OAK RIDGE, TENN 37830                                             00015850
C                                                                       00015860
C                                                                       00015870
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT                            00015880
      COMMON/PARM4/V11,V21,V12,V22,V13                                  00015890
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6                       00015900
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42              00015910
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C                               00015920
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00015930
C                                                                       00015940
C                                                                       00015950
      SQT=SQRT(T)                                                       00015960
      SQ1T=SQRT(1.-T)                                                   00015970
      ETA4=D33*SQT                                                      00015980
      ETA5=D32*SQ1T                                                     00015990
      ETA6=D12*SQ1T                                                     00016000
      ETA6SQ=ETA6*ETA6                                                  00016010
      IF(ETA6SQ.GT.EXPMAX) CALL ARGCHK(ETA6,ETA6SQ)                     00016020
C                                                                       00016030
      ARG1=T*XCT                                                        00016040
      EXP1=EXP(-ARG1)                                                   00016050
      TERM1=EXP1/SQT                                                    00016060
C                                                                       00016070
      IF(ETA4.EQ.0.) GO TO 10                                           00016080
      ETA4SQ=ETA4*ETA4                                                  00016090
      IF(ETA4SQ.GT.EXPMAX) CALL ARGCHK(ETA4,ETA4SQ)                     00016100
      TERM2=1.-SQPI*ETA4*(EXP(ETA4SQ)*ERFC(ETA4))                       00016110
      IF(TERM2.LT.0.) TERM2=0.                                          00016120
      GO TO 11                                                          00016130
```

```
   10 TERM2=1.
C
   11 IF(V22.EQ.0.) GO TO 12
      ETA5SQ=ETA5*ETA5
      IF(ETA5SQ.GT.EXPMAX) CALL ARGCHK(ETA5,ETA5SQ)
      T3A=EXP(ETA5SQ)*ERFC(ETA5)
      T3B=EXP(ETA6SQ)*ERFC(ETA6)
      TERM3=R12*T3A-R22*T3B
      IF(TERM3.LT.0.) TERM3=0.
      GO TO 13
C
   12 T3A=(1.+2.*ETA6SQ)*(EXP(ETA6SQ)*ERFC(ETA6))
      T3B=2.*ETA6/SQPI
      TERM3=T3A-T3B
      IF(TERM3.LT.0.) TERM3=0.
C
   13 FUN2=TERM1*TERM2*TERM3
      RETURN
      END
C
C
      DOUBLE PRECISION FUNCTION FUN3(T)
      REAL*8 T
C                 REAL*8 FUNCTION FUN3 (VERSION 82360), PART OF PEM.
C
C
C     INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION FOR AREA
C     SOURCES IN MAIN PROGRAM IS DEFINED HERE.
C
C
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982
C     K. SHANKAR RAO
C     NOAA-ATDL, P.O. BOX - E
C     OAK RIDGE, TENN 37830
C
C
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT
      COMMON/PARM2A/AA,BA
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2
      COMMON/PARM4/V11,V21,V12,V22,V13
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
C
      DN=SQRT2*AA
      BA1=1.-BA
      UTBA1=(UTAUC)**BA1
      P1=2.*V11*UTBA1/DN
      TBA1=T**BA1
      ETA1=P1*TBA1
      ETA1SQ=ETA1*ETA1
      IF(ETA1SQ.GT.EXPMAX) CALL ARGCHK(ETA1,ETA1SQ)
      TERM=EXP(ETA1SQ)*ERFC(ETA1)
      EXP1=EXP(-T)
C
      IF(WC1.NE.0.) GO TO 11
   10 SUM=TERM
      GO TO 13
C
   11 IF(V21.EQ.0.) GO TO 12
      P2=WC1*UTBA1/DN
      B1=P2*TBA1
      B1SQ=B1*B1
      IF(B1SQ.GT.EXPMAX) CALL ARGCHK(B1,B1SQ)
      SUM=EXP(-B1SQ)*(R11*TERM-R21*(EXP(B1SQ)*ERFC(B1)))
      GO TO 13
C
   12 RF1=1.+2.*ETA1SQ
      RS1=2.*ETA1/SQPI
      SUM=EXP(-ETA1SQ)*(RF1*TERM-RS1)
C
   13 IF(SUM.LT.0.) SUM=0.0
      FUN3=EXP1*SUM/VDC1
      RETURN
      END
C
```

```
C
      SUBROUTINE EXPO(BX,EX)
C                                 SUBROUTINE EXPO (VERSION 82360), PART OF PEM.
C
C
C
C     GIVEN THE ARGUMENT BX, SUBROUTINE EXPO CALCULATES AND
C     RETURNS EX=EXP(BX).  EXPO LIMITS THE ARGUMENT TO AVOID
C     OVERFLOW/UNDERFLOW ERRORS.
C
C
C
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982
C     K. SHANKAR RAO
C     NOAA-ATDL, P.O. BOX-E
C     OAK RIDGE, TENN 37830
C
C
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
C
      BXABS=ABS(BX)
      IF(BX) 5,10,15
    5 IF(BXABS-EXPMIN) 6,7,7
    6 EX=EXP(BX)
      GO TO 20
    7 EX=0.
      GO TO 20
   10 EX=1.
      GO TO 20
   15 IF(BXABS.GT.EXPMAX) BXABS=EXPMAX
      EX=EXP(BXABS)
   20 RETURN
      END
C
C
      SUBROUTINE ARGCHK(E,ESQ)
C                                 SUBROUTINE ARGCHK (VERSION 82360), PART OF PEM.
C
C
C     SUBROUTINE ARGCHK LIMITS THE ARGUMENTS OF EXP(ESQ)*ERFC(E)
C     TO AVOID OVERFLOW/UNDERFLOW ERRORS.
C
C
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT:  DECEMBER 1982
C     K. SHANKAR RAO
C     NOAA-ATDL, P.O. BOX-E
C     OAK RIDGE, TENN 37830
C
C
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
C
      ESQ=EXPMAX
      IF(E.LT.0.) NSIGN=-1
      IF(E.GE.0.) NSIGN=1
      E=NSIGN*ETAMAX
      RETURN
      END
C
C
      SUBROUTINE INMOD
C                                 SUBROUTINE INMOD  (VERSION 82360), PART OF PEM.
C
C
C
C  SUBROUTINE INMOD READS IN ALL INPUTS TO THE MODEL, SCREENS THEM,
C    PRINTS WARNING MESSAGES, AND INSERTS DEFAULT VALUES AS NEEDED.
C    THE SUBROUTINE PRINTS OUT LISTS OF THE CONTROL PARAMETERS,
C    SCENARIO PARAMETERS, AND SOURCE DATA FOR REFERENCE.
C    INMOD ALSO PROCESSES THE INPUT FOR EACH SCENARIO BEFORE
C    TRANSMITTING IT TO THE MAIN PROGRAM.
C
C
C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS,
C     NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830
C     DECEMBER 1982
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
```

```
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,     UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC
      COMMON/PARM1A/GAMMA
C
      DIMENSION NAME(2),WDINC(6),SUMAQ(2),SUMPQ(2),SUMAR(2),EAR(2),
     1 AMSG(2),CWS(6)
      DIMENSION DCR(24,2),NSC(24),NWD(24),NWS(24),ASCALE(2)
      DATA NAME/4H    ,4H    /
      DATA AMSG/4HVD1 ,4HVD2 /
      DATA WDINC/1.5707963,0.7853982,0.5235988,0.2617994,
     1           0.1745329,0.08726646/
      DATA CWS/1.5,2.46,4.47,6.93,9.61,12.52/
C
      IF(INDEX.NE.0) GO TO 300
C
      ISTOP=0
C
C  R E A D   A L L   I N P U T   D A T A.
C
C **** READ FIRST CONTROL PARAMETER CARD (TITLE).
C
      READ(IRD,800)TT
      WRITE(IWR,900) TT
C
C **** READ SECOND CONTROL PARAMETER CARD (OPTIONS).
C
C     NTOPT  = AVERAGING TIME OPTION (1 OR 2 OR 3).
C     NWDOPT = WIND DIRECTION INPUT OPTION (0 TO 7).
C     NWSOPT = WIND SPEED INPUT OPTION (0 OR 1).
C     NSCEN  = NUMBER OF SCENARIOS (1 TO 24).
C     NLIST  = OUTPUT OPTION: LISTS OF CONC AND SURF DEP FLUX (0 OR 1)
C     NARRAY = OUTPUT OPTION: MAPS OF CONC AND SURF DEP FLUX (0 TO 3)
C     NTAPE  = OUTPUT OPTION: TAPE OF CONC AND SURF DEP FLUX (0 OR 1)
C     NCSOPT = OUTPUT OPTION: POINT SOURCE CULPABILITY LIST (0 OR 1).
C     NMAX   = OUTPUT OPTION: MAXIMUM CONC. FOR EACH SCENARIO (0 OR 1).
C     NSTDWN = STACK-TIP DOWNWASH OPTION (0 OR 1).
C     INTER  = RECEPTOR INTERVAL ON TAPE OUTPUT (1,2,---).
C     NPRINT = OUTPUT OPTION: POINT SOURCE PLUME RISE INFO (0 OR 1)
C     INPTSC = INPUT OPTN: POINT SOURCE DATA ON UNIT IRD OR IDSK (1 OR 2)
C
      READ(IRD,805)NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,
     1 NCSOPT,NMAX,NSTDWN,INTER,NPRINT,INPTSC
C
      IF(NTOPT.GE.1 .AND. NTOPT.LE.3) GO TO 2
      WRITE(IWR,660) NTOPT
      NTOPT=1
    2 IF(NWDOPT.LE.1) GO TO 6
      IF(NWDOPT.GT.7) GO TO 5
      IF(NTOPT.EQ.1 .OR. NWDOPT.LE.1) GO TO 6
      WRITE(IWR,615)
    5 NWDOPT=0
    6 IF(NWSOPT.GT.1) NWSOPT=0
      IF(NSCEN.EQ.0) NSCEN=1
      IF(NTOPT.EQ.2 .AND. NSCEN.NE.24) GO TO 500
   10 IF(NSCEN.GT.24) GO TO 510
   20 IF(NLIST.EQ.0) GO TO 25
      IF(NLIST.GT.1) GO TO 22
      IF(NWDOPT.LE.1) GO TO 25
      WRITE(IWR,605)
   22 NLIST=0
   25 IF(NARRAY.GT.3) NARRAY=0
      IF(NTAPE.EQ.0) GO TO 40
      IF(NTAPE.GT.1) GO TO 30
      IF(NWDOPT.LE.1) GO TO 40
      WRITE(IWR,620)
   30 NTAPE=0
```

```
   40 IF(NCSOPT.GT.1) NCSOPT=0                                          00018440
      IF(NMAX.GT.1) NMAX=0                                              00018450
      IF(NSTDWN.GT.1) NSTDWN=0                                          00018460
      IF(INTER.EQ.0) INTER=1                                            00018470
      IF(NPRINT.GT.1) NPRINT=0                                          00018480
      IF(INPTSC.LT.1 .OR. INPTSC.GT.2) INPTSC=1                         00018490
C                                                                       00018500
C      SET LABEL FOR TIME AVERAGING                                     00018510
      IAV=1                                                             00018520
      IF(NTOPT.EQ.2) IAV=24                                             00018530
      IF (NTOPT.EQ.3) IAV=NSCEN                                         00018540
C                                                                       00018550
C **** READ THIRD CONTROL PARAMETER CARD (GRID, DTDZ)                   00018560
C                                                                       00018570
C    XRSWC,YRSWC = COORDINATES OF SOUTHWEST CORNER OF RECEPTOR GRID (KM)00018580
C    LX          = NUMBER OF COLUMNS IN RECEPTOR GRID.                  00018590
C    LY          = NUMBER OF ROWS IN RECEPTOR GRID.                     00018600
C    GRID        = SPACING BETWEEN ROWS AND COLUMNS OF RECEPTOR GRID (KM) 00018610
C                                                                       00018620
C    DTDZ(1&2) = VERTICAL POTENTIAL TEMPERATURE GRADIENT                00018630
C                     FOR STABILITY CLASSES E & F.                      00018640
C                                                                       00018650
      READ(IRD,810)XRSWC,YRSWC,LX,LY,GRID,DTDZ(1),DTDZ(2)               00018660
C                                                                       00018670
      IF(LX.EQ.0) LX=1                                                  00018680
      IF(LY.EQ.0) LY=1                                                  00018690
      IF(NTAPE.EQ.0) GO TO 115                                          00018700
C                                                                       00018710
      NRECS=((LX+1)/INTER)*((LY+1)/INTER)*NSCEN                         00018720
      IF(NTOPT.EQ.2) NRECS= NRECS/24                                    00018730
      IF(NTOPT.EQ.3) NRECS= NRECS/NSCEN                                 00018740
      IF(NRECS.LT.10000) GO TO 115                                      00018750
      WRITE(IWR,600)                                                    00018760
      NTAPE=0                                                           00018770
  115 CONTINUE                                                          00018780
C                                                                       00018790
C **** READ FOURTH CONTROL PARAMETER CARD (POLLUTANTS)                  00018800
C                                                                       00018810
C    NPOL  = NUMBER OF POLLUTANTS (1 OR 2)                              00018820
C    ICT   = CHEMICAL TRANSFORMATION OR DECAY OPTION (0 OR 1)           00018830
C    VD1   = DEPOSITION VELOCITY FOR POLLUTANT SPECIES-1 (CM/S)         00018840
C    W1    = SETTLING VELOCITY FOR POLLUTANT SPOECIES-1 (CM/S)          00018850
C    VD2   = DEPOSITION VELOCITY FOR POLLUTANT SPECIES-2 (CM/S)         00018860
C    W2    = SETTLING VELOCITY FOR POLLUTANT SPECIES-2 (CM/S)           00018870
C    XKT   = CHEMICAL TRANSFORMATION OR DECAY RATE OF POLLUTANT         00018880
C              SPECIES-1 (PERCENT PER HOUR)                             00018890
C    GAMMA = RATIO OF MOLECULAR WEIGHTS OF SPECIES-2 (PRODUCT)          00018900
C              TO SPECIES-1 (REACTANT) IN CHEMICAL TRANSFORMATION       00018910
C                                                                       00018920
C  NOTE: FOR DEPOSITION TO OCCUR, W SHOULD BE LESS THAN OR EQUAL TO VD. 00018930
C        FOR DEPOSITION OF GASES AND VERY SMALL PARTICLES, W=0.         00018940
C        FOR DEPOSITION OF SMALL PARTICLES, W IS LESS THAN VD.          00018950
C        FOR DEPOSITION OF MEDIUM AND LARGE PARTICLES, W=VD.            00018960
C                                                                       00018970
      READ (IRD,812) NPOL,ICT,VD1,W1,VD2,W2,XKT,GAMMA                   00018980
C                                                                       00018990
      IF(NPOL.LT.1 .OR. NPOL.GT.2) NPOL=1                               00019000
      IF(NPOL.EQ.1 .OR. NCSOPT.EQ.0) GO TO 116                          00019010
      WRITE(IWR,635)                                                    00019020
      NCSOPT=0                                                          00019030
  116 IF(W1.GT.VD1) W1=VD1                                              00019040
      IF(NPOL.EQ.2) GO TO 117                                           00019050
      VD2=0.0                                                           00019060
      W2=0.0                                                            00019070
      GO TO 118                                                         00019080
  117 IF(W2.GT.VD2) W2=VD2                                              00019090
  118 IF(ICT.EQ.1) GO TO 119                                            00019100
      XKT=0.0                                                           00019110
      GAMMA=0.0                                                         00019120
      GO TO 122                                                         00019130
  119 IF(XKT.GE.0.1 .AND. XKT.LE.100.) GO TO 120                        00019140
      TXKT=0.1                                                          00019150
      IF(XKT.GT.100.) TXKT=100.                                         00019160
      WRITE(IWR,640) XKT,TXKT                                           00019170
      XKT=TXKT                                                          00019180
C                                                                       00019190
C    CONVERT CHEMICAL TRANSFORMATION RATE XKT (PERCENT PER HOUR) TO     00019200
```

```
C     THE EQUIVALENT TIME SCALE TAUC (SECONDS).
  120 TAUC=0.36E06/XKT
C
  122 IF(NCSOPT.EQ.0 .OR. (LX.LE.25 .AND. LY.LE.25)) GO TO 125
      WRITE(IWR,645)
      NCSOPT=0
C
C     SHIFT THE RECEPTOR GRID TO THE COMPUTATION GRID.
  125 XSWC= XRSWC - 0.5*GRID
      YSWC= YRSWC - 0.5*GRID
C
  130 IF(DTDZ(1).LT.0.00001) DTDZ(1)=0.020
      IF(DTDZ(2).LT.0.00001) DTDZ(2)=0.035
C
C  IF GRID IS ZERO, SWITCH ON AUTOMATIC GRID OPTION.
      IGRID=0
      IF(GRID.LT.1.0E-5) IGRID=1
      IF(IGRID.EQ.1.AND.NTOPT.GT.1) GO TO 520
C
C **** READ 5TH CONTROL PARAMETER CARD (AREA SOURCE SCALING,CALIBRATION)
C
C     ASCALE(1&2) = AREA SOURCE EMISSION SCALING FACTORS
C                   FOR EACH POLLUTANT.
C     A(1&2)      = CONCENTRATION CALIBRATION FACTOR (INTERCEPT)
C                   FOR EACH POLLUTANT.
C     B(1&2)      = CONCENTRATION CALIBRATION FACTOR (SLOPE)
C                   FOR EACH POLLUTANT.
C
  135 READ(IRD,815) ASCALE,A(1),B(1),A(2),B(2)
C
      IF(ASCALE(1).LE.0.) ASCALE(1)=1.0
      IF(ASCALE(2).LE.0.) ASCALE(2)=1.0
C
C  **** READ CARD 6 (POLLUTANT AND CALIBRATION LABELS)
C
      READ(IRD,817)(POLNAM(I,1),I=1,3),(CALNAM(I,1),I=1,7),
     1             (POLNAM(I,2),I=1,3),(CALNAM(I,2),I=1,7)
C
C  **** READ ONE TO 24 SCENARIO PARAMETER CARDS.
C
C     NSC       = STABILITY CLASS NUMBER (1 TO 7)
C     NWS       = WIND SPEED CLASS NUMBER (1 TO 6)
C     NWD       = WIND SECTOR NUMBER (1 TO 16)
C     WS        = WIND SPEED (M/S)
C     WD        = WIND DIRECTION (DEGREES)
C     TA        = AMBIENT TEMPERATURE (DEGREES CELSIUS)
C     PEN       = INVERSION PENETRATION FACTOR (PEN .GE. 1.0)
C     HMIX      = MIXING HEIGHT (METERS)
C
      DO 150 IS=1,NSCEN
      READ(IRD,820)NSC(IS),NWS(IS),NWD(IS),WS(IS),WD(IS),TA(IS),
     1 PEN(IS),HMIX(IS)
C
      IF(NSC(IS).GE.1 .AND. NSC(IS).LE.7) GO TO 140
      NUM=1
      IF(NSC(IS).GT.7) NUM=7
      WRITE(IWR,535) IS,NSC(IS),NUM
      NSC(IS)=NUM
  140 IF(NWSOPT.EQ.0) GO TO 142
      IF(NWS(IS).GE.1 .AND. NWS(IS).LE.6) GO TO 144
      NUM=1
      IF(NWS(IS).GT.6) NUM=6
      WRITE(IWR,545) IS,NWS(IS),NUM
      NWS(IS)=NUM
      GO TO 144
  142 IF(WS(IS).GT.0.) GO TO 144
      WRITE(IWR,565) IS,WS(IS)
      WS(IS)=1.0
  144 IF(NWDOPT.NE.1) GO TO 146
      IF(NWD(IS).GE.1 .AND. NWD(IS).LE.16) GO TO 146
      NUM=1
      IF(NWD(IS).GT.16) NUM=16
      WRITE(IWR,555) IS,NWD(IS),NUM
      NWD(IS)=NUM
  146 IF(PEN(IS).LT.1.0) PEN(IS)=2.0
      IF(HMIX(IS).LT.1.0E-5) HMIX(IS)= 9999.9
  150 CONTINUE
```

```
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) NWSOPT
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) DTDZ(1),DTDZ(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(ICT.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(NWSOPT.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
```

```
C
C  **** READ UP TO 50 AREA SOURCE CARDS.
C
C    XA,YA    = COORDINATES OF SOUTHWEST CORNER OF AREA SOURCE (KM).
C    SIZE     = LENGTH OF A SIDE OF AREA SOURCE (M).
C    EA(1&2)  = EMISSION RATES OF 2 POLLUTANTS (G/S).
C
      WRITE(IWR,990) TT
      NAS=1
      SUMAQ(1)=0.
      SUMAQ(2)=0.
      SUMAR(1)=0.
      SUMAR(2)=0.
C
170   READ(IRD,825)XA(NAS),YA(NAS),SIZE(NAS),EA(NAS,1),EA(NAS,2)
C
      IF(NPOL.EQ.1) EA(NAS,2)=0.0
      IF((SIZE(NAS)+EA(NAS,1)+EA(NAS,2)).LT.1.0E-04) GO TO 180
      IF(SIZE(NAS).GE.1.0E-4) GO TO 172
      SIZE(NAS)=1.0E-4
      IF(GRID.NE.0.) SIZE(NAS)=GRID*1000.
      WRITE(IWR,585) NAS,SIZE(NAS)
172   DO 175 K=1,2
      EAR(K)=EA(NAS,K)
      SUMAR(K)=SUMAR(K)+EAR(K)
      EA(NAS,K)= EA(NAS,K)*ASCALE(K)
175   SUMAQ(K)=SUMAQ(K)+EA(NAS,K)
C
C   PRINT INPUT PARAMETERS FOR THIS AREA SOURCE
      WRITE(IWR,992)NAS,XA(NAS),YA(NAS),SIZE(NAS),EAR(1),EA(NAS,1),
     1EAR(2),EA(NAS,2)
C
      SIZE(NAS)=SIZE(NAS)*0.001
      IF(NAS/50*50.EQ.NAS) WRITE(IWR,990)TT
      NAS=NAS+1
      GO TO 170
180   NAS=NAS-1
      WRITE(IWR,994) SUMAR(1),SUMAQ(1),SUMAR(2),SUMAQ(2)
C
C   IF AREA SOURCE CALCULATIONS ARE TO BE MADE, THEN DEPOSITION VELOCITY
C    VALUE(S) MUST BE GREATER THAN ZERO
      IF(NAS.LT.1) GO TO 184
      IF(VD1.GT.0.) GO TO 181
      WRITE(IWR,655) AMSG(1)
      VD1=0.01
181   IF(NPOL.EQ.1 .OR. VD2.GT.0.) GO TO 184
      WRITE(IWR,655) AMSG(2)
      VD2=0.01
C
C
C  **** READ UP TO 300 POINT SOURCES
C
C    XP,YP    = COORDINATES OF POINT SOURCE (KM).
C    EP(1&2)  = EMISSION RATES OF 2 POLLUTANTS (G/S).
C    HP       = SOURCE HEIGHT (M).
C    DP       = INSIDE DIAMETER (M).
C    VP       = VELOCITY (M/S).
C    TP       = TEMPERATURE (DEGREES CELSIUS).
C    NAME     = IDENTIFICATION.
C
184   WRITE(IWR,980) TT
      NPS=1
      SUMPQ(1)=0.
      SUMPQ(2)=0.
C
185   IF(INPTSC.EQ.2)READ(IDSK,830)XP(NPS),YP(NPS),EP(NPS,1),EP(NPS,2),
     1 HP(NPS),DP(NPS),VP(NPS),TP(NPS),NAME(1),NAME(2)
      IF(INPTSC.EQ.1) READ(IRD,830)XP(NPS),YP(NPS),EP(NPS,1),EP(NPS,2),
     1 HP(NPS),DP(NPS),VP(NPS),TP(NPS),NAME(1),NAME(2)
C
      IF(NPOL.EQ.1) EP(NPS,2)=0.0
      IF(HP(NPS)+DP(NPS)+VP(NPS)+TP(NPS).LT.1.0E-4) GO TO 190
      IF(DP(NPS).GT.0.0) GO TO 187
      WRITE(IWR,575) NPS
      DP(NPS)=1.0E-4
C
C  PRINT INPUT PARAMETERS FOR THIS POINT SOURCE
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  187 WRITE(IWR,984) NPS,NAME(1),NAME(2),XP(NPS),YP(NPS),EP(NPS,1),
     1 EP(NPS,2),HP(NPS),DP(NPS),VP(NPS),TP(NPS)
C
      TP(NPS)=TP(NPS)+273.15
      IF(NPS/50*50.EQ.NPS) WRITE(IWR,980)TT
      SUMPQ(1)=SUMPQ(1)+EP(NPS,1)
      SUMPQ(2)=SUMPQ(2)+EP(NPS,2)
      NPS=NPS+1
      GO TO 185
  190 NPS= NPS-1
      WRITE(IWR,986) SUMPQ(1),SUMPQ(2)
C
C   IF THERE WERE SERIOUS ERRORS IN INPUT PARAMETERS, STOP
      IF(ISTOP.EQ.0) GO TO 195
      WRITE(IWR,630)
      STOP
C
C   INITIALIZE FOR FIRST CALL TO INMOD FOR SCENARIO PREPARATION
  195 IWDOPT= 0
      ISCEN=0
      RETURN
C
C
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.
C
  300 IF(NWDOPT.LE.1) GO TO 350
      IF(ISCEN.EQ.0.OR.IWDOPT.GE.4) GO TO 320
      IWDOPT= IWDOPT + 1
      WD(ISCEN)= WD(ISCEN) + WDINC(NWDOPT-1)
      IF(WD(ISCEN).GE.6.2831853) WD(ISCEN)=WD(ISCEN) - 6.2831853
      GO TO 353
  320 ISCEN= ISCEN + 1
      IWDOPT= 1
      GO TO 353
  350 ISCEN= ISCEN + 1
  353 ISC=NSC(ISCEN)
      IWD=NWD(ISCEN)
      D47= DCR(ISCEN,1)
      D80= DCR(ISCEN,2)
      D8047= D80 - D47
      IF(NCSOPT.EQ.0) GO TO 400
      DO 380 I=1,25
      DO 380 J=1,25
      DO 380 K=1,5
      NWORST(I,J,K)=0
  380 CWORST(I,J,K)=0.
  400 RETURN
C
C   ERROR MESSAGES
C
  500 WRITE(IWR,505)
  505 FORMAT(1H0,'WHEN TIME AVG OPTION NTOPT=2, NUMBER OF SCENARIOS MUST
     1 =24')
      ISTOP=1
      GO TO 10
  510 WRITE(IWR,515) NSCEN
  515 FORMAT(1H0,'MAXIMUM NUMBER OF SCENARIOS ALLOWED IS 24. NSCEN=',I4)
      ISTOP=1
      GO TO 20
  520 WRITE(IWR,525)
  525 FORMAT(1H0,'AUTOGRID MAY NOT BE USED WITH TIME AVG OPTION NTOPT>1'
     1)
      ISTOP=1
      GO TO 135
  535 FORMAT(1H0,'IN SCENARIO',I3,' STABILITY CLASS NUMBER NSC=',I2,
     1' IS OUT OF RANGE.  NSC SET TO',I2)
  545 FORMAT(1H0,'IN SCENARIO',I3,' WIND SPEED CLASS NUMBER NWS=',I2,
     1' IS OUT OF RANGE.  NWS SET TO',I2)
  555 FORMAT(1H0,'IN SCENARIO',I3,' WIND DIRECTION SECTOR NUMBER NWD=',
     1 I3,' IS OUT OF RANGE.  NWD SET TO',I3)
  565 FORMAT(1H0,'IN SCENARIO',I3,' SPECIFIED WIND SPEED MUST BE GREATER
     1 THAN ZERO.  WS SET TO 1.0 M/S')
  575 FORMAT(1H0,'POINT SOURCE',I4,':  INSIDE DIAMETER MUST BE GREATER T
     1HAN ZERO.  DP SET TO .0001 M')
  585 FORMAT(1H0,'AREA SOURCE',I3,':  LENGTH OF SIDE MUST BE GREATER THA
     1N ZERO.  SIZE SET TO ',F9.2)
  600 FORMAT(1H0,'RUN REQUESTED WOULD PRODUCE OVER 10000 RECORDS ON TAPE
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     1'/' OUTPUT OPTION NTAPE HAS BEEN SET TO ZERO')                    00022290
  605 FORMAT(1H0,'OUTPUT OPTION NLIST MAY NOT BE USED WITH AUTOMATIC WIN00022300
     1D SHIFT OPTION (NWDOPT>1)'/' NLIST HAS BEEN SET TO ZERO')         00022310
  615 FORMAT(1H0,'AUTOMATIC WIND SHIFT OPTION (NWDOPT>1) MAY NOT BE USED00022320
     1 WITH TIME AVG OPTION NTOPT>1'/' NWDOPT HAS BEEN SET TO ZERO')    00022330
  620 FORMAT(1H0,'OUTPUT OPTION NTAPE MAY NOT BE USED WITH AUTOMATIC WIN00022340
     1D SHIFT OPTION (NWDOPT>1)'/' NTAPE HAS BEEN SET TO ZERO')         00022350
  630 FORMAT(1H1//' SERIOUS ERROR(S) IN INPUT PARAMETERS',5X,           00022360
     1 'RUN CANNOT BE CONTINUED')                                       00022370
  635 FORMAT(1H0,'CONTROL STRATEGY OUTPUT OPTION NCSOPT MAY NOT BE USED 00022380
     1WITH TWO POLLUTANTS'/' NCSOPT HAS BEEN SET TO ZERO')              00022390
  640 FORMAT(1H0,'CHEMICAL TRANSFORMATION RATE XKT=',F7.3,' IS OUT OF RA00022400
     1NGE'/' XKT HAS BEEN SET TO',F8.3)                                 00022410
  645 FORMAT(1H0,'CONTROL STRATEGY OUTPUT OPTION NCSOPT MAY NOT BE USED 00022420
     1WHEN NUMBER OF COLUMNS OR ROWS IN RECEPTOR GRID IS GREATER THAN 2500022430
     2'/' NCSOPT HAS BEEN SET TO ZERO')                                 00022440
  655 FORMAT(1H0,'AREA SOURCE CALCULATIONS REQUIRE DEPOSITION VELOCITY G00022450
     1REATER THAN ZERO.',4X,A4,'HAS BEEN SET TO 0.01')                  00022460
  660 FORMAT(1H0,'TIME AVERAGING OPTION NTOPT=',I2,' IS OUT OF RANGE.  N00022470
     1TOPT SET TO 1')                                                   00022480
C                                                                       00022490
C   INPUT FORMATS                                                       00022500
C                                                                       00022510
  800   FORMAT(20A4)                                                    00022520
  805   FORMAT(13I5)                                                    00022530
  810   FORMAT(2F10.0,2I10,3F10.0)                                      00022540
  812   FORMAT(2I5,6F10.0)                                              00022550
  815   FORMAT(6F10.0)                                                  00022560
  817   FORMAT(3A4,7A4,3A4,7A4)                                         00022570
  820   FORMAT(3I5,5F10.0)                                              00022580
  825   FORMAT(5F10.0)                                                  00022590
  830   FORMAT(8F9.0,2A4)                                               00022600
C                                                                       00022610
C   OUTPUT FORMATS                                                      00022620
C                                                                       00022630
  900 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT CONTROL PARA00022640
     1METERS:  ',20A4//)                                                00022650
  902 FORMAT(10X,'AVERAGING TIME OPTION: NTOPT=',I1//                   00022660
     1 18X,'A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR'//  00022670
     2 13X,'1  1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO'/00022680
     3 13X,'2  24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE 00022690
     4AVERAGED'/13X,'3  VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN 00022700
     5NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED'//)                    00022710
  904 FORMAT(10X,'WIND DIRECTION OPTION: NWDOPT=',I1//                  00022720
     113X,'0  DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO'/  00022730
     213X,'1  SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO'/         00022740
     312X,'2-7 DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOU00022750
     4R SUB-SCENARIOS.'/17X,'FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRE00022760
     5CTION IS AUTOMATICALLY INCREASED'/17X,'BY 90,45,30,15,10,OR 5 DEGR00022770
     6EES, DEPENDING ON THE OPTION NUMBER SELECTED.'//)                 00022780
  906 FORMAT(10X,'WIND SPEED OPTION: NWSOPT=',I1//                      00022790
     113X,'0  SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO'/          00022800
     213X,'1  WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO'00022810
     3//)                                                               00022820
  908 FORMAT(10X,'NUMBER OF SCENARIOS: NSCEN=',I2//)                    00022830
  910 FORMAT(10X,'STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=',I1//    00022840
     1 13X,'0  ALGORITHM IS IN EFFECT'/                                 00022850
     2 13X,'1  ALGORITHM IS NOT USED'//)                                00022860
  914 FORMAT(10X,'AUTOMATIC RECEPTOR GRID OPTION IS IN EFFECT'//)       00022870
  916 FORMAT(10X,'RECEPTOR GRID:',                                      00022880
     16X,'COLUMNS: LX=',I3,4X,'ROWS: LY=',I3/                           00022890
     230X,'SPACING: GRID=',F7.3,' KM'/                                  00022900
     330X,'SOUTHWEST CORNER    XRSWC= ',F8.3,' KM W'/                   00022910
     450X,'YRSWC= ',F8.3,' KM S'//)                                     00022920
  920 FORMAT(10X,'POTENTIAL TEMPERATURE GRADIENT: DTDZ(1)= ',F7.3,      00022930
     1' DEG/M    STABILITY CLASS E'/                                    00022940
     242X,'DTDZ(2)= ',F7.3,' DEG/M    STABILITY CLASS F'//)             00022950
  921 FORMAT(1H+,85X,7A4)                                               00022960
  922 FORMAT(10X,'NUMBER OF POLLUTANTS: NPOL=',I1/                      00022970
     1 51X,'POLLUTANT-1: ',3A4)                                         00022980
  923 FORMAT(1H+,85X,'POLLUTANT-2: ',3A4)                               00022990
  924 FORMAT(/10X,'AREA SOURCE SCALING FACTOR:',17X,'ASCALE=',F9.3)     00023000
  925 FORMAT(10X,'CALIBRATION COEFFICIENTS:',                           00023010
     1 16X,'A=',F10.3,'  B=',F10.3)                                     00023020
  926 FORMAT(1H+,85X,'A=',F10.3,'  B=',F10.3)                           00023030
  927 FORMAT(10X,'CALIBRATION IDENTIFICATION:',14X,7A4,6X,7A4)          00023040
  928 FORMAT(10X,'DEPOSITION VELOCITY (CM/S):',20X,'VD1=',F8.3)         00023050
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929 FORMAT(10X,'SETTLING VELOCITY (CM/S):',23X,'W1=',F8.3)
930 FORMAT(//10X,'CHEMICAL TRANSFORMATION OPTION: ICT=',I1/)
931 FORMAT(1H+,91X,'VD2=',F8.3)
932 FORMAT(13X,'NPOL=1'/
   215X,'ICT=0  CHEMICAL TRANSFORMATION LOSS OF POLLUTANT IS IGNORED'/
   315X,'ICT=1  FIRST-ORDER CHEMICAL TRANSFORMATION LOSS OF POLLUTANT
   4IS CONSIDERED'//)
933 FORMAT(1H+,92X,'W2=',F8.3)
934 FORMAT(13X,'NPOL=2'/
   215X,'ICT=0  CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED'
   3/15X,'ICT=1  FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO
   4 POLLUTANT-2 IS CONSIDERED'//)
935 FORMAT(1H+,88X,'ASCALE=',F9.3)
936 FORMAT(10X,'CHEMICAL TRANSFORMATION RATE: XKT=',F7.3,
   1' PERCENT/HR'/)
938 FORMAT(10X,'RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO
   1 POLLUTANT-1 (REACTANT): GAMMA=',F6.3/)
940 FORMAT(//9X,'OUTPUT OPTIONS SELECTED:'/)
942 FORMAT(13X,'NLIST=',I1,3X,'LISTS OF CONCENTRATION AND SURFACE DEPO
   1SITION FLUX AT EACH RECEPTOR IN THE GRID,'/24X,'ONE COLUMN PER PAG
   2E')
944 FORMAT(13X,'NARRAY=',I1,2X,'MAPS OF CONCENTRATION AND SURFACE DEPO
   1SITION FLUX AT EACH RECEPTOR IN THE GRID,')
946 FORMAT(24X,'CALIBRATED AND UNCALIBRATED')
948 FORMAT(24X,'UNCALIBRATED ONLY')
950 FORMAT(24X,'CALIBRATED ONLY')
952 FORMAT(13X,'NTAPE=',I1,3X,'TAPE CONTAINING COORDINATES, CONCENTRAT
   1ION, AND SURFACE DEPOSITION FLUX'/24X,'AT EACH RECEPTOR IN THE GRI
   2D'/13X,'INTER=',I2,2X,'INTERVAL OF RECEPTORS WHICH WILL BE WRITTEN
   3 ON TAPE')
954 FORMAT(13X,'NCSOPT=',I1,2X,'LIST OF POINT SOURCE CULPABILITY FOR C
   1ONCENTRATION AND SURFACE DEPOSITION FLUX'/24X,'AT EACH RECEPTOR IN
   2 THE GRID')
956 FORMAT(13X,'NPRINT=',I1,2X,'LIST OF POINT SOURCE PARAMETERS AND EF
   1FECTIVE STACK HEIGHTS'/24X,'PRINTED AT BEGINNING OF EACH SCENARIO'
   2)
958 FORMAT(13X,'NMAX=',I1,4X,'LIST OF RECEPTORS WITH HIGHEST CONCENTRA
   1TION AND SURFACE DEPOSITION FLUX'/24X,'FOR EACH SCENARIO - PRINTED
   2 AT END OF RUN')
960 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT SCENARIO PAR
   1AMETERS:  ',20A4//26X,'WIND DIRECTIONS',27X,'WIND SPEED CLASSES',
   212X,'STABILITY CLASSES'/)
962 FORMAT(10X,'SECTOR    DIRECTION',6X,'SECTOR    DIRECTION',9X,
   1'CLASS   SPEED    CLASS',15X,'CLASS'/
   210X,'NUMBER',8X,'(DEG)',6X,'NUMBER',8X,'(DEG)',9X,'INDEX   (M/S)
   3 INTERVAL(KT)',9X,'INDEX   CLASS'//13X,'1    N',7X,'0.0',9X,'9
   4S',5X,'180.0'/13X,'2    NNE    22.5',8X,'10    SSW    202.5',11X,
   5'1',6X,'1.50',7X,'0-3',16X,'1',7X,'A'/13X,'3    NE',5X,'45.0',8X,
   6'11    SW    225.0',11X,'2',6X,'2.46',7X,'4-6',16X,'2',7X,'B')
963 FORMAT(13X,'4    ENE    67.5',8X,'12    WSW    247.5',11X,'3',6X,
   1'4.47',7X,'7-10',15X,'3',7X,'C'/13X,'5    E',6X,'90.0',8X,'13    W
   2',5X,'270.0',11X,'4',6X,'6.93',6X,'11-16',15X,'4',7X,'DD (DAY)'/
   313X,'6    ESE    112.5',8X,'14    WNW    292.5',11X,'5',6X,'9.61',
   46X,'17-21',15X,'5',7X,'DN (NIGHT)'/13X,'7    SE    135.0',8X,'15
   5  NW    315.0',11X,'6',5X,'12.52    OVER 21',15X,'6',7X,'E'/
   613X,'8    SSE    157.5',8X,'16    NNW    337.5',48X,'7',7X,'F'///)
964 FORMAT(5X,'SCENARIO',3X,'STABILITY',3X,'WIND SPEED',5X,'WIND',8X,
   1'WIND',6X,'WIND',8X,'AMBIENT',9X,'INVERSION',8X,'MIXING'/
   26X,'NUMBER',6X,'CLASS',7X,'CLASS',8X,'SPEED',6X,'SECTOR',3X,
   3'DIRECTION',3X,'TEMPERATURE',3X,'PENETRATION FACTOR',3X,'HEIGHT'/
   443X,'(M/S)',17X,'(DEG)',7X,'(DEG C)',27X,'(M)'/)
966 FORMAT(8X,I2,10X,A2)
970 FORMAT(1H+,31X,I1)
972 FORMAT(1H+,42X,F6.3)
974 FORMAT(1H+,55X,I2)
978 FORMAT(1H+,63X,F6.2,7X,F7.2,11X,F6.3,8X,F7.1)
980 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT POINT SOURCE
   1 PARAMETERS:  ',20A4///
   26X,'POINT SOURCE',10X,'COORDINATES',9X,'EMISSION RATE',
   36X,'EMISSION RATE',5X,'HEIGHT',4X,'DIAMETER',4X,'EXIT VEL',5X,
   4'EXIT TEMP'/5X,'NUMBER',3X,'LABEL',7X,'X(KM)',5X,'Y(KM)',6X,
   5'POLLUTANT-1 (G/S)',2X,'POLLUTANT-2 (G/S)',3X,'(M)',8X,'(M)',8X,
   6'(M/S)',8X,'(DEG C)'/)
984 FORMAT(6X,I3,3X,2A4,3X,F8.2,2X,F8.2,10X,F9.3,10X,F9.3,6X,F6.2,5X,
   1F6.3,6X,F7.3,6X,F8.3)
986 FORMAT(1H0,5X,'SUMS OF THE POINT SOURCE EMISSION RATES',6X,F9.3,
   1' G/S',6X,F9.3,' G/S')
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  990 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT AREA SOURCE
     1PARAMETERS:  ',20A4///
     270X,'POLLUTANT-1',17X,'POLLUTANT-2'/5X,'AREA SOURCE',8X,
     3'COORDINATES',9X,'LENGTH OF SIDE',11X,'EMISSION RATE',15X,
     4'EMISSION RATE'/
     57X,'NUMBER',9X,'X(KM)',5X,'Y(KM)',13X,'(M)',12X,'INPUT (G/S)',
     64X,'SCALED',7X,'INPUT (G/S)',4X,'SCALED'/)
  992 FORMAT(9X,I2,8X,F8.2,2X,F8.2,10X,F8.2,9X,F9.3,4X,F9.3,6X,
     1 F9.3,4X,F9.3)
  994 FORMAT(1H0,5X,'SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN'
     1,8X,F9.3,4X,F9.3,6X,F9.3,4X,F9.3)
      END
C
C
      SUBROUTINE OUTMOD
C                          SUBROUTINE OUTMOD (VERSION 82360), PART OF PEM.
C
C
C     SUBROUTINE OUTMOD COORDINATES OUTPUT OF THE CONCENTRATION(S)
C     AND SURFACE DEPOSITION FLUX(ES) CALCULATED FOR EACH RECEPTOR
C     IN THE GRID FOR EACH SCENARIO.
C     ON OPTION, THE OUTPUT MAY BE IN THE FORM OF LISTS, ARRAY
C     MAPS, OR TAPE.
C     OUTMOD CALLS SUBROUTINE SCENMX TO DETERMINE AND STORE THE
C     RECEPTORS WITH MAXIMUM CONCENTRATION(S) AND SURFACE DEPOSITION
C     FLUX(ES) FOR THE SCENARIO.
C
C
C *** PEM MODIFICATIONS AND FORMATS BY MARTHA M. STEVENS,
C     NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830
C     DECEMBER 1982
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC
      DIMENSION CON(2),CALCON(2),SD(2),CALSD(2)
C
C
      WOUT= WD(ISCEN)*180./3.1415927
C
C   CONTROL STRATEGY RESULTS OUTPUT BY SUBROUTINE WOROUT
      IF(NCSOPT.GT.0.AND.NTOPT.EQ.1) CALL WOROUT
C
C  PRINT AND/OR WRITE-ON-TAPE LISTS OF CONCENTRATION(S) AND
C     SURFACE DEPOSITION FLUX(ES)
      IF(NLIST.EQ.0 .AND. NTAPE.EQ.0) GO TO 350
      IF(NTAPE.EQ.1) WRITE(ITA,900)TT
      NREP=0
C
C  BEGIN LOOP ON COLUMNS
  100 DO 325 I=1,LX
      IF(NLIST.EQ.0) GO TO 250
      ISKIP=0
      DO 125 JM=1,LY
      DO 125 KM=1,2
      IF(CONC(I,JM,KM).NE.0.) GO TO 130
  125 CONTINUE
      ISKIP=1
      IF(NTAPE.EQ.0) GO TO 325
      GO TO 250
  130 IF(NREP.EQ.1) GO TO 150
      WRITE(IWR,905)TT,ISCEN,SCLAB(ISC),WS(ISCEN),WOUT,
     1 HMIX(ISCEN),IAV
      WRITE(IWR,910)(CALNAM(L,1),L=1,7),(CALNAM(L,2),L=1,7),
     1 (POLNAM(L,1),L=1,3),(POLNAM(L,2),L=1,3),(POLNAM(L,1),L=1,3),
     2 (POLNAM(L,2),L=1,3)
```

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      GO TO 250                                                         00024600
  150 WRITE(IWR,907) TT,ISCEN,SCLAB(ISC),WS(ISCEN),WOUT,                00024610
     1 HMIX(ISCEN),IAV                                                  00024620
      WRITE(IWR,912) (CALNAM(L,1),L=1,7), (CALNAM(L,2),L=1,7),          00024630
     1 (POLNAM(L,1),L=1,3),(POLNAM(L,2),L=1,3),(POLNAM(L,1),L=1,3),     00024640
     2 (POLNAM(L,2),L=1,3)                                              00024650
C                                                                       00024660
  250 XI=I                                                              00024670
      X=XSWC+(XI-0.5)*GRID                                              00024680
C  BEGIN LOOP ON ROWS IN THIS COLUMN                                    00024690
      DO 300 J=1,LY                                                     00024700
      YJ=J                                                              00024710
      Y=YSWC+(YJ-0.5)*GRID                                              00024720
C                                                                       00024730
C  INITIALIZE CONCENTRATION AND SDF VARIABLES                           00024740
      DO 260 K=1,2                                                      00024750
      CON(K)=0.                                                         00024760
      CALCON(K)=0.                                                      00024770
      SD(K)=0.                                                          00024780
      CALSD(K)=0.                                                       00024790
  260 CONTINUE                                                          00024800
C  SET CONCENTRATION AND SDF - APPLY CALIBRATION COEFFICIENTS           00024810
      DO 280 K=1,NPOL                                                   00024820
      IF(NREP.EQ.1) GO TO 270                                           00024830
      CON(K)=CONC(I,J,K)                                                00024840
      CALCON(K)= A(K) + B(K) * CON(K)                                   00024850
  270 SD(K)=SDF(I,J,K)                                                  00024860
      CALSD(K)= A(K) + B(K) * SD(K)                                     00024870
  280 CONTINUE                                                          00024880
C                                                                       00024890
      IF(NLIST.EQ.0 .OR. ISKIP.EQ.1) GO TO 290                          00024900
      IF(NREP.EQ.0) WRITE(IWR,970) I,J,X,Y,CON(1),CON(2),               00024910
     1 CALCON(1),CALCON(2)                                              00024920
      IF(NREP.EQ.1) WRITE(IWR,970) I,J,X,Y,SD(1),SD(2),                 00024930
     1 CALSD(1),CALSD(2)                                                00024940
  290 IF(NTAPE.EQ.0 .OR. NREP.EQ.1) GO TO 300                           00024950
      IF(((I-1)/INTER)*INTER.NE.(I-1).OR.((J-1)/INTER)*INTER.NE.        00024960
     1 (J-1)) GO TO 300                                                 00024970
      WRITE(ITA,975)X,Y,(CON(K),SD(K),CALCON(K),CALSD(K),K=1,2)         00024980
  300 CONTINUE                                                          00024990
  325 CONTINUE                                                          00025000
C                                                                       00025010
      IF(NLIST.EQ.0 .OR. NREP.EQ.1) GO TO 350                           00025020
C                                                                       00025030
C  IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT                       00025040
      IF(VD1.LE.0.01 .AND. VD2.LE.0.01) GO TO 350                       00025050
      NREP=1                                                            00025060
      GO TO 100                                                         00025070
C                                                                       00025080
C  PRINT ARRAY MAPS OF CONCENTRATIONS                                   00025090
  350 IF(NARRAY.GT.0) CALL ARRAY                                        00025100
C                                                                       00025110
C  DETERMINE MAXIMUM PREDICTED CONCENTRATION(S) FOR SCENARIO VIA SCENMX 00025120
      IF(NMAX.GT.0.AND.(NTOPT.EQ.1.OR.ISCEN.EQ.NSCEN)) CALL SCENMX      00025130
C                                                                       00025140
      RETURN                                                            00025150
C                                                                       00025160
  900 FORMAT(20A4)                                                      00025170
  905 FORMAT(1H1,'PEM OUTPUT:  PREDICTED CONCENTRATION:  ',             00025180
     120A4/' SCENARIO ',I2,', STABILITY=',A2,', WIND SPEED=',F5.2,' M/S,00025190
     2 WIND DIRECTION=',F6.2,' DEG, MIXING HEIGHT=',F7.1,' M, AVERAGING 00025200
     3TIME=',I3,' HR'//)                                                00025210
  907 FORMAT(1H1,'PEM OUTPUT:  PREDICTED SURFACE DEPOSITION FLUX:  ',   00025220
     120A4/' SCENARIO ',I2,', STABILITY=',A2,', WIND SPEED=',           00025230
     2F5.2,' M/S, WIND DIRECTION=',F6.2,' DEG, MIXING HEIGHT=',F7.1,    00025240
     3' M, AVERAGING TIME=',I3,' HR'//)                                 00025250
  910 FORMAT(33X,'UNCALIBRATED CONCENTRATION',11X,'CALIBRATED CONCENTRAT00025260
     1ION  POL-1: ',7A4/16X,'RECEPTOR',9X,'(MICROGRAMS PER CUBIC METER)'00025270
     2,9X,'CALIBRATED CONCENTRATION  POL-2: ',7A4/15X,'COORDINATES',7X, 00025280
     3'POLLUTANT-1',5X,'POLLUTANT-2',10X,'POLLUTANT-1',5X,'POLLUTANT-2'/00025290
     4' COL ROW',6X,'X(KM)',4X,'Y(KM)',5X,3A4,4X,3A4,9X,3A4,4X,3A4)     00025300
  912 FORMAT(32X,'UNCALIBRATED SURFACE DEPOSITION FLUX',4X,'CALIBRATED V00025310
     1ALUE  POLLUTANT-1: ',7A4/16X,'RECEPTOR',9X,'(MICROGRAMS PER SQ MET00025320
     2ER PER HOUR)',5X,'CALIBRATED VALUE  POLLUTANT-2: ',7A4/           00025330
     315X,'COORDINATES',7X,'POLLUTANT-1',5X,'POLLUTANT-2',12X,          00025340
     4'POLLUTANT-1',5X,'POLLUTANT-2'/' COL ROW',6X,'X(KM)',4X,'Y(KM)',  00025350
     55X,3A4,4X,3A4,11X,3A4,4X,3A4)                                     00025360
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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)                                                    00025380
2543            END                                                               00025390
2544      C                                                                       00025400
2545            SUBROUTINE ARRAY                                                  00025410
2546      C                                                                       00025420
2547      C                    SUBROUTINE ARRAY  (VERSION 82360), PART OF PEM.    00025430
2548      C                                                                       00025440
2549      C                                                                       00025450
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                                                                       00025510
2556      C                                                                       00025520
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                                                                       00025560
2561      C                                                                       00025570
2562            COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00025580
2563           1 XP(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,IDSK,         D80,D47,D8047,DIST,DELTA,              00025640
2569           7 ESH(2),PEAK,IBUOY,IRISE,IDWN,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,NCSOPT,NMAX,        00025670
2572           * NSTDWN,INTER,NPRINT                                              00025680
2573      C                                                                       00025690
2574            COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                          00025700
2575            DIMENSION X(50),CC(50),SSDF(50),DV(2)                             00025710
2576            INTEGER CC,SSDF                                                   00025720
2577      C                                                                       00025730
2578            DV(1)=VD1                                                         00025740
2579            DV(2)=VD2                                                         00025750
2580            WOUT= WD(ISCEN)*180./3.1415927                                    00025760
2581            NLX=1                                                             00025770
2582            NLY=1                                                             00025780
2583            IF(LX.GT.25) NLX=2                                                00025790
2584            IF(LY.GT.25) NLY=2                                                00025800
2585            NSECT=NLX*NLY                                                     00025810
2586      C                                                                       00025820
2587        100 ISECT=0                                                           00025830
2588            DO 700 JLX=1,NLX                                                  00025840
2589            MX2= JLX*25                                                       00025850
2590            IF(MX2.GT.LX) MX2=LX                                              00025860
2591            MX1=1                                                             00025870
2592            IF(JLX.EQ.2) MX1=26                                               00025880
2593            DO 125 I=MX1,MX2                                                  00025890
2594            XI=I                                                              00025900
2595        125 X(I)= XSWC + (XI-0.5)*GRID                                        00025910
2596            DO 600 JLY=1,NLY                                                  00025920
2597            ISECT=ISECT+1                                                     00025930
2598            IF(JLY.EQ.1) GO TO 150                                            00025940
2599            MY1=26                                                            00025950
2600            MY2=LY                                                            00025960
2601            GO TO 175                                                         00025970
2602        150 MY1=1                                                             00025980
2603            MY2=25                                                            00025990
2604            IF(LY.LT.25) MY2=LY                                               00026000
2605        175 DO 500 N=1,NPOL                                                   00026010
2606            NREP=0                                                            00026020
2607        180 IF(NARRAY.EQ.3) GO TO 320                                         00026030
2608            WRITE(IWR,900)ISECT,NSECT,ISCEN,TT                                00026040
2609            WRITE(IWR,902)SCLAB(ISC),WS(ISCEN),WOUT,HMIX(ISCEN),IAV,          00026050
2610           1          N,(POLNAM(L,N),L=1,3)                                   00026060
2611            IF(NREP.EQ.0) GO TO 185                                           00026070
2612      C    LOOP THROUGH SDF ARRAY TO FIND ANY VALUE GE 1000. IN THAT CASE,    00026080
2613      C    SET FLAG TO SCALE SDF VALUES AS THEY ARE SET IN SSDF ARRAY         00026090
2614            IFLAG=0                                                           00026100
2615            DO 182 NX=1,LX                                                    00026110
2616            DO 182 NY=1,LY                                                    00026120
2617            IF(SDF(NX,NY,N).GT.999.49) GO TO 184                              00026130
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  182 CONTINUE                                                          00026140
      WRITE(IWR,905)                                                    00026150
      GO TO 190                                                         00026160
  184 IFLAG=1                                                           00026170
      WRITE(IWR,910)                                                    00026180
      GO TO 190                                                         00026190
  185 WRITE(IWR,904)                                                    00026200
  190 WRITE(IWR,915) (X(I),I=MX1,MX2,2)                                 00026210
      DO 300 J=MY1,MY2                                                  00026220
      IY= MY2 + MY1 - J                                                 00026230
      Y=IY                                                              00026240
      Y= YSWC + (Y-0.5)*GRID                                            00026250
C                                                                       00026260
      IF(NREP.EQ.1) GO TO 240                                           00026270
      DO 230 I=MX1,MX2                                                  00026280
  230 CC(I)= CONC(I,IY,N) + 0.5                                         00026290
      WRITE(IWR,920)Y,(CC(I),I=MX1,MX2)                                 00026300
      GO TO 300                                                         00026310
  240 DO 250 I=MX1,MX2                                                  00026320
      IF(IFLAG.EQ.0) GO TO 245                                          00026330
      SSDF(I)=SDF(I,IY,N)*1.0E-03 + 0.5                                 00026340
      GO TO 250                                                         00026350
  245 SSDF(I)= SDF(I,IY,N) + 0.5                                        00026360
  250 CONTINUE                                                          00026370
      WRITE(IWR,920) Y,(SSDF(I),I=MX1,MX2)                              00026380
  300 WRITE(IWR,925)Y                                                   00026390
      WRITE(IWR,915)(X(I),I=MX1,MX2,2)                                  00026400
  320 IF(NARRAY.EQ.2) GO TO 450                                         00026410
      WRITE(IWR,900)ISECT,NSECT,ISCEN,TT                                00026420
      WRITE(IWR,902)SCLAB(ISC),WS(ISCEN),WOUT,HMIX(ISCEN),IAV,          00026430
     1          N,(POLNAM(L,N),L=1,3)                                   00026440
      IF(NREP.EQ.0) WRITE(IWR,906)(CALNAM(L,N),L=1,7),A(N),B(N)         00026450
      IF(NREP.EQ.1) WRITE(IWR,907) (CALNAM(L,N),L=1,7),A(N),B(N)        00026460
      WRITE(IWR,915)(X(I),I=MX1,MX2,2)                                  00026470
      DO 400 J=MY1,MY2                                                  00026480
      IY= MY2 + MY1 - J                                                 00026490
      Y=IY                                                              00026500
      Y= YSWC + (Y-0.5)*GRID                                            00026510
C                                                                       00026520
      IF(NREP.EQ.1) GO TO 340                                           00026530
      DO 330 I=MX1,MX2                                                  00026540
  330 CC(I)= A(N) + B(N)*CONC(I,IY,N) + 0.5                             00026550
      WRITE(IWR,920)Y,(CC(I),I=MX1,MX2)                                 00026560
      GO TO 400                                                         00026570
  340 DO 350 I=MX1,MX2                                                  00026580
  350 SSDF(I)= A(N) + B(N) * SDF(I,IY,N) + 0.5                          00026590
      WRITE(IWR,920) Y,(SSDF(I),I=MX1,MX2)                              00026600
  400 WRITE(IWR,925)Y                                                   00026610
      WRITE(IWR,915)(X(I),I=MX1,MX2,2)                                  00026620
  450 IF(NREP.EQ.1) GO TO 500                                           00026630
C   IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT                      00026640
      IF(DV(N).LE.0.01) GO TO 500                                       00026650
      NREP=1                                                            00026660
      GO TO 180                                                         00026670
  500 CONTINUE                                                          00026680
  600 CONTINUE                                                          00026690
  700 CONTINUE                                                          00026700
C                                                                       00026710
      RETURN                                                            00026720
C                                                                       00026730
  900 FORMAT(1H1,'PEM OUTPUT:  ','SECTION ',I1,' OF ',I1,', SCENARIO ', 00026740
     1 I2,2X,20A4)                                                      00026750
  902 FORMAT(' STABILITY=',A2,', WIND SPD=',F5.2,' M/S, WIND DIR=',F6.2,00026760
     1 ' DEG, MIXING HT=',F7.1,' M, AVERAGING TIME=',I3,' HR.',6X,      00026770
     2 'POLLUTANT-',I1,': ',3A4)                                        00026780
  904 FORMAT(' UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER')00026790
  905 FORMAT(' UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQU00026800
     1ARE METER PER HOUR')                                              00026810
  906 FORMAT(' CALIBRATED CONCENTRATION - ',7A4,18X,'CALIBRATION COEFFIC00026820
     1IENTS:  A =',F11.4,',  B =',F11.4)                                00026830
  907 FORMAT(' CALIBRATED SURFACE DEPOSITION FLUX - ',7A4,10X,          00026840
     1'CALIBRATION COEFFICIENTS:  A=',F10.4,5X,'B=',F10.4)              00026850
  910 FORMAT(' UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUA00026860
     1RE KILOMETER PER HOUR')                                           00026870
  915 FORMAT(1H0,14X,13F8.2)                                            00026880
  920 FORMAT(1H0,4X,F8.2,4X,25I4)                                       00026890
  925 FORMAT(1H+,122X,F8.2)                                             00026900
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```
      END
C
C
      SUBROUTINE WORST(I,J,CHI)
C                    SUBROUTINE WORST  (VERSION 82360), PART OF PEM.
C
C
C  SUBROUTINE WORST DETERMINES THE FIVE POINT SOURCES CONTRIBUTING THE
C    MOST TO THE TOTAL CONCENTRATION AT EACH RECEPTOR. SOURCE
C    IDENTIFICATIONS AND CONTRIBUTIONS ARE STORED IN NWORST AND CWORST
C    RESPECTIVELY, FOR OUTPUT BY SUBROUTINE WOROUT.
C
C
C *** PEM MODIFICATIONS BY M.M. STEVENS,
C     NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830
C     DECEMBER 1982
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,     UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)
C
C
      IF(CHI.LE.CWORST(I,J,5)) RETURN
      IF(CHI.GT.CWORST(I,J,4)) GO TO 205
      CWORST(I,J,5)= CHI
      NWORST(I,J,5)= IPS
      RETURN
  205 IF(CHI.GT.CWORST(I,J,3)) GO TO 210
      NW=1
      GO TO 225
  210 IF(CHI.GT.CWORST(I,J,2)) GO TO 215
      NW=2
      GO TO 225
  215 IF(CHI.GT.CWORST(I,J,1)) GO TO 220
      NW=3
      GO TO 225
  220 NW=4
  225 DO 250 IW=1,NW
      CWORST(I,J,6-IW)= CWORST(I,J,5-IW)
  250 NWORST(I,J,6-IW)= NWORST(I,J,5-IW)
      CWORST(I,J,5-NW)= CHI
      NWORST(I,J,5-NW)= IPS
      RETURN
      END
C
C
      SUBROUTINE WOROUT
C                    SUBROUTINE WOROUT (VERSION 82350), PART OF PEM.
C
C
C  SUBROUTINE WOROUT PRINTS A CULPABILITY LIST OF THE IDENTIFICATIONS
C    AND CONTRIBUTIONS OF THE FIVE POINT SOURCES CONTRIBUTING THE MOST
C    TO THE TOTAL CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH
C    RECEPTOR, USING DATA COMPILED BY SUBROUTINE WORST
C
C
C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS,
C     NOAA-ATDL, P.O. BOX E, OAK RIDGE, TN 37830
C     DECEMBER 1982
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
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     5 XSWC,YSWC,GRID,LX,LY,      A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,          D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,      UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)
C
C
      WOUT= WD(ISCEN)*180./3.1415927
      N=1
      IF(NTOPT.EQ.1) GO TO 250
      N=2
250   DO 400 I=1,LX
C     IF ALL CONCENTRATION VALUES ARE ZERO IN THIS COL, SKIP IT
      DO 275 JM=1,LY
      IF(CONC(I,JM,N).NE.0.) GO TO 280
275   CONTINUE
      GO TO 400
C
280   WRITE(IWR,905) TT,(POLNAM(L,1),L=1,3)
      WRITE(IWR,910) ISCEN,WOUT,WS(ISCEN),SCLAB(ISC),HMIX(ISCEN),IAV
      WRITE(IWR,915)
      XI=I
      X= XSWC + (XI-0.5)*GRID
      DO 400 J=1,LY
      IF(CONC(I,J,N).LT.1.0E-5) GO TO 303
      DO 300 L=1,5
300   CWORST(I,J,L)= CWORST(I,J,L)*100./CONC(I,J,N)
303   YJ=J
      Y= YSWC + (YJ-0.5)*GRID
      WRITE(IWR,925)I,J,X,Y,NWORST(I,J,1),CWORST(I,J,1),NWORST(I,J,2),
     1 CWORST(I,J,2),NWORST(I,J,3),CWORST(I,J,3),NWORST(I,J,4),
     2 CWORST(I,J,4),NWORST(I,J,5),CWORST(I,J,5),CONC(I,J,N),SDF(I,J,N)
400   CONTINUE
C
      RETURN
C
905   FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'OUTPUT:  ',20A4//
     14X,'LIST OF THE FIVE POINT SOURCES WHICH PRODUCE THE HIGHEST VALUE
     2S OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR'//
     34X,'POLLUTANT: ',3A4,'  -  CONCENTRATION IN MICROGRAMS PER CUBIC M
     4ETER'/32X,'SURFACE DEPOSITION FLUX IN MICROGRAMS PER SQUARE METER
     5PER HOUR'/)
910   FORMAT(4X,'SCENARIO',6X,'WIND DIRECTION',6X,'WIND SPEED',6X,'STABI
     1LITY CLASS',6X,'MIXING HEIGHT',6X,'AVERAGING TIME'/
     25X,'NUMBER',11X,'(DEG)',13X,'(M/S)',34X,'(M)',17X,'(HR)'/
     37X,I2,13X,F5.1,13X,F5.2,15X,A2,15X,F7.2,15X,I3/)
915   FORMAT(45X,'POINT SOURCE SEQUENCE NUMBER AND PERCENT'/
     115X,'COORDINATES',15X,'OF TOTAL CONCENTRATION AND SURFACE DEPOSITI
     2ON FLUX',14X,'TOTAL',8X,'TOTAL SURFACE'/
     3' COL ROW',4X,'X (KM)',4X,'Y (KM)',9X,'HIGHEST',6X,'SECOND',8X,
     4'THIRD',7X,'FOURTH',8X,'FIFTH',6X,'CONCENTRATION',3X,'DEPOSITION F
     5LUX'/)
925   FORMAT(2(2X,I2),3X,F8.2,2X,F8.2,3X,5(3X,I3,F7.2),6X,F8.2,9X,F8.2)
C
      END
C
C
      SUBROUTINE SCENMX
C                    SUBROUTINE SCENMX (VERSION 82360), PART OF PEM.
C
C
C  SUBROUTINE SCENMX LOCATES AND STORES THE COORDINATES, CONCENTRATION,
C  AND SURFACE DEPOSITION FLUX AT THE RECEPTOR GRID POINTS RECORDING
C  THE HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX OF EACH
C  POLLUTANT IN EACH SCENARIO.  STORED VALUES ARE PRINTED BY SUBROUTINE
C  MAXOUT AT THE END OF THE RUN.
C
C
C *** PEM MODIFICATIONS BY M.M. STEVENS,
C     NOAA-ATDL, P.O.BOX - E, OAK RIDGE, TN 37830
C     DECEMBER 1982
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
```

```
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,      A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,          D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,     UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/MAX/XMX(24,4,2),YMX(24,4,2),ZMX(24,4,2),SMX(24,4,2)
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC
C
C
      IF(NTOPT.EQ.1) GO TO 120
      I= 1
      GO TO 130
120   I= ISCEN
130   IF(NWDOPT.LE.1) GO TO 140
      J= IWDOPT
      GO TO 150
140   J= 1
150   DO 400 K=1,NPOL
      Z= 0.
      DO 350 NX=1,LX
      DO 350 NY=1,LY
      IF(CONC(NX,NY,K).LT.Z) GO TO 350
      Z= CONC(NX,NY,K)
      ZS=SDF(NX,NY,K)
      ZX=NX
      ZY=NY
350   CONTINUE
      ZMX(I,J,K)= Z
      SMX(I,J,K)=ZS
      XMX(I,J,K)= XSWC + (ZX - 0.5)*GRID
      YMX(I,J,K)= YSWC + (ZY - 0.5)*GRID
400   CONTINUE
      RETURN
      END
C
C
      SUBROUTINE MAXOUT
C                    SUBROUTINE MAXOUT (VERSION 82350), PART OF PEM.
C
C
C  SUBROUTINE MAXOUT PRINTS THE COORDINATES, CONCENTRATION, AND
C  SURFACE DEPOSITION FLUX AT THE RECEPTOR GRID POINTS RECORDING
C  THE HIGHEST CONCENTRATION OF EACH POLLUTANT IN EACH SCENARIO.
C  THESE VALUES WERE SELECTED AND STORED BY SUBROUTINE SCENMX.
C
C
C
C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS,
C     NOAA-ATDL, P.O.BOX E, OAK RIDGE, TN 37830
C     DECEMBER 1982
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,      A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,          D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,     UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/MAX/XMX(24,4,2),YMX(24,4,2),ZMX(24,4,2),SMX(24,4,2)
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC
      DIMENSION ZC(2),ZS(2)
C
C  CHECK WHETHER SURF DEP FLUX WAS CALCULATED AND SET FLAG
      NREP=1
      IF(VD1.LE.0.01 .AND. VD2.LE.0.01) NREP=0
```

```
C
      IF(NWDOPT.GT.1) GO TO 300
C
      J=1
      N=1
      IF(NTOPT.EQ.1) N=NSCEN
C   PRINT HIGHEST CONCENTRATIONS
      WRITE(IWR,900) TT
      WRITE(IWR,902) (CALNAM(L,1),L=1,7)
      IF(NPOL.EQ.2) WRITE(IWR,903) (CALNAM(L,2),L=1,7)
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)
      WRITE(IWR,912)
      WRITE(IWR,915)
      DO 200 I=1,N
      DO 120 K=1,NPOL
  120 ZC(K)= A(K) + B(K)*ZMX(I,1,K)
      WRITE(IWR,920)
      WRITE(IWR,925) I,J,(XMX(I,1,K),YMX(I,1,K),ZMX(I,1,K),ZC(K),
     1 K=1,NPOL)
  200 CONTINUE
C
C   PRINT SURFACE DEPOSITION FLUX VALUES
C   IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT
      IF(NREP.EQ.0) RETURN
      WRITE(IWR,900) TT
      WRITE(IWR,932) (CALNAM(L,1),L=1,7)
      IF(NPOL.EQ.2) WRITE(IWR,933) (CALNAM(L,2),L=1,7)
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)
      WRITE(IWR,942)
      WRITE(IWR,915)
      DO 250 I=1,N
      DO 220 K=1,NPOL
  220 ZS(K)= A(K) + B(K)*SMX(I,1,K)
      WRITE(IWR,920)
      WRITE(IWR,925) I,J,(XMX(I,1,K),YMX(I,1,K),SMX(I,1,K),ZS(K),
     1 K=1,NPOL)
  250 CONTINUE
C
      RETURN
C
C   PRINT FOR CASE OF NWDOPT>1 -  SUB-SCENARIOS
  300 N=NSCEN
C   PRINT HIGHEST CONCENTRATIONS
      DO 500 I=1,N
      IF(((I-1)/8)*8.NE.I-1) GO TO 310
      WRITE(IWR,900) TT
      WRITE(IWR,902) (CALNAM(L,1),L=1,7)
      IF(NPOL.EQ.2) WRITE(IWR,903) (CALNAM(L,2),L=1,7)
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)
      WRITE(IWR,912)
      WRITE(IWR,915)
  310 WRITE(IWR,920)
      DO 400 J=1,4
      DO 320 K=1,NPOL
  320 ZC(K)= A(K) + B(K)*ZMX(I,J,K)
      WRITE(IWR,925) I,J,(XMX(I,J,K),YMX(I,J,K),ZMX(I,J,K),ZC(K),
     1 K=1,NPOL)
  400 CONTINUE
  500 CONTINUE
C
C   PRINT SURFACE DEPOSITION FLUX VALUES
C   IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT
      IF(NREP.EQ.0) RETURN
      DO 600 I=1,N
      IF(((I-1)/8)*8.NE.I-1) GO TO 510
      WRITE(IWR,900) TT
      WRITE(IWR,932) (CALNAM(L,1),L=1,7)
      IF(NPOL.EQ.2) WRITE(IWR,933) (CALNAM(L,2),L=1,7)
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)
      WRITE(IWR,942)
      WRITE(IWR,915)
  510 WRITE(IWR,920)
      DO 550 J=1,4
```

```
      DO 520 K=1,NPOL
  520 ZS(K)= A(K) + B(K)*SMX(I,J,K)
      WRITE(IWR,925) I,J,(XMX(I,J,K),YMX(I,J,K),SMX(I,J,K),ZS(K),
     1 K=1,NPOL)
  550 CONTINUE
  600 CONTINUE
C
  700 RETURN
C
  900 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'OUTPUT:  ',20A4//)
  902 FORMAT(4X,'HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR E
     1ACH SCENARIO'//4X,'UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CU
     2BIC METER  -  CALIBRATION, POLLUTANT-1: ',7A4)
  903 FORMAT(65X,'CALIBRATION, POLLUTANT-2: ',7A4)
  910 FORMAT(//40X,'POLLUTANT-1: ',3A4)
  911 FORMAT(1H+,93X,'POLLUTANT-2: ',3A4)
  912 FORMAT(/' SCENARIO  WIND DIRECTION',7X,'COORDINATES',14X,
     1'CONCENTRATION',16X,'COORDINATES',14X,'CONCENTRATION')
  915 FORMAT(2X,'NUMBER',4X,'SUB-SCENARIO',6X,'X(KM)',5X,'Y(KM)',6X,
     1'UNCALIBRATED',4X,'CALIBRATED',7X,'X(KM)',5X,'Y(KM)',6X,
     2'UNCALIBRATED',4X,'CALIBRATED'/)
  920 FORMAT(1X)
  925 FORMAT(4X,I2,11X,I2,8X,F9.2,1X,F9.2,5X,F11.4,4X,F11.4,4X,F9.2,1X,
     1F9.2,5X,F11.4,4X,F11.4)
  932 FORMAT(4X,'HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLU
     1TANT FOR EACH SCENARIO'//4X,'UNCALIBRATED VALUES IN MICROGRAMS PER
     2 SQUARE METER PER HOUR  -  CALIBRATION, POLLUTANT-1: ',7A4)
  933 FORMAT(68X,'CALIBRATION, POLLUTANT-2: ',7A4)
  942 FORMAT(/' SCENARIO  WIND DIRECTION',7X,'COORDINATES',9X,
     1'SURFACE DEPOSITION FLUX',11X,'COORDINATES',9X,'SURFACE DEPOSITION
     2 FLUX')
      END
C
C
      SUBROUTINE RISE
C                    SUBROUTINE RISE   (VERSION 82360), PART OF PEM.
C
C
C  SUBROUTINE RISE CALCULATES PLUME RISE VIA ONE OF SIX EQUATIONS
C  (BRIGGS,1969). IF IRISE=1, DISTANCE DEPENDENT EFFECTIVE SOURCE
C  HEIGHT (ESH(1)) IS RETURNED. IF IRISE=2, MAXIMUM EFFECTIVE SOURCE
C  HEIGHT (ESH(2)) IS RETURNED. RISE IS CALLED ONCE PER SOURCE PER
C  SCENARIO WITH IRISE=2. IT IS CALLED WITH IRISE=1 WHENEVER THE
C  DOWNWIND DISTANCE (DIST) IS LESS THAN THE DISTANCE TO MAXIMUM
C  PLUME RISE (PEAK).
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,      A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      IDWN=1
      IF(IRISE.EQ.1) GO TO 300
      DWNWSH= 1.0
      IF(IBUOY.EQ.0) GO TO 205
      IF(EFF.GE.55.) GO TO 150
C
C XS,CTB, AND CTMU ARE INDEPENDENT OF DISTANCE, AND ARE THEREFORE
C  CALCULATED ONCE PER SOURCE PER SCENARIO (WHEN IRISE=2).
      XS= 49.*EFF**0.625
      GO TO 160
  150 XS=119.*EFF**0.4
  160 CTB= 1.6*UINV*EFF**0.333333
      IF(ISC.GE.6) GO TO 170
C
C PEAK PLUME RISE: BUOYANCY-DOMINATED PLUME, UNSTABLE AIR (A-D).
      DELTAH= CTB*XS**0.666667
      GO TO 250
C
```

```
C  PEAK PLUME RISE: BUOYANCY-DOMINATED PLUME, STABLE AIR (E,F).
170   DELTAH= 2.6*(EFF*UINV*TA(ISCEN)/(9.8*DTDZ(ISC-5)))**0.333333
      GO TO 250
205   IF(ISC.GE.6) GO TO 230
      CTMU= 1.89*(VP(IPS)*VP(IPS)*DP(IPS)*UINV/(VP(IPS)+3./UINV))**0.66600
     1667
C
C  PEAK PLUME RISE: MOMENTUM-DOMINATED PLUME, UNSTABLE AIR (A-D).
      DELTAH= 3.0*VP(IPS)*DP(IPS)*UINV
      GO TO 250
C
C  PEAK PLUME RISE: MOMENTUM-DOMINATED PLUME, STABLE AIR (E,F).
230   DELTAH= 1.5*(0.5*VP(IPS)*DP(IPS))**0.666667*UINV**0.333333
     1 *(TA(ISCEN)/(DTDZ(ISC-5)*9.8))**0.166667
250   IF(NSTDWN.EQ.1) GO TO 270
      IF(VP(IPS)*UINV.GT.1.5) GO TO 270
      CDELH= 2.0*(1.5 - VP(IPS)*UINV)*DP(IPS)
      IDWN=3
      IF(CDELH.GE.DELTAH) GO TO 260
      DWNWSH= (DELTAH-CDELH)/DELTAH
      GO TO 270
260   DWNWSH= 0.
270   ESH(2)= HP(IPS) + DELTAH*DWNWSH
      RETURN
C
300   IF(IBUOY.EQ.0) GO TO 500
C
C  DISTANCE-DEPENDENT PLUME RISE: BUOYANCY-DOMINATED PLUME,
C    ANY STABILITY (A-F).
      ESH(1)= DWNWSH*CTB*(DIST*1000.)**0.666667 + HP(IPS)
      IF(ESH(1).GT.ESH(2)) ESH(1)=ESH(2)
      RETURN
C
C  DISTANCE-DEPENDENT PLUME RISE: MOMENTUM-DOMINATED PLUME,
C    UNSTABLE AIR (A-D).
500   ESH(1)= DWNWSH*CTMU*(DIST*1000.)**0.333333 + HP(IPS)
      IF(ESH(1).GT.ESH(2)) ESH(1)=ESH(2)
      RETURN
C
C  THERE IS NO DISTANCE-DEPENDENT PLUME RISE GIVEN FOR A
C    MOMENTUM-DOMINATED PLUME IN STABLE AIR. DISTANCE TO MAXIMUM PLUME
C    RISE FOR THIS SITUATION IS SET EQUAL TO ZERO IN THE MAIN PROGRAM,
C    SO THE MAXIMUM HEIGHT, ESH(2), IS USED AT ALL DISTANCES.
      END
C
C
C
      SUBROUTINE AUTGRD
C                    SUBROUTINE AUTGRD (VERSION 82360), PART OF PEM.
C
C
C  SUBROUTINE AUTGRID CALCULATES THE FIVE PARAMETERS DEFINING THE
C    RECEPTOR GRID (XSWC,YSWC,LX,LY,GRID) WHEN THE AUTOMATIC GRID
C    OPTION IS USED. THIS IS DONE BY SETTING GRID=0.0 IN THE INPUT
C    DATA. GRID PARAMETERS WILL BE CHOSEN FOR EACH SCENARIO SO AS
C    TO INSURE GOOD COVERAGE BY RECEPTORS NEAR THE POINT OF
C    MAXIMUM CONCENTRATION.  THIS POINT IS DETERMINED USING GAUSSIAN
C    PLUME ALGORITHMS WITHOUT POLLUTANT REMOVAL MECHANISMS.  THIS
C    POINT IS THEREFORE ONLY APPROXIMATE FOR PROBLEMS WHICH INCLUDE
C    DEPOSITION, SEDIMENTATION, AND CHEMICAL DECAY/TRANSFORMATION.
C    THE OPTIMUM RECEPTOR GRID IN THIS CASE SHOULD BE DETERMINED BY
C    TRIAL AND ERROR, USING THE RECEPTOR GRID DEFINED BY AUTGRD AS
C    THE FIRST APPROXIMATION.
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
```

```
C
      DIMENSION XCRNR(4),YCRNR(4),HL(2),DL(2),XTM(2)
      DIMENSION AG(7,2),BG(7,2),DG(7)
      DATA AG/.0383,.1393,.112,.0856,.0818,.1094,.05645,
     1        .0002539,.04396,.1014,.2591,.2527,.2452,.1930/
      DATA BG/1.281,.9467,.9100,.865,.8155,.7657,.805,
     1        2.089,1.114,.926,.6869,.6341,.6358,.6072/
      DATA DG/.873,.897,.908,.916,.916,.912,.911/
C
C
      E= 1.570796 -WVEC
      SINEE= SIN(E)
      COSNE= COS(E)
      GX1= XP(1)*COSNE  + YP(1)*SINEE
      GX2= GX1
      GY1= YP(1)*COSNE  - XP(1)*SINEE
      GY2= GY1
      DO 200 I=1,NPS
      XT= XP(I)*COSNE  + YP(I)*SINEE
      YT= YP(I)*COSNE  - XP(I)*SINEE
      IBUOY=1
      IF(VP(I).GT.90.67*(TP(I)-TA(ISCEN))*SQRT(TA(ISCEN))/TP(I)) IBUOY=
      IRISE=2
      UINV = 1./WS(ISCEN)
      IF(HP(I).GT.10.) UINV = UINV*((10./HP(I))**P(ISC))
      EFF= 2.45*VP(I)*DP(I)*DP(I)*(TP(I)-TA(ISCEN))/TP(I)
      IPS=I
      HL(1)= HP(I)
      CALL RISE
      HL(2)= ESH(2)
      DO 170 J=1,2
      DL(J)=(BG(ISC,2)*HL(J)*HL(J)/(AG(ISC,2)*AG(ISC,2)*(BG(ISC,2)+DG(IS
     1C))))**(0.5/BG(ISC,2))*0.001
      IF(DL(J).GE.400.) GO TO 170
      DL(J)=(BG(ISC,1)*HL(J)*HL(J)/(AG(ISC,1)*AG(ISC,1)*(BG(ISC,1)+DG(IS
     1C))))**(0.5/BG(ISC,1))*0.001
  170 XTM(J)= XT + DL(J)
      IF(XTM(2).GT.GX2) GX2= XTM(2)
      IF(XTM(1).LT.GX1) GX1= XTM(1)
      IF(YT.GT.GY2)     GY2= YT
      IF(YT.LT.GY1)     GY1= YT
  200 CONTINUE
      XCRNR(1)= GX1
      XCRNR(2)= GX2
      XCRNR(3)= GX2
      XCRNR(4)= GX1
      YCRNR(1)= GY1
      YCRNR(2)= GY1
      YCRNR(3)= GY2
      YCRNR(4)= GY2
      DO 300 J=1,4
      XCRNRT= XCRNR(J)
      XCRNR(J)= XCRNR(J)*COSNE  - YCRNR(J)*SINEE
  300 YCRNR(J)= YCRNR(J)*COSNE + XCRNRT*SINEE
      XSWC= XCRNR(1)
      XNEC= XSWC
      YSWC= YCRNR(1)
      YNEC= YSWC
      DO 400 I=2,4
      IF(XCRNR(I).GT.XNEC) XNEC= XCRNR(I)
      IF(XCRNR(I).LT.XSWC) XSWC= XCRNR(I)
      IF(YCRNR(I).GT.YNEC) YNEC= YCRNR(I)
  400 IF(YCRNR(I).LT.YSWC) YSWC= YCRNR(I)
      XT= XNEC - XSWC
      YT= YNEC - YSWC
      DMAX= XT
      IF(YT.GT.XT) DMAX= YT
      IF(DMAX.LT.10.) GO TO 500
      IF(XT.GT.YT) GO TO 420
      LY=  50
      GRID= YT/50.
      LX= XT/GRID
      IF(LX.LT.50) LX= LX+1
      GO TO 600
  420 LX= 50
      GRID= XT/50.
      LY= YT/GRID
```

```
      IF(LY.LT.50) LY=LY+1                                              00032300
      GO TO 600                                                         00032310
  500 IF(DMAX.LT.5.) GO TO 540                                          00032320
      GRID= 0.2                                                         00032330
      LX= XT/GRID                                                       00032340
      LY= YT/GRID                                                       00032350
      IF(LX.LT.50) LX=LX+1                                              00032360
      IF(LY.LT.50) LY=LY+1                                              00032370
      GO TO 600                                                         00032380
  540 IF(DMAX.LT.0.25) GO TO 580                                        00032390
      IF(XT.GT.YT) GO TO 560                                            00032400
      LY= 25                                                            00032410
      GRID= YT/25.                                                      00032420
      LX= XT/GRID                                                       00032430
      IF(LX.LT.25) LX=LX+1                                              00032440
      GO TO 600                                                         00032450
  560 LX= 25                                                            00032460
      GRID= XT/25.                                                      00032470
      LY= YT/GRID                                                       00032480
      IF(LY.LT.25) LY=LY+1                                              00032490
      GO TO 600                                                         00032500
  580 GRID= 0.01                                                        00032510
      LX= XT/GRID                                                       00032520
      LY= YT/GRID                                                       00032530
      IF(LX.LT.25) LX=LX+1                                              00032540
      IF(LY.LT.25) LY=LY+1                                              00032550
  600 XSWC= XSWC - 0.5*GRID                                             00032560
      YSWC= YSWC - 0.5*GRID                                             00032570
      IF(NCSOPT.LT.1.OR.(LX.LE.25.AND.LY.LE.25)) GO TO 700              00032580
      XL=LX                                                             00032590
      YL=LY                                                             00032600
      IF(LX.GT.LY) GO TO 640                                            00032610
      DELG= YL/25.                                                      00032620
      LY=25                                                             00032630
      GRID= GRID*DELG                                                   00032640
      LX= XL/DELG                                                       00032650
      IF(LX.LT.25) LX=LX+1                                              00032660
      GO TO 700                                                         00032670
  640 DELG= XL/25.                                                      00032680
      LX=25                                                             00032690
      GRID= GRID*DELG                                                   00032700
      LY= YL/DELG + 1.                                                  00032710
  700 CONTINUE                                                          00032720
      WRITE(IWR,900)ISCEN,IWDOPT,TT                                     00032730
      XRSWC=XSWC+0.5*GRID                                               00032740
      YRSWC=YSWC+0.5*GRID                                               00032750
      WRITE(IWR,905)LX,LY,GRID,XRSWC,YRSWC                              00032760
  900 FORMAT(1H1,'PEM:   AUTOMATICALLY GENERATED RECEPTOR GRID PARAMETER00032770
     1S FOR SCENARIO ',I2,'  (WIND DIRECTION SUB-SCENARIO ',I2,')'//    00032780
     221X,20A4/1X,120('-')//)                                           00032790
  905 FORMAT(' RECEPTOR GRID CONSISTS OF ',I2,' COLUMNS AND ',I2,' ROWS 00032800
     1OF SPACING =',F7.4,' KM. SOUTHWEST CORNER OF GRID =',F8.3,' KM W, 00032810
     2',F8.3,' KM S.')                                                  00032820
      RETURN                                                            00032830
      END                                                               00032840
C                                                                       00032850
C                                                                       00032860
C                                                                       00032870
      BLOCK DATA                                                        00032880
C                 BLOCK DATA (VERSION 82360), PART OF PEM.              00032890
C                                                                       00032900
C                                                                       00032910
C                                                                       00032920
C     THIS SUBPROGRAM INITIALIZES VARIABLES IN COMMON/PEMCOM/           00032930
C                                                                       00032940
C *** PEM MODIFICATIONS BY M.M.STEVENS,                                 00032950
C     NOAA-ATDL, P.O.BOX-E, OAK RIDGE, TENN 37830                       00032960
C     DECEMBER 1982                                                     00032970
C                                                                       00032980
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00032990
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00033000
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00033010
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00033020
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00033030
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),     00033040
     6 ITA,IRD,IWR,IDSK,         D80,D47,D8047,DIST,DELTA,              00033050
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00033060
```

```
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
C
      DATA INDEX,NAS,NPS/0,0,0/
      DATA ITA,IRD,IWR,IDSK/1,5,6,8/
      DATA SCLAB/2HA ,2HB ,2HC ,2HDD,2HDN,2HE ,2HF /
      DATA P/0.1,0.15,0.2,0.25,0.25,0.3,0.3/
      DATA AX/.0383,.1393,.112,.0856,.0818,.1094,.05645,
     1 .0002539,.04936,.1014,.2591,.2527,.2452,.1930,
     2 .0002539,.04936,.1154,.7368,1.297,.9204,1.505/
      DATA BX/1.281,.)467,.9100,.865,.8155,.7657,.805,
     1  2.089,1.114,.926,.6869,.6341,.6358,.6072,
     2 2.089,1.114,.9109,.5642,.4421,.4805,.3662/
      DATA SECTAN/0.,.39270,.78540,1.17810,1.57080,1.96350,2.35620,
     1 2.74890,3.14159,3.53429,3.92699,4.31969,4.71239,5.10509,
     2 5.49779,5.89049/
C
      END
C
C
C
      SUBROUTINE D01AJF(F, A, B, EPSABS, EPSREL, RESULT, ABSERR,WORK,
     * LWORK, IWORK, LIWORK, IFAIL)
C                    SUBROUTINE D01AJF, PART OF PEM (VERSION 82360).
C
C     MARK 8 RELEASE. NAG COPYRIGHT 1980
C
C     D01AJF IS A GENERAL PURPOSE INTEGRATOR WHICH CALCULATES
C     AN APPROXIMATION TO THE INTEGRAL OF A FUNCTION OVER A FINITE
C     INTERVAL (A,B).  THIS ROUTINE CAN BE USED WHEN THE INTEGRAND
C     HAS SINGULARITIES, ESPECIALLY WHEN THESE ARE OF ALGEBRAIC OR
C     LOGARITHMIC TYPE.  D01AJF IS AN ADAPTIVE ROUTINE, USING THE
C     GAUSS 10-POINT AND KRONROD 21-POINT RULES.  THE ALGORITHM
C     INCORPORATES A GLOBAL ACCEPTANCE CRITERION TOGETHER WITH
C     EPS-ALGORITHM TO PERFORM EXTRAPOLATION.  THE LOCAL ERROR IS
C     ESTIMATED.
C
C     THE GENERAL PURPOSE INTEGRATOR D01AJF INCLUDES THE FOLLOWING:
C     SUBROUTINES (1) D01AJF, (2) D01AJV, (3) D01AJX, (4) D01AJY,
C     (5) D01AJZ, INTEGER FUNCTION P01AAF, DOUBLE PRECISION FUNCTIONS
C     (1) X02AAF, (2) X02ABF, (3) X02ACF, AND SUBROUTINE X04AAF.
C     THE PROGRAM LISTINGS FOR THESE SUBROUTINES AND FUNCTIONS, COPIED
C     HERE FROM ORNL - NAG LIBRARY, FOLLOW.  THESE ARE DEVELOPED BY
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C          DOWNERS GROVE, ILLINOIS 60515
C     WHICH HOLDS THE COPYRIGHT (NAG FORTRAN MINI MANUAL, MARK8, 1980).
C     THESE PROGRAM LISTINGS ARE INCLUDED HERE WITH THEIR
C     KIND PERMISSION.  THEY ARE RELEASED BY
C          COMPUTER SCIENCES DEPARTMENT
C          OAK RIDGE NATIONAL LABORATORY (ORNL)
C          OAK RIDGE, TENNESSEE 37830
C     EXCLUSIVELY FOR USE IN THE PEM.  THESE LIBRARY SUB-
C     ROUTINES AND PROGRAMS SHOULD NOT BE USED FOR ANY OTHER
C     PURPOSE WITHOUT PRIOR APPROVAL FROM NAG AND ORNL.
C
C     D01AJF ITSELF IS ESSENTIALLY A DUMMY ROUTINE WHOSE FUNCTION IS TO
C     PARTITION THE WORK ARRAYS WORK AND IWORK FOR USE BY D01AJV.
C     WORK IS PARTITIONED INTO 4 ARRAYS EACH OF SIZE LWORK/4.
C     IWORK IS A SINGLE ARRAY IN D01AJV.
C
C     .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION A, ABSERR, B, EPSABS, EPSREL, RESULT
      INTEGER IFAIL, LIWORK, LWORK
C     .. ARRAY ARGUMENTS ..
      DOUBLE PRECISION WORK(LWORK)
      INTEGER IWORK(LIWORK)
C     .. FUNCTION ARGUMENTS ..
      DOUBLE PRECISION F
C     ..
C     .. LOCAL SCALARS ..
C$P 1
      DOUBLE PRECISION SRNAME
      INTEGER IBL, IEL, IER, IRL, LIMIT
C     .. FUNCTION REFERENCES ..
```

```
      INTEGER P01AAF                                                    00033840
C     .. SUBROUTINE REFERENCES ..                                       00033850
C     D01AJV                                                            00033860
C     ..                                                                00033870
      EXTERNAL F                                                        00033880
      DATA SRNAME /8H D01AJF /                                          00033890
C     CHECK THAT MINIMUM WORKSPACE REQUIREMENTS ARE MET                 00033900
      IF (LWORK.LT.4) GO TO 20                                          00033910
      IF (LIWORK.LT.LWORK/8+2) GO TO 20                                 00033920
C     LIMIT = UPPER BOUND ON NUMBER OF SUBINTERVALS                     00033930
      LIMIT = LWORK/4                                                   00033940
C     SET UP BASE ADDRESSES FOR WORK ARRAYS                             00033950
      IBL = LIMIT + 1                                                   00033960
      IEL = LIMIT + IBL                                                 00033970
      IRL = LIMIT + IEL                                                 00033980
C     PERFORM INTEGRATION                                               00033990
      CALL D01AJV(F, A, B, DABS(EPSABS), DABS(EPSREL), WORK(1),WORK(IBL)00034000
     *, WORK(IEL), WORK(IRL), LIMIT, IWORK, LIWORK,RESULT, ABSERR, IER) 00034010
      IF (IER.NE.0) GO TO 40                                            00034020
      IFAIL = 0                                                         00034030
      GO TO 60                                                          00034040
C     ERROR 6 = INSUFFICIENT WORKSPACE                                  00034050
   20 IER = 6                                                           00034060
   40 IFAIL = P01AAF(IFAIL,IER,SRNAME)                                  00034070
   60 RETURN                                                            00034080
      END                                                               00034090
C                                                                       00034100
C                                                                       00034110
      SUBROUTINE D01AJV(F, A, B, EPSABS, EPSREL, ALIST, BLIST,ELIST,    00034120
     * RLIST, LIMIT, IORD, LIORD, RESULT, ABSERR, IER)                  00034130
C                    SUBROUTINE D01AJV, PART OF PEM (VERSION 82360).    00034140
C                                                                       00034150
C     MARK 8 RELEASE. NAG COPYRIGHT 1979                                00034160
C     BASED ON QUADPACK ROUTINE DQAGS (FORMERLY QAGS)                   00034170
C     ****************************************************************  00034180
C                                                                       00034190
C        PURPOSE                                                        00034200
C           THE ROUTINE CALCULATES AN APPROXIMATION                     00034210
C           /RESULT/ TO A GIVEN DEFINITE INTEGRAL   I =                 00034220
C           INTEGRAL OF /F/ OVER (A,B), HOPEFULLY                       00034230
C           SATISFYING FOLLOWING CLAIM FOR ACCURACY .                   00034240
C           ABS(I-RESULT) .LE. MAX(EPSABS,EPSREL*ABS(I)).               00034250
C                                                                       00034260
C         CALLING SEQUENCE                                              00034270
C           CALL D01AJV (F,A,B,EPSABS,EPSREL,ALIST,BLIST,ELIST,         00034280
C                        RLIST,LIMIT,IORD,LIORD,RESULT,ABSERR,IER)      00034290
C                                                                       00034300
C        PARAMETERS                                                     00034310
C           F      - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND         00034320
C                    FUNCTION F(X). THE ACTUAL NAME FOR F               00034330
C                    NEEDS TO BE DECLARED E X T E R N A L               00034340
C                    IN THE DRIVER PROGRAM                              00034350
C                                                                       00034360
C           A      - LOWER LIMIT OF INTEGRATION                         00034370
C                                                                       00034380
C           B      - UPPER LIMIT OF INTEGRATION                         00034390
C                                                                       00034400
C           EPSABS - ABSOLUTE ACCURACY REQUESTED                        00034410
C                                                                       00034420
C           EPSREL - RELATIVE ACCURACY REQUESTED                        00034430
C                                                                       00034440
C           ALIST,BLIST,ELIST,RLIST                                     00034450
C                  - WORK ARRAYS (FUNCTIONS DESCRIBED BELOW)            00034460
C                                                                       00034470
C           LIMIT  - UPPER BOUND FOR NUMBER OF SUBINTERVALS             00034480
C                                                                       00034490
C           IORD   - WORK ARRAY                                         00034500
C                                                                       00034510
C           LIORD  - LENGTH OF IORD (AT LEAST LIMIT/2 + 2)              00034520
C                                                                       00034530
C           RESULT - APPROXIMATION TO THE INTEGRAL                      00034540
C                                                                       00034550
C           ABSERR - ESTIMATE OF THE MODULUS OF THE ABSOLUTE ERROR,     00034560
C                    WHICH SHOULD EQUAL OR EXCEED ABS(I-RESULT)         00034570
C                                                                       00034580
C           IER    - IER   = 0 NORMAL AND RELIABLE                      00034590
C                            TERMINATION OF THE ROUTINE.                00034600
```

```
C                                IT IS ASSUMED THAT THE
C                                REQUESTED  ACCURACY HAS BEEN
C                                ACHIEVED.
C                      - IER   .NE. 0 ABNORMAL TERMINATION OF
C                                THE ROUTINE. THE ESTIMATES
C                                FOR INTEGRAL AND ERROR ARE
C                                LESS RELIABLE. IT IS ASSUMED
C                                THAT THE  REQUESTED ACCURACY
C                                HAS NOT BEEN ACHIEVED.
C                            = 1 MAXIMUM NUMBER OF SUBDIVISIONS ALLOWED
C                                HAS BEEN ACHIEVED. THE USER CAN
C                                ALLOW MORE SUB DIVISIONS BY
C                                INCREASING THE DIMENSIONS OF THE
C                                WORK ARRAYS WORK AND IWORK.
C                                HOWEVER, THIS MAY
C                                YIELD NO  IMPROVEMENT, AND IT
C                                IS RATHER ADVISED TO HAVE A
C                                CLOSE LOOK AT THE INTEGRAND,
C                                IN ORDER TO DETERMINE THE
C                                INTEGRATION  DIFFICULTIES. IF
C                                THE POSITION OF A LOCAL
C                                DIFFICULTY CAN BE DETERMINED
C                                (I.E.  SINGULARITY,
C                                DISCONTINUITY WITHIN THE
C                                INTERVAL) ONE WILL PROBABLY
C                                GAIN FROM  SPLITTING UP THE
C                                INTERVAL AT THIS POINT AND
C                                CALLING THE INTEGRATOR ON THE
C                                SUB-RANGES. IF POSSIBLE, AN
C                                APPROPRIATE SPECIAL-PURPOSE
C                                INTEGRATOR SHOULD BE USED
C                                WHICH IS DESIGNED FOR
C                                HANDLING THE TYPE  OF
C                                DIFFICULTY INVOLVED.
C                            = 2 THE OCCURRENCE OF ROUNDOFF
C                                ERROR IS DETECTED WHICH
C                                PREVENTS THE REQUESTED
C                                TOLERANCE  FROM BEING
C                                ACHIEVED. THE ERROR MAY BE
C                                UNDER-ESTIMATED.
C                            = 3 EXTREMELY BAD INTEGRAND BEHAVIOUR
C                                OCCURS AT SOME INTERIOR POINTS OF THE
C                                INTEGRATION INTERVAL.
C                            = 4 IT IS PRESUMED THAT THE REQUESTED
C                                TOLERANCE CANNOT BE ACHIEVED,
C                                AND THAT THE RETURNED RESULT
C                                IS THE BEST WHICH CAN BE
C                                OBTAINED.
C                            = 5 THE INTEGRAL IS PROBABLY DIVERGENT, OR
C                                SLOWLY CONVERGENT. IT MUST BE NOTED
C                                THAT DIVERGENCY CAN OCCUR
C                                WITH ANY OTHER VALUE OF IER.
C
C     ***********************************************************
C     .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION A, ABSERR, B, EPSABS, EPSREL, RESULT
      INTEGER IER, LIMIT, LIORD
C     .. ARRAY ARGUMENTS ..
      DOUBLE PRECISION ALIST(LIMIT), BLIST(LIMIT), ELIST(LIMIT),
     * RLIST(LIMIT)
      INTEGER IORD(LIORD)
C     .. FUNCTION ARGUMENTS ..
      DOUBLE PRECISION F
C     ..
C     .. SCALARS IN COMMON ..
      INTEGER JUPBND
C     ..
C     .. LOCAL SCALARS ..
      DOUBLE PRECISION A1, A2, ABSEPS, AREA12, AREA1, AREA2, AREA, B1,
     * B2,CORREC, DEFAB1, DEFAB2, DEFABS, DRES, EPMACH, ERLARG,ERLAST,
     * ERRBND, ERRMAX, ERRO12, ERROR1, ERROR2, ERRSUM,ERTEST, OFLOW,
     * RESABS, RESEPS, SMALL, UFLOW
      INTEGER ID, IERRO, IROFF1, IROFF2, IROFF3, K, KSGN, KTMIN,LAST1,
     * LAST, MAXERR, NRES, NRMAX, NUMRL2
      LOGICAL EXTRAP, NOEXT
C     .. LOCAL ARRAYS ..
      DOUBLE PRECISION RES3LA(3), RLIST2(52)
```

```
C     .. FUNCTION REFERENCES ..
      DOUBLE PRECISION X02AAF, X02ABF, X02ACF
C     .. SUBROUTINE REFERENCES ..
C     D01AJX, D01AJY, D01AJZ
C     ..
      EXTERNAL F
      COMMON /AD01AJ/ JUPBND
C
C          THE DIMENSION OF /RLIST2/ IS DETERMINED BY
C          DATA /LIMEXP/ IN SUBROUTINE D01AJY (/RLIST2/
C          SHOULD BE OF DIMENSION (LIMEXP+2) AT LEAST).
C
      EPMACH = X02AAF(0.0D0)
      UFLOW = X02ABF(1.0D0)
      OFLOW = X02ACF(1.0D0)
C
C          LIST OF MAJOR VARIABLES
C          -----------------------
C
C         ALIST     - LIST OF LEFT END-POINTS OF ALL SUBINTERVALS
C                     CONSIDERED UP TO NOW
C
C         BLIST     - LIST OF RIGHT END-POINTS OF ALL SUBINTERVALS
C                     CONSIDERED UP TO NOW
C
C         RLIST(I)  - APPROXIMATION TO THE INTEGRAL OVER
C                     (ALIST(I),BLIST(I))
C
C         RLIST2    - ARRAY OF DIMENSION AT LEAST LIMEXP+2
C                     CONTAINING THE PART OF THE EPSILON TABLE
C                     WHICH IS STILL NEEDED FOR FURTHER
C                     COMPUTATIONS
C
C         ELIST(I)  - ERROR ESTIMATE APPLYING TO RLIST(I)
C
C         MAXERR    - POINTER TO THE INTERVAL WITH LARGEST ERROR
C                     ESTIMATE
C
C         ERRMAX    - ELIST(MAXERR)
C
C         ERLAST    - ERROR ON THE INTERVAL CURRENTLY SUBDIVIDED
C                     (BEFORE THAT SUBDIVISION HAS TAKEN PLACE)
C
C         AREA      - SUM OF THE INTEGRALS OVER THE SUBINTERVALS
C
C         ERRSUM    - SUM OF THE ERRORS OVER THE SUBINTERVALS
C
C         ERRBND    - REQUESTED ACCURACY MAX(EPSABS,EPSREL*
C                     ABS(RESULT))
C
C         *****1    - VARIABLE FOR THE LEFT INTERVAL
C
C         *****2    - VARIABLE FOR THE RIGHT INTERVAL
C
C         LAST      - INDEX FOR SUBDIVISION
C
C         NRES      - NUMBER OF CALLS TO THE EXTRAPOLATION ROUTINE
C
C         NUMRL2    - NUMBER OF ELEMENTS CURRENTLY IN
C                     RLIST2. IF AN APPROPRIATE
C                     APPROXIMATION TO THE COMPOUNDED
C                     INTEGRAL HAS BEEN OBTAINED IT IS
C                     PUT IN RLIST2(NUMRL2) AFTER NUMRL2
C                     HAS BEEN INCREASED BY ONE.
C
C         SMALL     - LENGTH OF THE SMALLEST INTERVAL CONSIDERED
C                     UP TO NOW, MULTIPLIED BY 1.5
C
C         ERLARG    - SUM OF THE ERRORS OVER THE INTERVALS LARGER
C                     THAN THE SMALLEST INTERVAL
C                     CONSIDERED UP TO NOW
C         EXTRAP    - LOGICAL VARIABLE DENOTING THAT THE
C                     ROUTINE IS ATTEMPTING TO PERFORM
C                     EXTRAPOLATION. I.E. BEFORE
C                     SUBDIVIDING THE SMALLEST INTERVAL
C                     WE TRY TO DECREASE THE VALUE OF
C                     ERLARG
```

```
C          NOEXT      - LOGICAL VARIABLE DENOTING THAT EXTRAPOLATION
C                       IS NO LONGER ALLOWED(/TRUE/ VALUE)
C
C          FIRST APPROXIMATION TO THE INTEGRAL
C          ----------------------------------
C
      LAST1 = 1
      IER = 0
      IERRO = 0
      CALL D01AJZ(F, A, B, RESULT, ABSERR, DEFABS, RESABS)
C
C          TEST ON ACCURACY
C
      DRES = DABS(RESULT)
      ERRBND = DMAX1(EPSABS,EPSREL*DRES)
      IF (ABSERR.LE.1.0D+02*EPMACH*DEFABS .AND. ABSERR.GT.ERRBND)IER = 2
      IF (LIMIT.LT.2 .AND. ABSERR.GT.ERRBND) IER = 1
      IF (IER.NE.0 .OR. ABSERR.LE.ERRBND) GO TO 320
C
C          INITIALIZATION
C          --------------
C
      ALIST(1) = A
      BLIST(1) = B
      RLIST(1) = RESULT
      RLIST2(1) = RESULT
      ERRMAX = ABSERR
      MAXERR = 1
      AREA = RESULT
      ERRSUM = ABSERR
      ABSERR = OFLOW
      NRMAX = 1
      NRES = 0
      NUMRL2 = 2
      KTMIN = 0
      EXTRAP = .FALSE.
      NOEXT = .FALSE.
      IROFF1 = 0
      IROFF2 = 0
      IROFF3 = 0
      KSGN = -1
      IF (DRES.GE.(0.1D+01-0.5D+02*EPMACH)*DEFABS) KSGN = 1
C
C          MAIN DO-LOOP
C          ------------
C
      IF (LIMIT.LT.2) GO TO 220
      DO 200 LAST=2,LIMIT
C
C          BISECT THE SUBINTERVAL WITH THE NRMAX-TH LARGEST
C          ERROR ESTIMATE
C
        LAST1 = LAST
        A1 = ALIST(MAXERR)
        B1 = 0.5D+00*(ALIST(MAXERR)+BLIST(MAXERR))
        A2 = B1
        B2 = BLIST(MAXERR)
        ERLAST = ERRMAX
        CALL D01AJZ(F, A1, B1, AREA1, ERROR1, RESABS, DEFAB1)
        CALL D01AJZ(F, A2, B2, AREA2, ERROR2, RESABS, DEFAB2)
C
C          IMPROVE PREVIOUS APPROXIMATION OF INTEGRAL
C          AND ERROR AND TEST FOR ACCURACY
C
        AREA12 = AREA1 + AREA2
        ERRO12 = ERROR1 + ERROR2
        ERRSUM = ERRSUM + ERRO12 - ERRMAX
        AREA = AREA + AREA12 - RLIST(MAXERR)
        IF (DEFAB1.EQ.ERROR1 .OR. DEFAB2.EQ.ERROR2) GO TO 40
        IF (DABS(RLIST(MAXERR)-AREA12).GT.0.1D-04*DABS(AREA12) .OR.
     *  ERRO12.LT.0.99D+00*ERRMAX) GO TO 20
        IF (EXTRAP) IROFF2 = IROFF2 + 1
        IF (.NOT.EXTRAP) IROFF1 = IROFF1 + 1
   20   IF (LAST.GT.10 .AND. ERRO12.GT.ERRMAX) IROFF3 = IROFF3 + 1
   40   RLIST(MAXERR) = AREA1
        RLIST(LAST) = AREA2
        ERRBND = DMAX1(EPSABS,EPSREL*DABS(AREA))
```

```
      IF (ERRSUM.LE.ERRBND) GO TO 280
C
C        TEST FOR ROUNDOFF ERROR AND EVENTUALLY
C        SET ERROR FLAG
C
      IF (IROFF1+IROFF2.GE.10 .OR. IROFF3.GE.20) IER = 2
      IF (IROFF2.GE.5) IERRO = 3
C
C        SET ERROR FLAG IN THE CASE THAT THE NUMBER OF INTERVAL
C         BISECTIONS EXCEEDS /LIMIT/
C
      IF (LAST.EQ.LIMIT) IER = 1
C
C        SET ERROR FLAG IN THE CASE OF BAD INTEGRAND BEHAVIOUR
C        AT INTERIOR POINTS OF INTEGRATION RANGE
C
      IF (DMAX1(DABS(A1),DABS(B2)).LE.(0.1D+01+0.1D+03*EPMACH)*
     * (DABS(A2)+0.1D+04*UFLOW)) IER = 4
      IF (IER.NE.0) GO TO 220
C
C        APPEND THE NEWLY-CREATED INTERVALS TO THE LIST
C
      IF (ERROR2.GT.ERROR1) GO TO 60
      ALIST(LAST) = A2
      BLIST(MAXERR) = B1
      BLIST(LAST) = B2
      ELIST(MAXERR) = ERROR1
      ELIST(LAST) = ERROR2
      GO TO 80
   60 ALIST(MAXERR) = A2
      ALIST(LAST) = A1
      BLIST(LAST) = B1
      RLIST(MAXERR) = AREA2
      RLIST(LAST) = AREA1
      ELIST(MAXERR) = ERROR2
      ELIST(LAST) = ERROR1
C
C        CALL SUBROUTINE D01AJX TO MAINTAIN THE
C        DESCENDING ORDERING IN THE LIST OF ERROR
C        ESTIMATES AND SELECT THE SUBINTERVAL WITH
C        NRMAX-TH LARGEST ERROR ESTIMATE (TO BE BISECTED
C        NEXT)
C
   80 CALL D01AJX(LIMIT, LAST, MAXERR, ERRMAX, ELIST, IORD,LIORD,
     *  NRMAX)
      IF (LAST.EQ.2) GO TO 180
      IF (NOEXT) GO TO 200
      ERLARG = ERLARG - ERLAST
      IF (DABS(B1-A1).GT.SMALL) ERLARG = ERLARG + ERRO12
      IF (EXTRAP) GO TO 100
C
C        TEST WHETHER THE INTERVAL TO BE BISECTED NEXT IS THE
C        SMALLEST INTERVAL
C
      IF (DABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200
      EXTRAP = .TRUE.
      NRMAX = 2
  100 IF (IERRO.EQ.3 .OR. ERLARG.LE.ERTEST) GO TO 140
C
C        THE SMALLEST INTERVAL HAS THE LARGEST ERROR.
C        BEFORE BISECTING DECREASE THE SUM OF THE ERRORS
C        OVER THE LARGER INTERVALS(ERLARG) AND PERFORM
C        EXTRAPOLATION
C
      ID = NRMAX
      DO 120 K=ID,JUPBND
         MAXERR = IORD(NRMAX)
         ERRMAX = ELIST(MAXERR)
         IF (DABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200
         NRMAX = NRMAX + 1
  120 CONTINUE
C
C        PERFORM EXTRAPOLATION
C
  140 NUMRL2 = NUMRL2 + 1
      RLIST2(NUMRL2) = AREA
      CALL D01AJY(NUMRL2, RLIST2, RESEPS, ABSEPS, RES3LA, NRES)
```

```
      KTMIN = KTMIN + 1                                                 00037690
      IF (KTMIN.GT.5 .AND. ABSERR.LT.0.1D-02*ERRSUM) IER = 5            00037700
      IF (ABSEPS.GE.ABSERR) GO TO 160                                   00037710
      KTMIN = 0                                                         00037720
      ABSERR = ABSEPS                                                   00037730
      RESULT = RESEPS                                                   00037740
      CORREC = ERLARG                                                   00037750
      ERTEST = DMAX1(EPSABS,EPSREL*DABS(RESEPS))                        00037760
      IF (ABSERR.LE.ERTEST) GO TO 220                                   00037770
C                                                                       00037780
C        PREPARE  BISECTION OF THE SMALLEST INTERVAL                    00037790
C                                                                       00037800
  160 IF (NUMRL2.EQ.1) 'IOEXT = .TRUE.                                  00037810
      IF (IER.EQ.5) GO TO 220                                           00037820
      MAXERR = IORD(1)                                                  00037830
      ERRMAX = ELIST(MAXERR)                                            00037840
      NRMAX = 1                                                         00037850
      EXTRAP = .FALSE.                                                  00037860
      SMALL = SMALL*0.5D+00                                             00037870
      ERLARG = ERRSUM                                                   00037880
      GO TO 200                                                         00037890
  180 SMALL = DABS(B-A)*0.375D+00                                       00037900
      ERLARG = ERRSUM                                                   00037910
      ERTEST = ERRBND                                                   00037920
      RLIST2(2) = AREA                                                  00037930
  200 CONTINUE                                                          00037940
C                                                                       00037950
C        SET  FINAL RESULT AND ERROR ESTIMATE                           00037960
C        ------------------------------------                           00037970
C                                                                       00037980
  220 IF (ABSERR.EQ.OFLOW) GO TO 280                                    00037990
      IF (IER+IERRO.EQ.0) GO TO 260                                     00038000
      IF (IERRO.EQ.3) ABSERR = ABSERR + CORREC                          00038010
      IF (IER.EQ.0) IER = 3                                             00038020
      IF (RESULT.NE.0.D+00.AND .AREA. NE.0.D+00) GO TO 240              00038030
      IF (ABSERR.GT.ERRSUM) GO TO 280                                   00038040
      IF (AREA.EQ.0.D+00) GO TO 320                                     00038050
      GO TO 260                                                         00038060
  240 IF (ABSERR/DABS(RESULT).GT.ERRSUM/DABS(AREA)) GO TO 280           00038070
C                                                                       00038080
C        TEST ON DIVERGENCY                                             00038090
C                                                                       00038100
  260 IF (KSGN.EQ.-1 .AND. DMAX1(DABS(RESULT),DABS(AREA)).LE.DEFABS*     00038110
     *0.1D-01) GO TO 320                                                00038120
      IF (0.1D-01.GT.(RESULT/AREA) .OR. (RESULT/AREA).GT.0.1D+03.OR.    00038130
     * ERRSUM.GT.DABS(AREA)) IER = 6                                    00038140
      GO TO 320                                                         00038150
C                                                                       00038160
C        COMPUTE GLOBAL INTEGRAL SUM                                    00038170
C                                                                       00038180
  280 RESULT = 0.D+00                                                   00038190
      DO 300 K=1,LAST                                                   00038200
         RESULT = RESULT + RLIST(K)                                     00038210
  300 CONTINUE                                                          00038220
      ABSERR = ERRSUM                                                   00038230
  320 IF (IER.GT.2) IER = IER - 1                                       00038240
      IORD(1) = 4*LAST1                                                 00038250
      RETURN                                                            00038260
      END                                                               00038270
C                                                                       00038280
C                                                                       00038290
      SUBROUTINE D01AJX(LIMIT, LAST, MAXERR, ERMAX, ELIST, IORD,LIORD,  00038300
     * NRMAX)                                                           00038310
C                    SUBROUTINE D01AJX, PART OF PEM (VERSION 82360).    00038320
C                                                                       00038330
C     MARK 8 RELEASE. NAG COPYRIGHT 1979                                00038340
C     BASED ON QUADPACK ROUTINE ORDER                                   00038350
C     ***************************************************               00038360
C                                                                       00038370
C        PURPOSE                                                        00038380
C           THIS ROUTINE MAINTAINS THE DESCENDING ORDERING              00038390
C           IN THE LIST OF THE LOCAL ERROR ESTIMATES                    00038400
C           RESULTING FROM THE INTERVAL SUBDIVISION                     00038410
C           PROCESS. AT EACH CALL TWO ERROR ESTIMATES                   00038420
C           ARE INSERTED USING THE SEQUENTIAL SEARCH                    00038430
C           METHOD . TOP-DOWN FOR THE LARGEST ERROR                     00038440
C           ESTIMATE,  BOTTOM-UP FOR THE SMALLEST ERROR                 00038450
```

```
C              ESTIMATE.
C
C          CALLING SEQUENCE
C              CALL D01AJX
C              (LIMIT,LAST,MAXERR,ERMAX,ELIST,IORD,LIORD,NRMAX)
C
C           PARAMETERS (MEANING AT OUTPUT)
C              LIMIT  - MAXIMUM NUMBER OF ERROR ESTIMATES THE LIST
C                       CAN CONTAIN
C
C              LAST   - NUMBER OF ERROR ESTIMATES CURRENTLY
C                       IN THE LIST. ELIST(LAST) CONTAINS
C                       THE SMALLEST ERROR ESTIMATE.
C
C              MAXERR - MAXERR POINTS TO THE NRMAX-TH LARGEST ERROR
C                       ESTIMATE CURRENTLY IN THE LIST.
C
C              ERMAX  - NRMAX-TH LARGEST ERROR ESTIMATE
C                       ERMAX = ELIST(MAXERR)
C
C              ELIST  - ARRAY OF DIMENSION LAST CONTAINING
C                       THE ERROR ESTIMATES
C
C              IORD   - ARRAY CONTAINING POINTERS TO ELIST SO
C                       THAT IORD(1) POINTS TO THE LARGEST
C                       ERROR ESTIMATE,...,IORD(LAST) TO THE
C                       SMALLEST ERROR ESTIMATE
C
C              LIORD  - DIMENSION OF IORD
C
C              NRMAX  - MAXERR = IORD(NRMAX)
C
C      ***************************************************
C
C      .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION ERMAX
      INTEGER LAST, LIMIT, LIORD, MAXERR, NRMAX
C     .. ARRAY ARGUMENTS ..
      DOUBLE PRECISION ELIST(LAST)
      INTEGER IORD(LIORD)
C     ..
C     .. SCALARS IN COMMON ..
      INTEGER JUPBND
C     ..
C     .. LOCAL SCALARS ..
      DOUBLE PRECISION ERRMAX, ERRMIN
      INTEGER I, IBEG, IDO, ISUCC, J, JBND, K
C     ..
      COMMON /AD01AJ/ JUPBND
C
C          CHECK WHETHER THE LIST CONTAINS MORE THAN
C          TWO ERROR ESTIMATES
C
      IF (LAST.GT.2) GO TO 20
      IORD(1) = 1
      IORD(2) = 2
      GO TO 180
C
C          THIS PART OF THE ROUTINE IS ONLY EXECUTED
C          IF, DUE TO A DIFFICULT INTEGRAND, SUBDIVISION
C          INCREASED THE ERROR ESTIMATE. IN THE NORMAL CASE
C          THE INSERT PROCEDURE SHOULD START AFTER THE
C          NRMAX-TH LARGEST ERROR ESTIMATE.
C
   20 ERRMAX = ELIST(MAXERR)
      IF (NRMAX.EQ.1) GO TO 60
      IDO = NRMAX - 1
      DO 40 I=1,IDO
         ISUCC = IORD(NRMAX-1)
         IF (ERRMAX.LE.ELIST(ISUCC)) GO TO 60
         IORD(NRMAX) = ISUCC
         NRMAX = NRMAX - 1
   40 CONTINUE
C
C          COMPUTE THE NUMBER OF ELEMENTS IN THE LIST TO
C          BE MAINTAINED IN DESCENDING ORDER. THIS NUMBER
C          DEPENDS ON THE NUMBER OF SUBDIVISIONS STILL
```

```
C          ALLOWED
C
   60 JUPBND = LAST
      IF (LAST.GT.(LIMIT/2+2)) JUPBND = LIMIT + 3 - LAST
      ERRMIN = ELIST(LAST)
C
C          INSERT ERRMAX BY TRAVERSING THE LIST TOP-DOWN
C          STARTING COMPARISON FROM THE ELEMENT
C          ELIST(IORD(NRMAX+1))
C
      JBND = JUPBND - 1
      IBEG = NRMAX + 1
      IF (IBEG.GT.JBND) GO TO 100
      DO 80 I=IBEG,JBND
         ISUCC = IORD(I)
         IF (ERRMAX.GE.ELIST(ISUCC)) GO TO 120
         IORD(I-1) = ISUCC
   80 CONTINUE
  100 IORD(JBND) = MAXERR
      IORD(JUPBND) = LAST
      GO TO 180
C
C          INSERT ERRMIN BY TRAVERSING THE LIST BOTTOM-UP
C
  120 IORD(I-1) = MAXERR
      K = JBND
      DO 140 J=I,JBND
         ISUCC = IORD(K)
         IF (ERRMIN.LT.ELIST(ISUCC)) GO TO 160
         IORD(K+1) = ISUCC
         K = K - 1
  140 CONTINUE
      IORD(I) = LAST
      GO TO 180
  160 IORD(K+1) = LAST
C
C          SET MAXERR AND ERMAX
C
  180 MAXERR = IORD(NRMAX)
      ERMAX = ELIST(MAXERR)
      RETURN
      END
C
C
      SUBROUTINE D01AJY(N, EPSTAB, RESULT, ABSERR, RES3LA, NRES)
C                    SUBROUTINE D01AJY, PART OF PEM (VERSION 82360).
C
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE EPSALG
C     ************************************************
C
C        PURPOSE
C           THE ROUTINE TRANSFORMS A GIVEN SEQUENCE OF
C           APPROXIMATIONS, BY MEANS OF THE EPSILON
C           ALGORITHM OF P. WYNN.
C
C           AN ESTIMATE OF THE ABSOLUTE ERROR IS ALSO GIVEN.
C           THE CONDENSED EPSILON TABLE IS COMPUTED. ONLY THOSE
C           ELEMENTS NEEDED FOR THE COMPUTATION OF THE
C           NEXT DIAGONAL ARE PRESERVED.
C
C        CALLING SEQUENCE
C           CALL D01AJY (N,EPSTAB,RESULT,ABSERR,RES3LA,NRES)
C
C        PARAMETERS
C           N      - EPSTAB(N) CONTAINS THE NEW ELEMENT IN THE
C                    FIRST COLUMN OF THE EPSILON TABLE.
C
C           EPSTAB - ONE DIMENSIONAL ARRAY CONTAINING THE
C                    ELEMENTS OF THE TWO LOWER DIAGONALS OF
C                    THE TRIANGULAR EPSILON TABLE.
C                    THE ELEMENTS ARE NUMBERED STARTING AT THE
C                    RIGHT-HAND CORNER OF THE TRIANGLE.
C                    THE DIMENSION SHOULD BE AT LEAST N+2.
C
C           RESULT - RESULTING APPROXIMATION TO THE INTEGRAL
C
```

```
C              ABSERR - ESTIMATE OF THE ABSOLUTE ERROR COMPUTED FROM
C                       RESULT AND THE 3 PREVIOUS /RESULTS/
C
C              RES3LA - ARRAY CONTAINING THE LAST 3 /RESULTS/
C
C              NRES   - NUMBER OF CALLS TO THE ROUTINE
C                       (SHOULD BE ZERO AT FIRST CALL)
C
C      ***********************************************
C      .. SCALAR ARGUMENTS ..
       DOUBLE PRECISION ABSERR, RESULT
       INTEGER N, NRES
C      .. ARRAY ARGUMENTS ..
       DOUBLE PRECISION EPSTAB(52), RES3LA(3)
C      ..
C      .. LOCAL SCALARS ..
       DOUBLE PRECISION DELTA1, DELTA2, DELTA3, E0, E1, E1ABS, E2, E3,
     * EPMACH,EPSINF, ERR1, ERR2, ERR3, ERROR, OFLOW, RES, SS, TOL1,
     * TOL2,TOL3
       INTEGER I, IB2, IB, IE, IND, K1, K2, K3, LIMEXP, NEWELM, NUM
C      .. FUNCTION REFERENCES ..
       DOUBLE PRECISION X02AAF, X02ACF
       ..
C
C              MACHINE DEPENDENT CONSTANTS
C               -------------------------
C              /LIMEXP/ IS THE MAXIMUM NUMBER OF ELEMENTS THE EPSILON
C              TABLE CAN CONTAIN. IF THIS NUMBER IS REACHED, THE UPPER
C              DIAGONAL OF THE EPSILON TABLE IS DELETED.
C
       DATA LIMEXP /50/
       EPMACH = X02AAF(1.0D0)
       OFLOW = X02ACF(1.0D0)
C
C              LIST OF MAJOR VARIABLES
C              -----------------------
C              E0     - THE 4 ELEMENTS ON WHICH THE
C              E1       COMPUTATION OF A NEW ELEMENT IN
C              E2       THE EPSILON TABLE IS BASED
C              E3                  E0
C                            E3    E1     NEW
C                                  E2
C              NEWELM - NUMBER OF ELEMENTS TO BE COMPUTED IN THE NEW
C                       DIAGONAL
C              ERROR  - ERROR = ABS(E1-E0)+ABS(E2-E1)+ABS(NEW-E2)
C              RESULT - THE ELEMENT IN THE NEW DIAGONAL WITH LEAST
C                       ERROR
C
       NRES = NRES + 1
       ABSERR = OFLOW
       RESULT = EPSTAB(N)
       IF (N.LT.3) GO TO 200
       EPSTAB(N+2) = EPSTAB(N)
       NEWELM = (N-1)/2
       EPSTAB(N) = OFLOW
       NUM = N
       K1 = N
       DO 80 I=1,NEWELM
          K2 = K1 - 1
          K3 = K1 - 2
          RES = EPSTAB(K1+2)
          E0 = EPSTAB(K3)
          E1 = EPSTAB(K2)
          E2 = RES
          E1ABS = DABS(E1)
          DELTA2 = E2 - E1
          ERR2 = DABS(DELTA2)
          TOL2 = DMAX1(DABS(E2),E1ABS)*EPMACH
          DELTA3 = E1 - E0
          ERR3 = DABS(DELTA3)
          TOL3 = DMAX1(E1ABS,DABS(E0))*EPMACH
          IF (ERR2.GT.TOL2 .OR. ERR3.GT.TOL3) GO TO 20
C
C         IF E0, E1 AND E2 ARE EQUAL TO WITHIN MACHINE
C         ACCURACY, CONVERGENCE IS ASSUMED
C         RESULT = E2
C         ABSERR = ABS(E1-E0)+ABS(E2-E1)
```

```
C
      RESULT = RES
      ABSERR = ERR2 + ERR3
      GO TO 200
   20 E3 = EPSTAB(K1)
      EPSTAB(K1) = E1
      DELTA1 = E1 - E3
      ERR1 = DABS(DELTA1)
      TOL1 = DMAX1(E1ABS,DABS(E3))*EPMACH
C
C        IF TWO ELEMENTS ARE VERY CLOSE TO EACH OTHER, OMIT
C        A PART OF THE TABLE BY ADJUSTING THE VALUE OF N
C
      IF (ERR1.LT.TOL1 .OR. ERR2.LT.TOL2 .OR. ERR3.LT.TOL3) GOTO 40
      SS = 0.1D+01/DELTA1 + 0.1D+01/DELTA2 - 0.1D+01/DELTA3
      EPSINF = DABS(SS*E1)
C
C        TEST TO DETECT IRREGULAR BEHAVIOUR IN THE TABLE, AND
C        EVENTUALLY OMIT A PART OF THE TABLE ADJUSTING THE VALUE
C        OF N
C
      IF (EPSINF.GT.0.1D-03) GO TO 60
   40 N = I + I - 1
      GO TO 100
C
C        COMPUTE A NEW ELEMENT AND EVENTUALLY ADJUST
C        THE VALUE OF RESULT
C
   60 RES = E1 + 0.1D+01/SS
      EPSTAB(K1) = RES
      K1 = K1 - 2
      ERROR = ERR2 + DABS(RES-E2) + ERR3
      IF (ERROR.GT.ABSERR) GO TO 80
      ABSERR = ERROR
      RESULT = RES
   80 CONTINUE
C
C        SHIFT THE TABLE
C
  100 IF (N.EQ.LIMEXP) N = 2*(LIMEXP/2) - 1
      IB = 1
      IF ((NUM/2)*2.EQ.NUM) IB = 2
      IE = NEWELM + 1
      DO 120 I=1,IE
         IB2 = IB + 2
         EPSTAB(IB) = EPSTAB(IB2)
         IB = IB2
  120 CONTINUE
      IF (NUM.EQ.N) GO TO 160
      IND = NUM - N + 1
      DO 140 I=1,N
         EPSTAB(I) = EPSTAB(IND)
         IND = IND + 1
  140 CONTINUE
  160 IF (NRES.GE.4) GO TO 180
      RES3LA(NRES) = RESULT
      ABSERR = OFLOW
      GO TO 200
C
C        COMPUTE ERROR ESTIMATE
C
  180 ABSERR = DABS(RESULT-RES3LA(3)) + DABS(RESULT-RES3LA(2)) +
     *DABS(RESULT-RES3LA(1))
      RES3LA(1) = RES3LA(2)
      RES3LA(2) = RES3LA(3)
      RES3LA(3) = RESULT
  200 ABSERR = DMAX1(ABSERR,5.0D+00*EPMACH*DABS(RESULT))
      RETURN
      END
C
C
      SUBROUTINE D01AJZ(F, A, B, RESULT, ABSERR, RESABS, RESASC)
C                 SUBROUTINE D01AJZ, PART OF PEM (VERSION 82360).
C
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE QUARUL
C     ***********************************************
```

```
C
C     PURPOSE
C        TO COMPUTE I = INTEGRAL OF F OVER (A,B), WITH ERROR
C                       ESTIMATE
C                  J = INTEGRAL OF ABS(F) OVER (A,B)
C
C     CALLING SEQUENCE
C        CALL D01AJZ (F,A,B,RESULT,ABSERR,RESABS,RESASC)
C
C     PARAMETERS
C        F      - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND
C                 FUNCTION F(X). THE ACTUAL NAME FOR F NEEDS
C                 TO BE DECLARED E X T E R N A L IN THE
C                 CALLING PROGRAM
C
C        A      - LOWER LIMIT OF INTEGRATION
C
C        B      - UPPER LIMIT OF INTEGRATION
C
C        RESULT - APPROXIMATION TO THE INTEGRAL I.
C                 RESULT IS CALCULATED BY APPLYING
C                 THE 21-POINT GAUSS-KRONROD RULE
C                 (RESK), OBTAINED BY OPTIMAL
C                 ADDITION OF ABSCISSAE TO THE
C                 10-POINT GAUSS  RULE (RESG).
C
C        ABSERR - ESTIMATE OF THE MODULUS OF THE
C                 ABSOLUTE ERROR, WHICH SHOULD NOT
C                 EXCEED ABS(I-RESULT)
C        RESABS - APPROXIMATION TO THE INTEGRAL J
C
C        RESASC - APPROXIMATION TO THE INTEGRAL OF
C                 ABS(F-I/(B-A)) OVER (A,B)
C
C     ***********************************************
C     .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION A, ABSERR, B, RESABS, RESASC, RESULT
C     .. FUNCTION ARGUMENTS ..
      DOUBLE PRECISION F
C     ..
C     .. LOCAL SCALARS ..
      DOUBLE PRECISION ABSC, CENTRE, DHLGTH, EPMACH, FC, FSUM, FVAL1,
     * FVAL2,HLGTH, RESG, RESK, RESKH, UFLOW
      INTEGER J
C     .. LOCAL ARRAYS ..
      DOUBLE PRECISION FV1(10), FV2(10), WG(10), WGK(11), XGK(11)
C     .. FUNCTION REFERENCES ..
      DOUBLE PRECISION X02AAF, X02ABF
C     ..
C
C        THE ABSCISSAE AND WEIGHTS ARE GIVEN FOR THE
C        INTERVAL (-1,1) . BECAUSE OF SYMMETRY ONLY THE
C        POSITIVE ABSCISSAE AND THEIR CORRESPONDING
C        WEIGHTS ARE GIVEN.
C        XGK    - ABSCISSAE OF THE 21-POINT GAUSS-KRONROD RULE
C                 XGK(2), XGK(4), .... ABSCISSAE OF THE 10-POINT
C                 GAUSS RULE
C                 XGK(1), XGK(3), .... ABSCISSAE WHICH
C                 ARE OPTIMALLY ADDED TO THE 10-POINT
C                 GAUSS RULE
C        WGK    - WEIGHTS OF THE 21-POINT GAUSS-KRONROD RULE
C        WG     - WEIGHTS OF THE 10-POINT GAUSS RULE,
C                 CORRESPONDING TO THE ABSCISSAE XGK(2),
C                 XGK(4), ... WG(1), WG(3), ... ARE SET
C                 TO ZERO.
C
      DATA XGK(1), XGK(2), XGK(3), XGK(4), XGK(5), XGK(6), XGK(7),XGK(8)
     *, XGK(9), XGK(10), XGK(11) /0.9956571630258080807355272807D+00,
     *0.9739065285171717200779640121D+00,
     *0.9301574913557082260012071801D+00,
     *0.8650633666889845107320966884D+00,
     *0.7808177265864168970637175783D+00,
     *0.6794095682990244062343273651D+00,
     *0.5627571346686046833390000993D+00,
     *0.4333953941292471907992659432D+00,
     *0.2943928627014601981311266031D+00,
     *0.1488743389816312108848260011D+00,0.0D0/
```

```
      DATA WGK(1), WGK(2), WGK(3), WGK(4), WGK(5), WGK(6), WGK(7),WGK(8)
     *, WGK(9), WGK(10), WGK(11) /0.1169463886737187427806439606D-01,
     *0.3255816230796472747881897246D-01,
     *0.5475589657435199603138130024D-01,
     *0.7503967481091995276704314092D-01,
     *0.9312545458369760553506546508D-01,
     *0.1093871588022976418992105903D+00,
     *0.1234919762620658510779581098D+00,
     *0.1347092173114733259280540018D+00,
     *0.1427759385770600807970942731D+00,
     *0.1477391049013384913748415160D+00,
     *0.1494455540029169056649364684D+00/
      DATA WG(1), WG(2), WG(3), WG(4), WG(5), WG(6), WG(7), WG(8),WG(9),
     * WG(10) /0.0D0,0.6667134430868813759356880989D-01,0.0D0,
     *0.1494513491505805931457763397D+00,0.0D0,
     *0.2190863625159820439955349342D+00,0.0D0,
     *0.2692667193099963550912269216D+00,0.0D0,
     *0.2955242247147528701738929947D+00/
      EPMACH = X02AAF(1.0D0)
      UFLOW = X02ABF(1.0D0)
C
C          LIST OF MAJOR VARIABLES
C          -----------------------
C          CENTRE - MID POINT OF THE INTERVAL
C          HLGTH  - HALF LENGTH OF THE INTERVAL
C          ABSC   - ABSCISSA
C          FVAL*  - FUNCTION VALUE
C          RESG   - 10-POINT GAUSS FORMULA
C          RESK   - 21-POINT GAUSS-KRONROD FORMULA
C          RESKH  - APPROXIMATION TO MEAN VALUE OF F OVER
C                   (A,B), I.E. TO I/(B-A)
C
      CENTRE = 0.5D+00*(A+B)
      HLGTH = 0.5D+00*(B-A)
      DHLGTH = DABS(HLGTH)
C
C          COMPUTE THE 21-POINT GAUSS-KRONROD APPROXIMATION TO
C          THE INTEGRAL, AND ESTIMATE THE ABSOLUTE ERROR
C
      RESG = 0.0D+00
      FC = F(CENTRE)
      RESK = WGK(11)*FC
      RESABS = DABS(RESK)
      DO 20 J=1,10
         ABSC = HLGTH*XGK(J)
         FVAL1 = F(CENTRE-ABSC)
         FVAL2 = F(CENTRE+ABSC)
         FV1(J) = FVAL1
         FV2(J) = FVAL2
         FSUM = FVAL1 + FVAL2
         RESG = RESG + WG(J)*FSUM
         RESK = RESK + WGK(J)*FSUM
         RESABS = RESABS + WGK(J)*(DABS(FVAL1)+DABS(FVAL2))
   20 CONTINUE
      RESKH = RESK*0.5D+00
      RESASC = WGK(11)*DABS(FC-RESKH)
      DO 40 J=1,10
         RESASC = RESASC + WGK(J)*(DABS(FV1(J)-RESKH)+DABS(FV2(J)-RESKH)
     *   )
   40 CONTINUE
      RESULT = RESK*HLGTH
      RESABS = RESABS*DHLGTH
      RESASC = RESASC*DHLGTH
      ABSERR = DABS((RESK-RESG)*HLGTH)
      IF (RESASC.NE.0.D+00) ABSERR = RESASC*DMIN1(0.1D+01,(0.2D+03*
     *ABSERR/RESASC)**1.5D0)
      IF (RESABS.GT.UFLOW/(0.5D+02*EPMACH)) ABSERR =DMAX1(EPMACH*RESABS*
     *0.5D+02,ABSERR)
      RETURN
      END
C
C
      INTEGER FUNCTION P01AAF(IFAIL, ERROR, SRNAME)
C                                FUNCTION P01AAF, PART OF PEM (VERSION 82360).
C
C     MARK 1 RELEASE.  NAG COPYRIGHT 1971
C     MARK 3 REVISED
```

```
C     MARK 4A REVISED, IER-45
C     MARK 4.5 REVISED
C     MARK 7 REVISED (DEC 1978)
C     RETURNS THE VALUE OF ERROR OR TERMINATES THE PROGRAM.
      INTEGER ERROR, IFAIL, NOUT
C$P 1
      DOUBLE PRECISION SRNAME
C     TEST IF NO ERROR DETECTED
      IF (ERROR.EQ.0) GO TO 20
C     DETERMINE OUTPUT UNIT FOR MESSAGE
      CALL X04AAF (0,NOUT)
C     TEST FOR SOFT FAILURE
      IF (MOD(IFAIL,10).EQ.1) GO TO 10
C     HARD FAILURE
      WRITE (NOUT,99999) SRNAME, ERROR
C     STOPPING MECHANISM MAY ALSO DIFFER
      STOP
C     SOFT FAIL
C     TEST IF ERROR MESSAGES SUPPRESSED
   10 IF (MOD(IFAIL/10,10).EQ.0) GO TO 20
      WRITE (NOUT,99999) SRNAME, ERROR
   20 P01AAF = ERROR
      RETURN
99999 FORMAT (1H0, 38HERROR DETECTED BY NAG LIBRARY ROUTINE , A8,
     * 11H - IFAIL = , I5//)
      END
C
C
      DOUBLE PRECISION FUNCTION X02AAF(X)
C                          FUNCTION X02AAF, PART OF PEM (VERSION 82360).
C
C     NAG COPYRIGHT 1975
C     MARK 4.5 RELEASE
      DOUBLE PRECISION X
C     * EPS *
C
C     IBM DOUBLE PRECISION VERSION
C
C     RETURNS THE VALUE EPS WHERE EPS IS THE SMALLEST
C     POSITIVE
C     NUMBER SUCH THAT 1.0 + EPS > 1.0
C     THE X PARAMETER IS NOT USED
C     FOR ICL 1900
C     X02AAF = 2.0**(-37.0)
C     FOR IBM 360/370
C     X02AAF = 2.0D0**(-52.0D0)
      DOUBLE PRECISION Z
      DIMENSION ZZ(2)
      EQUIVALENCE (ZZ(1),Z)
      DATA ZZ /O171410000000,O000000000000/
C     DATA Z/Z3410000000000000/
      X02AAF = Z
      RETURN
      END
C
C
      DOUBLE PRECISION FUNCTION X02ABF(X)
C                          FUNCTION X02ABF, PART OF PEM (VERSION 82360).
C
C     NAG COPYRIGHT 1975
C     MARK 4.5 RELEASE
      DOUBLE PRECISION X
C     * RMIN *
C
C     IBM DOUBLE PRECISION VERSION
C
C     RETURNS THE VALUE OF THE SMALLEST POSITIVE REAL FLOATING-
C     POINT NUMBER EXACTLY REPRESENTABLE ON THE COMPUTER
C     THE X PARAMETER IS NOT USED
C     FOR ICL 1900
C     X02ABF = 2.0**(-257.0)
C     FOR IBM 360/370
C     X02ABF = 16.0D0**(-65.0D0)
      DOUBLE PRECISION Z
      DIMENSION ZZ(2)
      EQUIVALENCE (ZZ(1),Z)
      DATA ZZ /O000110000000,O000000000000/
```

```
      C     DATA Z/Z0010000000000000/                                  00043790
            X02ABF = Z                                                 00043800
            RETURN                                                     00043310
            END                                                        00043820
      C                                                                00043830
      C                                                                00043840
            DOUBLE PRECISION FUNCTION X02ACF(X)                        00043850
      C                          FUNCTION X02ACF, PART OF PEM (VERSION 82360). 00043860
      C                                                                00043870
      C     NAG COPYRIGHT 1975                                         00043880
      C     MARK 4.5 RELEASE                                           00043890
            DOUBLE PRECISION X                                         00043900
      C     * RMAX *                                                   00043910
      C                                                                00043920
      C     IBM DOUBLE PRECISION VERSION                               00043930
      C                                                                00043940
      C     RETURNS THE VALUE OF THE LARGEST POSITIVE REAL  FLOATING-  00043950
      C     POINT NUMBER REPRESENTABLE ON THE COMPUTER                 00043960
      C     FOR ICL 1900                                               00043970
      C     X02ACF = (2.0 - 2.0**(-36.0))*2.0**254.0                   00043980
      C     FOR IBM 360/370                                            00043990
      C     X02ACF = (1.0D0-16.0D0**(-14.0D0))*16.0D0**63.0D0          00044000
            DOUBLE PRECISION Z                                         00044010
            DIMENSION ZZ(2)
            EQUIVALENCE (ZZ(1),Z)
            DATA ZZ /O377777777777,O777777777777/
      C     DATA Z/Z7FFFFFFFFFFFFFFF/                                  00044020
            X02ACF = Z                                                 00044030
            RETURN                                                     00044040
            END                                                        00044050
      C                                                                00044060
      C                                                                00044070
            SUBROUTINE X04AAF(I,NERR)                                  00044080
      C                   SUBROUTINE X04AAF, PART OF PEM (VERSION 82360). 00044090
      C                                                                00044100
      C     MARK 7 RELEASE. NAG COPYRIGHT 1978                         00044110
      C     MARK 7C REVISED IER-190 (MAY 1979)                         00044120
      C     IF I = 0, SETS NERR TO CURRENT ERROR MESSAGE UNIT NUMBER   00044130
      C     (STORED IN NERR1).                                         00044140
      C     IF I = 1, CHANGES CURRENT ERROR MESSAGE UNIT NUMBER TO     00044150
      C     VALUE SPECIFIED BY NERR.                                   00044160
      C                                                                00044170
      C     *** NOTE ***                                               00044180
      C     THIS ROUTINE ASSUMES THAT THE VALUE OF NERR1 IS SAVED      00044190
      C     BETWEEN CALLS.  IN SOME IMPLEMENTATIONS IT MAY BE          00044200
      C     NECESSARY TO STORE NERR1 IN A LABELLED COMMON              00044210
      C     BLOCK /AX04AA/ TO ACHIEVE THIS.                            00044220
      C                                                                00044230
      C     .. SCALAR ARGUMENTS ..                                     00044240
            INTEGER I, NERR                                            00044250
      C     ..                                                         00044260
      C     .. LOCAL SCALARS ..                                        00044270
            INTEGER NERR1                                              00044280
      C     ..                                                         00044290
            DATA NERR1 /6/                                             00044300
            IF (I.EQ.0) NERR = NERR1                                   00044310
            IF (I.EQ.1) NERR1 = NERR                                   00044320
            RETURN                                                     00044330
            END                                                        00044340
**
@BRKPT  PRINT$
```