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DEVELOPMENT OF AN URBAN AIR QUALITY SIMULATION MODEL WITH COMPATIBLE RAPS DATA VOLUME I

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by

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San Jose, California 95193

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Final Report

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Abstract

An advanced generalized urban air quality model (IBMAQ-2) is developed based on the theory utilized in an existing model (IBMAQ-1) as prescribed in Ref. 1. The model, based on numerical integration of the concentration equation, computes temporal and three-dimensional spatial concentration distributions resulting from specified urban point and area sources by using NEDS (National Emission Data System) and simulated RAMS (Regional Air Monitoring System) data. The urban surface roughness values, estimated from measured mean building heights and calculated building density, are treated explicity as input parameters. The UTM (Universal Transverse Metric) coordinates are used in all geographical, source emission, and monitoring data. A new method to incorporate point sources into the grid computation is developed by using a Lagrange trajectory method. Many model options are provided which enable users to study conveniently the significant effects which these options have on the final concentration distributions. These options offer the user not only flexibility in the adoption of data, but also offer one timely optimization of the model.

The program description is included to provide a guide for users. The program is constructed in a modular form which allows users to change or improve each component conveniently. The input auxiliary model, which processes geographical, source emission, and monitoring data, is also included.

The model was tested using simulated meteorological conditions for a three-day period. The significant effects of urban surface roughness on concentration distribution were also investigated.

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I. MODEL DESCRIPTION

1. Introduction

An urban air quality simulation model can be used to study the complex relation between the source emissions and ambient concentrations, and the dependence of this relation on the meteorological and urban surface conditions. The development of such a model depends on current knowledge of urban air pollutant transport, on the diffusion mechanism, and on the availability and quality of source emission, meteorological, and surface condition data. In addition, the purpose and computation requirements of the model should be taken into consideration. Therefore, the degree of sophistication of a model should be commensurate with data availability, computational facility, and application purposes. A brief summary of the development of various modeling approaches and the objectives of developing a grid model are discussed in Ref. 1, which is included in the appendix.

We are concerned herein with a research-oriented model. Its purpose is not only to understand air pollutant transport phenomena, but also to study various significant parameters which affect the urban air quality. Although the model utilizes currently available data, through study of its results one can infer additional characteristics or types of data that may be useful and therefore should be collected in the future. In

addition, the model can be used to study and verify various assumptions used in simpler model formulations. Therefore, it can serve as a guide for the future development of an improved simpler model.

In this work, an advanced urban air quality simulation model is developed based on the numerical integration of the concentration equation over a specified set of grid elements. The model offers a large degree of flexibility by taking into account the temporal and spatial variation of meteorological variables and surface conditions. These parameters are not normally incorporated in most simplified models. Moreover, the model is designed to be able to accept both extensive and limited amounts of data. It is especially developed to adopt RAPS and RAMS data collected in the St. Louis metropolitan area for evaluation and validation. However, during the course of model development, the data acquisition system of these programs had not yet been completed. Therefore, the model development could not benefit from the proposed extensive data collection, and further improvement or modification may be needed when this data becomes available. The model is applied to determine the SO_2 distribution in St. Louis. It also can be extended to study multiple-species distributions without extensive modification.

2. Model Formulation

2-A. Simulation Region and Grid System

The region of interest is the St. Louis metropolitan area as defined in the RAPS project. The factors which are considered, are as follows: spatial distributions of point and area sources, area sources inventory resolution, monitoring station distribution, computational grid resolution and computational requirements. Most of the area sources are concentrated in a region of 20 by 20 km in the St. Louis area. The point sources are distributed along the Mississippi river, extending from the Alton area in the north to 60 km south downstream. A region of 60 km north-south by 40 km east-west centered at RAMS station 101 is sufficient to cover the major point and area sources as well as most of the RAMS stations. The individual area source inventory grid elements in the St. Louis urban area are 1 km square. Using a uniform 1 km grid system, a 40 x 60 network with a total of 2400 grid elements is required for the region. This number is too large for our computation. In view of this, a "stretch" grid system is designed to obtain optimum resolution and economical computations. This system is composed of 30 grid elements east-west and 40 grid elements north-south. In additions, there are finer grid elements 1 km square at the center urban region, and coarser grid elements of 1 km by 2 km

rectangular size and 2 km x 2 km size on the outer suburban region. The total volume in the region and under the mixing height is to be simulated. There are four remote RAMS stations outside the region which may provide some information about the background concentrations. There are also three significant point sources outside the region, and their effects on the concentrations inside the region require a further investigation.

2-B. Equations, Boundary Conditions and Initial Conditions

Since this area has a reasonably flat terrain, the effects of topography are neglected. The surface roughness parameter z_o is used to represent the effects of urban buildings, forests, and rolling hills. SO_2 emission is considered passive and therefore does not alter the meteorological conditions. The turbulent diffusion of SO_2 is assumed to be of the gradient diffusion type. The governing equation of SO_2 in the atmosphere based on the mass conservation law is

$$\frac{\partial C}{\partial t} + \nabla \cdot \underset{\rightarrow}{V} C = K_H \nabla_H^2 C + \frac{\partial}{\partial z} K \frac{\partial C}{\partial z} + Q + R \quad , \qquad (1)$$

where C is the mean concentration of SO_2, $\underset{\rightarrow}{V} = (U, V, W)$ is the mean wind vector, Q is the source strength rate, R is the chemical reaction rate, K_H is the horizontal eddy

diffusivity, ∇_H^2 is the horizontal Laplacian operator, and K is the vertical eddy diffusivity. The upper and lower boundary conditions are:

$$K \frac{\partial C}{\partial z} = 0 \quad , \quad z = 0, H \quad , \tag{2}$$

where $H = H(t)$, the mixing depth of the planetary boundary layer, is assumed constant in space due to the fact that the data for a spatially varying H are difficult to obtain and not likely to be available in the near future. The absorption of the SO_2 by the ground surface is neglected because it requires data describing the surface properties and their absorption rate. The significance of the spatially varying mixing height and surface absorption rate must be investigated, so that their priority in a data base can be established. As these data become available, their incorporation into the model is a simple matter. The inflow lateral boundary conditions are:

$$C = C_b \quad , \quad \text{if } \underset{\rightarrow}{V} \cdot \underset{\rightarrow}{n} < 0 \quad ; \tag{3}$$

where C_b is the background concentration, and $\underrightarrow{n}$ is the unit outward vector normal to the lateral surface. The outflow lateral boundary conditions are:

$$\frac{\partial^2 C}{\partial x^2} = 0 \quad , \quad x = 0, \; x_{max} \quad , \qquad (4)$$

and

$$\frac{\partial^2 C}{\partial y^2} = 0 \quad , \quad y = 0, \; y_{max} \quad . \qquad (5)$$

Where x_{max} and y_{max} are the east and north boundries of the area respectively. The data required to specify the exact lateral boundary conditions are not available. These conditions in (4), (5), which extrapolate the concentration outside the region, serve as a reasonable approximation when the region of computation is large enough. In practice, and as we have found, the lack of well-posed boundary conditions (due to the absence of data required for the proper conditions) does not cause serious problems. This is because the horizontal advection terms, which dominate the horizontal diffusion terms, are only first order in the

space derivative. The computation may be affected by the inflow boundary conditions. However, if there is no high concentration outside the inflow boundary this influence is minimal, and the linear extrapolation could offer a fair approximation. In this study, the computational region is about ten times larger than the urban area in which major sources are located. Moreover, there is no nearby major urban area to influence the inflow boundary conditions, although there are three major point sources located to the west and south of this region. Their influences may not be negligible under certain meteorological conditions. The effects of these remote point sources and return flow cannot be treated by this model alone. One approach would be an experimental study to determine the background concentration in order to evaluate the necessity of developing a larger regional model to estimate the background concentration. Since the background concentrations may be from elevated sources, the surface concentration measurement alone may not be sufficient to describe their three-dimensional spatial distributions.

The initial conditions of concentration are arbitrarily set to zero. The required three-dimensional initial concentration distributions cannot be generated easily from the surface measurements alone. The model requires the initialization of the surface concentration distributions based on the observed data from the monitoring stations as

well as the vertical distributions of concentration. These input data are not usually available. However, the computations show that the concentrations reach observed levels approximately within two hours under average wind speed conditions. Hence, the initial conditions are not important for the concentration computations after this initial time. This required time period depends on the wind speed and the region of interest. This time interval can be estimated by $T_u \simeq L/u$, here L is the distance downwind from the sources and u is average wind speed. However, this may not be valid when the wind changes its direction drastically during this time period. In this case, the initial period may need to be longer. However, it is better, if possible, to select an initial period in which the wind directions do not vary too much. The model simulation can begin at an arbitrary time. However, it is simplest to begin at a time which is consistent with the time period used for acquisition of the input data (e.g., if the air quality measurements are on a 24 hourly basis beginning 1400 LST, then the model computations should be started at 1400 LST). In addition, in order to compare the computed and observed results, one should have compatible average time periods of computations and field measurments.

2-C. Parameterization

The parameters required for the integration of the equation

(2) are $\vec{V}$, K_H, K, Q, R, and H, which, except for Q, are not provided explicitly or sufficiently. The following discussion outlines the methods which were used to obtain the required input data for the model.

It must be pointed out that the choice of parameterization is a very delicate matter and may be somewhat controversial. The parameterization of a model depends on the availability and the accuracy of input data, the best available theory, and computer resources available. Since none of these factors is static, but all are continuously changing and improving, one must leave some leeway in the model for future improvement. In addition, the model can also be used to study the significance and ramifications of various atmospheric variables available from future measurements. Thus, more parameterization options than are essential should be included in order to allow users to study their potential effect, to optimize the model, and to point the way for future data acquisition. The following methods of parameterization represent the best efforts of the authors based on available data, current theory, and computer capability. We emphasize that many options of the parameterization have been included in the model for the purposes of optimization, sensitivity testing, directing future data acquisition, and future model improvement. When all RAPS and RAMS data become available, one may have to re-examine these parameterizations.

2-C-a) Wind field

(i) Horizontal wind distribution

The wind vector $\underset{\rightarrow}{V} = \underset{\rightarrow}{V}(x, y, z, t)$ is required at every grid element for each time step of integration. The time-averaged surface wind field for the total region was obtained by using a weighted interpolation scheme. Data from the measurement stations were interpolated to a square grid. The choice of the grid size for this analysis grid system requires an empirical study. In general, it depends on the spatial distribution and density of the observation network of wind vector and the spatial variability of the wind field within the region of the study. Currently, the grid size of 4 KM is used. Several schemes have been tested in this analysis. It was found that reasonable results can be obtained from the equations:

$$\bar{u}_{ij} = \frac{\sum_{m,n} (\tilde{u}_{mn}/r_{mn}^2)}{\sum_{m,n} (1/r_{mn}^2)} \quad \text{and} \quad \bar{v}_{ij} = \frac{\sum_{m,n} (\tilde{v}_{mn}/r_{mn}^2)}{\sum_{m,n} (1/r_{mn}^2)} \; .$$

where u_{ij} and v_{ij} are components of the wind vector at analysis grid points in x and y directions, respectively;

$\tilde{u}_{mn}$ and $\tilde{v}_{mn}$ are initial guess field values at analysis grid points and r_{mn} is the distance from grid point point (i,j) to grid point (m,n). The initial-guess field is obtained by assuming

$$\left.\begin{aligned} \tilde{u}_{mn} &= u_k \\ \tilde{v}_{mn} &= v_k \end{aligned}\right\} \quad \text{for minimum of } r_k \quad ,$$

where u_k and v_k are wind vector components measured at station k and r_k is the distance from a grid point to station k.

From this analyzed wind field a linear interpolation is employed to obtain a wind vector at each grid point used in the numerical scheme. The interpolation formula for the u component of the wind vector is

$$u_{k\ell} = (1-a)\cdot(1-b)\cdot\bar{u}_{ij} + a\cdot(1-b)\cdot\bar{u}_{i+1,j} + (1-a)\cdot b\cdot\bar{u}_{ij+1} + a\cdot b\cdot\bar{u}_{i+1,j+1} \quad ,$$

where $0 \le a = \delta x/D \le 1$; $0 \le b = \delta y/D \le 1$. δx and δy are

the distances between numerical grid point (k,l) and wind analysis grid point (i,j) in x and y direction respectively. D is the grid size of wind analysis grid. Similar expression is used for V component of the wind vector.

In summary, the procedure for computing the wind vector at each grid point used in the numerical scheme is as follows:

- A square grid system (wind field analysis grid) is selected which is 4 km in size.

- An initial-guess wind vector $(\tilde{u},\tilde{v})$ is obtained at each grid point (m,n) from nearest available observation station.

- The weighted interpolation formula is applied to the initial-guess field to obtain the wind vector at each analysis grid point.

- Simple linear interpolation is used to obtain the wind vector at each grid point used in the numerical scheme from the wind vector values at the four nearest adjacent analysis grid points.

The analysis of a mesoscale wind field is a very complex problem. In reality, we do not expect the simple method

employed here will be able to handle all possible meteorological conditions. Due to the unavailability of RAMS data, whether a more complex method is necessary has yet to be determined.

The model also includes an option to use a subjective wind field analysis. This is included in order to compare the reliability of various wind-analysis schemes. It also includes two other options; using a uniform wind field, and generating the wind field directly from RAMS data. The former could be used to study the significance of non-uniform distribution of wind, and the latter is included for future daily operation of the model.

(ii) Vertical distribution of wind

The spatial distribution of upper layer wind data was not available, and the present knowledge of urban meteorology cannot offer much information about this distribution. Fortunately, the concentration at those locations where the local sources dominated are not sensitive to the upper wind. The vertical wind profiles at each grid location are assumed to be of power-law form:

$$|\underset{\rightarrow}{V}| = |\underset{\rightarrow}{V}_s| \ (z/z_s)^p \quad , \qquad (6)$$

where $\underset{\rightarrow}{V}$ and $\underset{\rightarrow s}{V}$ are the upper and surface wind velocities at the height z and z_s respectively. The power constant p is determined by

$$p = \ell n\ (|\underset{\rightarrow}{V}_3|/|\underset{\rightarrow}{V}_1|)/\ \ell n(z_3/z_1) \quad , \qquad (7)$$

where $\underset{\rightarrow}{V}$ and $\underset{\rightarrow 1}{V}$ are the winds at the height z_3 and z_1. The values of p are restricted between 0.15 and 0.65 which are the usually observed values (Ref. 2). The direction of the upper wind is also unknown. It is understood that the upper wind usually has a direction to the right of the surface wind in the northern hemisphere. However, this angle cannot be determined quantitatively from any theory under general conditions. Two methods have been previously tested. One method assumes no directional change and the other assumes equal angle change with height from z_s to z_3. Results from both methods differ very little. Since the upper air sounding data for RAPS were not available, it did not seem profitable to develop any new scheme to use these unavailable data.

(iii) Vertical wind components

The vertical winds are important under certain meteorological conditions such as strong convergence due to the urban heat island effect or to frontal passage. However, these data are usually not available. Thus, the vertical winds were calculated from horizontal winds through the continuity equation. In the previous study, the interpolated horizontal winds are so smooth that the vertical winds are too small to influence the concentration distributions significantly. In addition, the incomplete knowledge of the vertical winds resulting from the urban heat island effects make the simulation of the vertical wind difficult. Moreover, when the upper air sounding data are not recorded at a fixed location, substantial pre-analysis is required before they can be used for the model. The effects of vertical wind on the urban atmospheric transport remain to be investigated.

2-C-b) Atmospheric stability

It is well known that turbulent diffusion of air pollutants is the second most important mechanism next to the wind transport in affecting air pollutant dispersion. Its magnitude is directly related to the atmospheric turbulence intensity. However, due to the complex and heteorogeneous distribution of the atmospheric turbulence, it is not simple

to describe or categorize the turbulence intensity. The most significant factors influencing the turbulence are wind, atmospheric stability, and surface conditions. The surface condition, parameterized here as surface roughness, has been especially neglected in most of the previous air pollution diffusion theories and air pollution models. However, it is the fundamental mechanical property influencing the atmospheric flows. A practical method to categorize the turbulence by considering the three components, namely, wind, stability, and surface roughness, has been developed and described in detail in Ref. 1. The method first entails the calculation of the gross modified Pasquill's stability class, which is a continuous function, and then estimates the Monin-Obukhov length by the following expressions:

$$1/L = \pm [d \cdot \ell n\ (1.2 + 10/z_o)]^2 \cdot 10^{f(S)} \quad , \quad (8)$$

and

$$f(S) = -a/(1+b|S|^c) \quad , \quad (9)$$

where S is the stability class; a=4, b=1.3, c=.85, d=0.216586, and $z_o=z_o$ (x,y) is the surface roughness parameter in meters. The stability parameter S=0 denotes neutral conditions, and negative and positive values of S denote unstable and stable conditions respectively. Thus, the sign of L in equation (8) must be the same as that of S. Moreover, the continuous values of S as discussed previously allow smooth changes between stability classes.

Since this method which requires minimal data of wind, insolation, and surface roughness, is much easier to use than measuring vertical temperature distributions, its merits should not be overlooked. Certainly, it may require further improvements such as continuous insolation classifications, non-uniform spatial stability distributions, and effects of precipitation. The accuracy of this method has to be evaluated using available data. Future RAMS data will provide the vertical temperature difference at 12 stations. It is not yet clear how to more usefully utilize these data to describe the spatial distribution of turbulence than the method used here because these data are not yet available.

From the previous study, we did not find any systematic errors (the difference between the computed and observed concentration) with respect to the stability parameter. Hence, no obvious errors from this method of determining

stability can be determined.

2-C-c) Eddy diffusivity

The treatment of turbulent diffusion as gradient diffusion is a classical method. In view of the scarcity of the relevent meteorological data needed to describe the heteorogeneous turbulence distributions over an urban area and test any turbulence theory, it is doubtful that a more sophisticated method is necessary. The method to determine the eddy diffusivity developed here is based on experimental data and computed results from the turbulent transport model which is described in Ref. 1, and can be expressed as follows:

$$K = u_* \ell / \phi_h \ , \quad \ell = k_o z e^{-b_o z/H} \ , \qquad (10)$$

where u_*, ϕ_h, k_o and H are friction velocity, non-dimensional temperature gradient, von Karman constant, and the height of the boundary layer, respectively. The factor b_o, which should be a function of stability, has a value of 4 determined by the turbulent transport model (Ref. 3). Its dependence on the stability requires further investigation. From given L and $\vec{V}_s$ (wind velocity at z = 10m), we can calculate K_s from the following procedures:

1. Calculate u_* from $\underset{\rightarrow}{V}_s$, L and z_o by

$$u_* = k_o |\underset{\rightarrow}{V}_s| / \psi_m, \tag{11}$$

where

$$\psi_m = \int_{z_o}^{z} (\phi_m / \tilde{z})\, d\tilde{z}, \tag{12}$$

ϕ_m is the non-dimensional wind shear. According to Businger, et al (Ref.4), ϕ_m can be expressed as follows:

$$\phi_m = \begin{cases} 1 + \alpha\zeta & , \zeta \geq 0; \\ (1 - \beta\zeta)^{-1/4} & , \zeta < 0, \end{cases}$$

where

$$\zeta = z/L, \quad \alpha = 4.7, \quad \text{and} \quad \beta = 15.$$

By use of last equations, equation (12) after integration becomes

$$\psi_m = \begin{cases} \ell n\ (1 + z/z_o) + \alpha\zeta & \text{for } \zeta \geq 0; \\ \ell n\ (1 + z/z_o) - 2\ell n\ [(1 + \omega)/2] - \ell n\ [(1 + \omega^2)/2] & \\ \quad + 2\tan^{-1}\omega - \pi/2 \quad , \quad \text{for } \zeta < 0, & \end{cases} \tag{13}$$

where

$$\omega = 1/\phi_m \quad .$$

2. Calculate K from u_* and ϕ_h by

$$K = u_* \ell/\phi_h \quad , \tag{14}$$

where

$$\phi_h = \begin{cases} \gamma + \alpha\zeta & , \quad \zeta \geq 0 \ ; \\ \gamma(1 - \beta'\zeta)^{-1/2} & , \quad \zeta < 0 \ , \end{cases}$$

and

$$\gamma = 0.74, \ \beta' = 9 \ .$$

Formulas (12) to (14) are valid in the surface layer. We calculate $K_s = K(z=10m)$ and then extrapolate K to higher altitude by $K = K_S \, \ell/\ell_s$. This approach by no means implies that the turbulent diffusion of air pollutants over an urban area is really so simple. These formulas, derived from experimental data, are based on the assumption of equilibrium for the turbulence. This assumption may not hold over an urban area where the horizontal inhomogeneity plays an important role, because turbulence is not in equilibrium in the vicinity of a change in surface roughness and temperature. However, little information is available about the urban effects on the eddy diffusivity. The formulas used here are subject to improvement when more knowledge is available. However, we feel that this method is a significant improvement over existing methods because the effects of the surface roughness are taken into account

in the calculation of L and K. The effects of the surface roughness which are neglected in most other approaches, can influence the concentration distribution significantly.

The horizontal eddy diffusivity, K_H, has less effect on the surface concentration distributions than K, the vertical eddy diffusivity. However, it does significantly affect the concentration from point sources and may not be neglected. As the numerical scheme for the advection is significantly improved, the artificial diffusion from finite difference approximation error is reduced. This will require the horizontal eddy diffusivity to be estimated more accurately. Both the horizontal and the vertical eddy diffusivity depend on the height, wind, stability, and surface roughness. Moreover, K also depends on the meso-scale wind motion which may be prominent under stable conditions. The meso-scale wind influences are too complex to describe in a simple formula. As a preliminary formulation, we have found that the horizontal eddy diffusivity can be related to the vertical eddy diffusivity K by the relation:

$$K_H = f_k\ (z,S)\ K \quad ,$$

where to a first approximation, f_k is dependent on height

and atmosphere stability conditions. Although it is not possible to determine the form of f analytically, its behavior and values as an empirical representation can be infered in principle from experimental data or from calculation with an appropriate turbulent transport model. Recently our study indicated that the value of f_k varies slowly with height and stability conditions, and is about 10 near neutral conditions toward the top of the surface layer. However, further study is required to obtain more precise results and a more adequate functional representation of $f_k(Z,S)$. Currently, $f_k = 10$ is assumed in the model computations.

2-C-d) Surface roughness

The surface roughness, which is the fundamental mechanical surface property affecting the atmospheric flow, is neglected in most air quality models. There may be several reasons for this. In the past, both Gaussian Plume diffusion theory and the empirical determination of the diffusion parameters (σ_z, σ_y) do not explicitly include the effects of surface roughness. Recently, Pasquill (Ref. 5) included the effects of surface roughness on the σ_x and σ_y. Another reason for omitting the effect of surface roughness is related to the lack of such data over an urban area. Thus, surface roughness effects may be treated implicitly

through a "tune up" process rather than calculated explicitly. The most widely used "tune up" method for including the surface roughness in a Gaussian plume model is to modify the initial values of σ_z according to the average building height of the area source grid elements.

The following simple formula was used to estimate the roughness length of the urban area (Ref. 6):

$$z_o = 0.5 \quad rh \quad , \tag{15}$$

where r is the silhouette area ratio and h is the effective mean height of the roughness elements. Data for the mean building heights and mean surface altitudes are available for the St. Louis area. Those of natural roughness elements, such as forest, and the silhouette ratio are not available. The silhouette ratio, which is the density of the roughness elements, has values ranging from about 0.05 to 0.5 from rural to urban area, respectively. One crude method to estimate the building density is to assume that the building density is proportional to the annual area source emission from space heating. This enables one to estimate the urban surface roughness approximately without extensive survey data. Although this method is not totally

satisfactory, it constitutes a plausible effort to include the effects of surface roughness when sufficient data are not available.

The formulas used to estimate the silhoutte ratio and the effective mean height of the roughness elements are the following:

$$r = 0.04\ (1 + Q_a(x,y)/\bar{Q}_a) \quad , \qquad (16)$$

$$h = h_b + 0.2\ h_t + 5 \quad ,$$

where Q_a and $\bar{Q}_a$ are the annual mean areas source strength and its spatial average value respectively; h_b and h_t are the mean building height and terrain height respectively. Inclusion of the terrain height is based on the assumption that the rolling hills in the south-west area also contribute to the turbulent mixing. The validity of equation (16) requires further investigation. The constant 5m term in the formula for h represents our assumption of the contribution of the natural roughness elements to the effective mean height. This term leads to a minimum value of surface roughness of 10 cm from the formula for z_o. This method will be used until the extensive survey data become

available. The effects of surface roughness on the distribution of the surface concentration are significant. The magnitude of influence depends on the atmospheric stability condition and heights of emitting sources. In St. Louis area, our model computations indicate that a reasonable results of the surface concentration values can still be achieved by the use of a less complicated method for estimating surface roughness. However, it is important that the estimated values of surface roughness should represent the characteristics of the surface obstacles in the simulation region.

2-C-e) The mixing height

The mixing height is an important parameter to determine the volume in which air pollutants can be diluted by turbulent mixing. This mixing height usually varies temporally and spatially, and is difficult to predict accurately by either surface measurements alone or planetary boundary layer theory. However, when the source-receptor distance is not too large such as in St. Louis, and the mixing height is greater than 1000 m, it does not have profound effects on the surface concentration in the central urban area because the time of advection is shorter than the time of diffusion. In general, the determination of the mixing height requires at least two measurements: one each for the daily maximum and minimum height. In this study, since no data were

available, the average values of previously measured data are used. In modeling the mixing height, the air pollutants can be totally confined within the mixing height during its diurnal variation. This approach seems to be reasonable in the morning during the growth period of mixing height. On the other hand, in the evening period, the temperature lapse rate usually approaches a neutral profile and then a stable lapse rate starts to grow near the surface. This causes a certain portion of the air pollutants to be left above the mixing height. When this type of discontinuous mixing height occurs, the air pollutants can no longer be assumed totally confined underneath the mixing height.

2-C-f) Chemical reaction rate

The chemical reaction rates of SO_2 is expressed by $R = -k_a c$, where k_a is the reaction rate constant. The chemical reaction parameterization in the model could be considered controversial due to its complexity. Its dependencies on various factors such as insolation, water vapor, and other pollutants are not yet completely clear. These chemical reaction effects could be significant under low wind-speed condition, when the time scale of a chemical reation is comparable to the time scale of advection. A high value for the chemical reaction rate, namely a half-life about two hours, was used in the previous study. The results

nonetheless showed that the model constantly over-predicted values for the low wind-speed cases. This is not easily explained by the choice of the chemical reaction rate alone. It involves more complex factors such as the assumed emission rate and emission height of the area sources. With the current magnitude of the uncertainty in the area source emission, this discrepancy requires further investigation of both the chemical reactions and area source emission inventory.

2-D. Methods of Analysis

2-D-a) Grid specifications

The three dimensional 30x40x14 grid system consists of 16800 grid elements (Fig. I-1). The x, y, z axes are oriented E-W, N-S and vertically, respectively.

The horizontal grid sizes are specified as follows:

$$\Delta x_i = 1000 \text{ m} \quad , \quad 6 \leq i \leq 25 \quad ,$$
$$= 2000 \text{ m} \quad , \quad \text{otherwise} \quad ,$$

$$\Delta y_j = 1000 \text{ m} \quad , \quad 11 \leq j \leq 30 \quad ,$$
$$= 2000 \text{ m} \quad , \quad \text{otherwise} \quad .$$

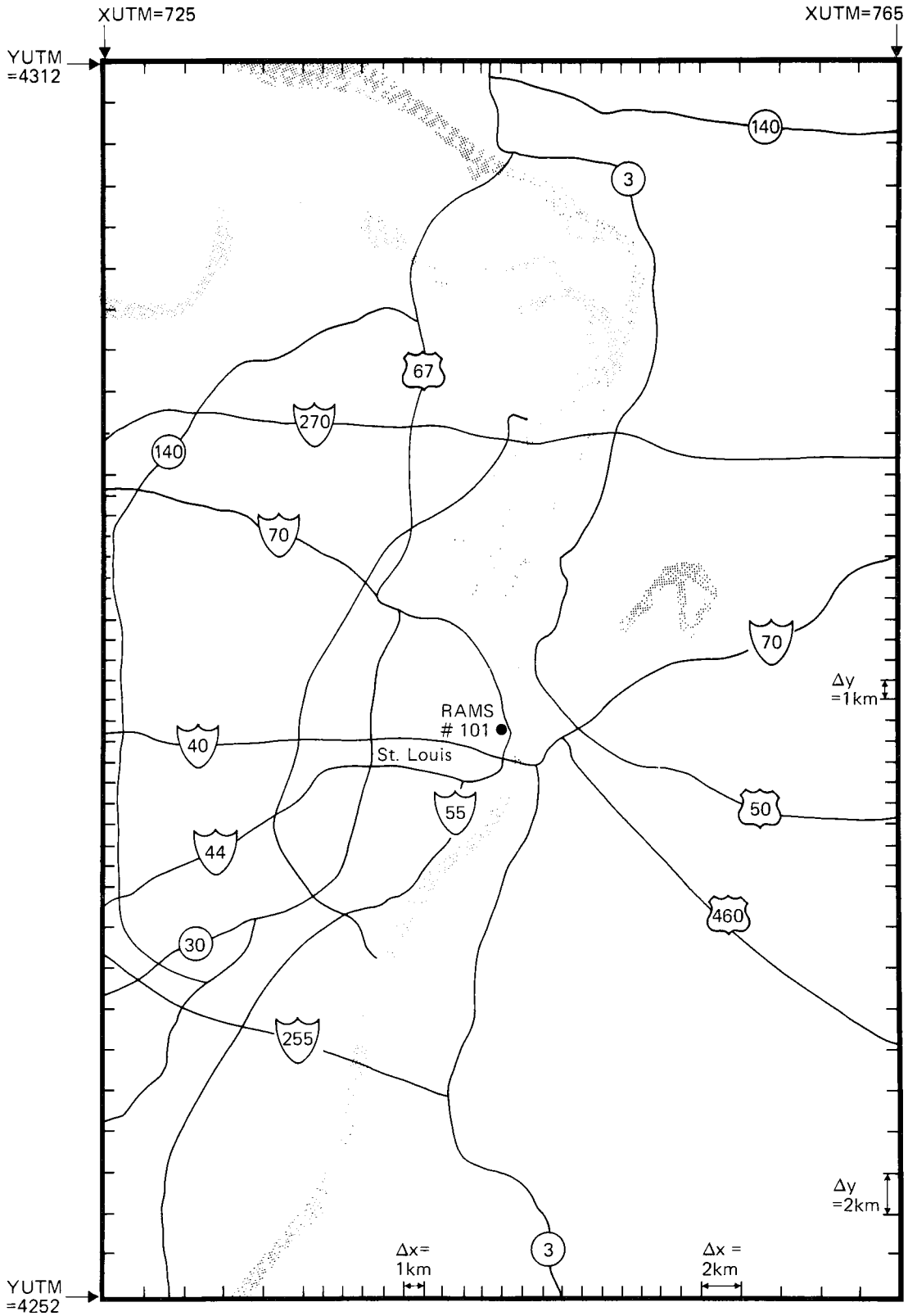

Fig. I-1 The St. Louis metropolitan area and horizontal numerical grid specification.

This system, which may be termed a "stretched" grid system, can cover a 40x60 square km area, and encompass smaller grid sub-elements compatible with the area source inventory grid size at the central urban area. It also has other advantages such as the program is invariant to grid size, and excessive index computation can be avoided. It must be noted that the horizontal coordinate system used here is the Universal Transverse Mercator (UTM) system (Ref. 7). The vertical grid sizes are specified as follows:

$$\Delta z_k = \begin{cases} 20\text{m} & , \ 1 \leq k \leq 5 \ ; \\ 25\text{m} & , \ 6 \leq k \leq 9 \ ; \\ (H-200)/4 & , \ 10 \leq k \leq 13, \text{ for } H \geq 300\text{m}; \\ 25\text{m} & , \ 10 \leq k \leq 13, \text{ for } H < 300\text{m}, \end{cases}$$

where H is the mixing height when $H \geq 300m$. The lower nine grid points under 200m have a fixed spatial size because the effective heights of point and area sources are within this layer. The levels of the upper four grid points are determined by the hourly varying mixing height. The grid spacing for these four grid points is set to be larger than or equal to 25m. Thus, the minimum height of the grid system is 300m. When the mixing height is lower than the top of the grid system, the grid spacing remains constant. However, small values of eddy diffusivity were forced at those levels located in the inversion layer the mixing height, where the mixing is small.

2-D-b) Numerical Methods

A second-order central finite-difference scheme was used to integrate the advection and horizontal diffusion term. Since the concentration fields usually have large variations, phase errors and damping resulting from the finite difference method are large, and careful treatment is required. Our finite difference approximation to the concentration equation is

$$C_{ijk}^{n+1} = C_{ijk}^{n} + U[C_{ijk}^{n}] + V[C_{ijk}^{*}] + W[C_{ijk}^{**}] + \mathcal{D}_{xy}[C_{ijk}^{n}] \quad (17)$$

$$+ \mathcal{D}_{z}[C_{ijk}] + \Delta t\, Q_{ijk}/\Delta V - \Delta t\, k_a\, C_{ijk}^{n} \ ,$$

where $\Delta V = \Delta x \Delta y \Delta z$ is the grid volume, and U, V, W are finite difference operators for horizontal (U,V) and vertical (W) advection, and $\mathcal{D}_{xz}$ and $\mathcal{D}_{z}$ are analogous operators for horizontal and vertical diffusion. The time step index is denoted by n, and i, j, k are grid indices

along the x, y, z directions respectively. The asterisk denotes the interim values when a time-splitting operation which will be explained later has been performed. The operators U, V, and W are defined by

$$U[C_{ijk}] = F_x\,[C_{ijk}] - F_x'[C_{ijk}],$$

and

$$V[C_{ijk}] = F_y\,[C_{ijk}] - F_y'[C_{ijk}],$$

$$W[C_{ijk}] = F_z\,[C_{ijk}] - F_z'[C_{ijk}],$$

where the F-factors, representing the amount of the concentration flux on the boundary of the grid element, are defined as follows:

$$F_x = \min\,(C_{i-1,jk},\ \hat{F}_x)\ ,\ \text{if } \alpha_{xi} > 0\ ; \qquad (18a)$$

$$= \min\,(C_{ijk}\ ,\ \hat{F}_x)\ ,\ \text{if } \alpha_{xi} < 0\ ,$$

$$F_x' = \min\,(C_{ijk}\ ,\ \hat{F}_x')\ ,\ \text{if } \alpha_{x\,i}^{*} > 0\ ; \qquad (18b)$$

$$= \min\,(C_{i+1,jk}\ ,\ \hat{F}_x')\ ,\ \text{if } \alpha_{x\,i}^{*} < 0\ ;$$

where

$$\hat{F}_x\,[C_{ijk}] = \frac{\alpha_{xi}}{(1+r_{xi})}\,[(1+\alpha_{xi})C_{i-1,jk} + (1-\alpha_{xi})C_{ijk}], \quad (18c)$$

$$\hat{F}_x'[C_{ijk}] = \frac{\alpha_{xi}r_{xi}}{(1+r_{xi})}\,[(1+\alpha_{xi})C_{ijk} + (1-\alpha_{xi})C_{i+1,jk}], \quad (18d)$$

$$r_{xi} = \Delta x_i/\Delta x_{i-1},\ \alpha_{xi} = \Delta t\ U_{i-\frac{1}{2},jk}/\Delta x_{i-1} \quad ,$$

and

$$\alpha^*_{xi} = \Delta t\ U_{i+\frac{1}{2},jk}/\Delta x_i \quad .$$

The similar expressions for F_y and F'_y can be obtained by interchanging the index i by j in equations (18). Similarly, for F_z and F'_z, we replace x and i by z and k, respectively. Equations (18) apply to non-uniform grid spacings. If grid space is uniform in x and y directions, $\Delta x_i = \Delta x$, $\Delta y_j = \Delta y$, $r_{xi} = 1$ and $r_{yj} = 1$. The time-splitting method employed is such that the new values of C calculated from the U operator are used for the V operator. Thus, we have

$$C^{*}_{ijk} = C^{n}_{ijk} + U[C^{n}_{ijk}] \quad ,$$

and

$$C^{**}_{ijk} = C^{*}_{ijk} + V[C^{*}_{ijk}] \quad .$$

The derivation of finite difference scheme for horizontal advection is given in Appendix 6. This method preserves the amount of concentration when it is transported from one grid element to the next. Because the method restricts the flux advected from any grid elements to be larger than or equal to the mass in that elements. In addition, it prevents the concentration values from becoming negative due to phase errors. For x direction advection, by comparing a Taylor series expansion and the finite-difference formula used in the model, it can be shown that the truncation error ε for an uniform grid is

$$\varepsilon = \frac{(1 - \alpha^2)\Delta x^2}{6} \left[U\Delta t \frac{\partial^3 C}{\partial x^3} - 3 \frac{\partial N}{\partial x} \right] \qquad (19)$$

where

$$N = \min\left(0, \frac{2C}{(1+\alpha)\Delta x} - \frac{\partial C}{\partial x}\right) \quad ,$$

$$\alpha = U\Delta t/\Delta x \quad .$$

The detailed characteristics of this finite difference operator are not easily analyzed. The reason for this lies in the non-linearity which causes interaction between modes of different wavelengths. The first term of the error is that of the second-order central difference error. The second term is due to the flux correction described in equation (18a) and (18b). One always can use a method with higher accuracy at the expense of computing time. However, this extra expense is meaningful only when it produces a commensurate improvement. The sophistication of the difference scheme should be compatible with the sophistication of the remainder of the model and the accuracy of the available data. We have attempted to achieve an appropriate balance among these factors in this model.

The operators $\mathcal{D}_{xy}$ and $\mathcal{D}_z$ are defined by

$$\mathcal{D}_{xy}[C_{ijk}] = \Delta t\, K_H[r_{xi}\, C_{i-1,jk} - (1 + r_{xi})C_{ijk} + C_{i+1,jk})/\Delta x^2 + (r_{yj}C_{i,j-1,k} - (1+r_{yk})C_{ijk} + C_{i,j+1,k})/\Delta y^2] \quad , \qquad (20)$$

and

$$\mathcal{D}_z[C^{n+1}_{ijk}] = \gamma_k(\theta\mathcal{D}[C^{n+1}_{ijk}] + (i-\theta)\mathcal{D}[C^{n}_{ijk}]) \quad , \qquad (21)$$

where

$$\mathcal{D}[C_{ijk}] = r_k K_{k-\frac{1}{2}}\, C_{ij,k-1} - (r_k K_{k-\frac{1}{2}} + K_{k+\frac{1}{2}})\, C_{ijk} + K_{k+\frac{1}{2}}\, C_{ij,k+1} \quad ;$$

$$\gamma_k = \Delta t/(\Delta z_k + \Delta z_{k-1})) \quad ,$$

$$r_k = \Delta z_k/\Delta z_{k-1}$$

and θ is a parametric constant.

The stability criteria for the terms of advection, horizontal diffusion, and chemical reaction rate are well known (Ref. 8) as follows:

α_a, $\alpha_a^* < 1$, where subscript a denotes x, y, or z;

$\Delta t\ K_H/(\Delta x^2 + \Delta y^2) \leq 1/4$, and $\Delta t\ k_a \leq 1$.

and

$$K_{k+\frac{1}{2}}\gamma_k \leq \frac{1}{4(1-\theta)} \quad . \tag{22}$$

Condition (22) is used to determine the value of θ in equation (21). The value of θ must be close to 1, if a large value of γ_k is used. When the grid spacing is a function of time, a correction due to the changing volume is needed, because equation (17) only applies to a constant grid spacing system. It can be shown that $-C_{ijk}\ \alpha \ell n \Delta z_k/\alpha t$ should be added on the right hand side of equation (17). The implementation of this correction is simplified by changing the height H(t) for each hourly period. With this arrangement, the concentrations at the upper five grid points are adjusted hourly according to the height, H as follows:

$$C_{ijk}^{n+1} = \begin{cases} C_{ijk}^n/s_n & , \quad k \geq k_n + 1; \\ \left(\dfrac{1 + r_n/s_n}{1 + r_k}\right) C_{ijk}^n & , \quad k = k_n \quad , \end{cases} \tag{23}$$

where

$$s_n = (H^{n+1} - z_{k_n})/(H^n - z_{k_n}), \text{ and } k_n = 10.$$

When a sudden decrease of the mixing height occurs, one should use an alternative method. One such approach provided as an option in the model avoids a compression of the concentration by allowing some concentration to be left above the mixing height. The same concentration profile is therefore kept at the same height. This method is as follows:

$$C^{n+1}_{ijk} = (1-r)\ C^{n}_{ijk'} + r\ C^{n}_{ij,k'-1} \quad , \qquad (24)$$

where

$$r = (z^{n}_{k'} - z^{n+1}_{k})/\Delta z^{n}_{k'-1} \quad ,$$

$$k' = k_n + (k-k_n)\ s_n + 1 \quad .$$

2-D-c) Point source formulation

One of the prevailing criticisms of the grid model is related to the accuracy of the incorporation of the point sources into the grid system. These comments are usually qualitative rather than quantitative in nature. One particular problem is related to initial diffusion. When the concentration due to point source is injected into the grid system, the concentration at a grid element represents only the mean value over the grid element volume. The sub-grid variation can only be accommodated by a separate sub-grid system which has not yet been developed. In this study, an experimental method utilizing a Lagrange plume trajectory is introduced. That is, one keeps track of the location of the plume center and the plume width initially, and incorporates the plume into the grid system when the plume width is comparable with the grid size (see Section 2-E-e). In other words, the effective point source location is calculated according to the wind field and the diffusion speed. The method can be described as follows:

$$\underset{\rightarrow}{r} = \underset{\rightarrow}{r}_o + \underset{\rightarrow}{V}\, T \quad ,$$

$$T = \min\left(\frac{h^2}{4K} \quad , \quad \frac{\Delta x \Delta y}{16\ \ell n(10) K_H}\right) \quad , \qquad (25)$$

where $\underset{\rightarrow}{r}_o$, $\underset{\rightarrow}{r}$, and $\underset{\rightarrow}{V}$ are the initial, and new point source location, and the wind vector at the initial point source location, respectively. The effective height of the point source is h and K is the average vertical eddy diffusivity below the stack height. The time scale of relocation is the minimum of the time which the surface concentration requires to reach its maximum, (first term on the right-hand side of equation 25) or the time required for the horizontal plume area to become comparable with the grid element area (Second term on the right-hand side of equation 25).

2-E. Modeling Options

The model developed does not consist of a single method, and perhaps should be thought of as a family of methods, which aim to describe the phenomena of air pollutant transport in as realistic a manner as possible. This is achieved by introducing a variety of options which offer the user the ability to study the significance of the components as parameters. It also makes the model more general in dealing with input data, and offers a convenient method of optimization. The optimization of the model here means to select the most realistic and effective method to describe the nature of air pollutant transport with available input data. It is the most essential and time-consuming task during the development of an air quality model. The existence of these options makes the model a useful and

general tool to understand and describe the physical system under investigation. The options included are as follows:

2-E-a) Choice of surface wind field

The surface wind field is the most important input to the model other than the sources. Four options are available, namely, a subjectively analyzed wind field, an objectively analyzed wind field, data from RAMS stations, and a uniform wind. The subjective wind field can provide a reference with which to compare various objective wind analysis schemes. The wind-field generating program which generates the surface wind field over the simulated region by using the observed wind data from the monitoring stations as described in section (2-C-a i), is included, thus, it saves one step of preanalysis of the wind field. The option of uniform wind field can be used to test the effects of non-uniform distributions of the wind field.

2-E-b) Choice of vertical variation of wind field

One can construct the upper wind aligning it with the surface wind, or can specify an angle change from the surface wind, or uniform distribution of the upper wind. The upper wind affects the high point sources more than surface area sources, especially when the plume travels a long distance.

2-E-c) Choice of vertical wind components

The surface concentration could be significantly sensitive to the vertical wind components. However, such data are usually not available. Three options are included: no vertical wind components, calcuating raw vertical wind components from the continuity equation, and smoothing the calculated vertical wind components.

2-E-d) Choice of concentration adjustment with mixing height variation

The hourly variation of the mixing height influences the concentration distributions. One of the options included is to keep the total mass constant below the mixing height. Thus, the concentrations below the mixing height are compressed or diluted accordingly. Another option is to keep the concentration distribution unchanged with respect to altitude, while the grid size is changed.

2-E-e) Choice of point source modeling

The options included are: to calculate the relocation of a plume by using the local wind speed and appropriate time scale of plume diffusion according to the specified formula, equation (25), or simply specify the relocation of all

plumes by a single time scale which is just equal to one time step used for numerical time integration. It is noted that this time scale is used for calculating relocation--not for integration. The latter is used when hypothetical eddy diffusivity is employed. For instance, if one assumes the urban area is extremely smooth with roughness length less than 1 cm, then one will have very small values of eddy diffusivity which, according to equation (25), may lead to an unusually large time scale. Other options included are: to incorporate the relocated plume into the grid element nearest to the center of the plume or distribute the plume into the nearby four grid elements.

3. Discussions and Recommendations

A research-oriented urban air quality simulation model such as described herein is a powerful tool to understand the phenomena of transport and diffusion of air pollutants over an urban area. It is an attempt to put together in a practical balance as much as we know about air pollution and urban meteorology, atmospheric turbulence, source emission, and mathematical technique, to describe the phenomena, along with a little atmospheric chemistry. Moreover, the availability and quality of the input data, and computer capability should be considered simultaneously. We hope the model has been designed such that it is easily used and

modified by other users for their purposes.

Among all of these considerations, the most important item is still the quality of the input data. A poor quality of data introduces uncertainty or confusion, and makes validation or evaluation of the model difficult.

In particular, the quality of the emission data, either directly measured or derived, is the most important factor in the process of development and validation of an urban air pollution model. No sensible validation can be made without good quality emission data. In addition, the quality of the meteorological data, surface condition data, and air pollution observation data are also important. However, the required detail and accuracy of these data is not easily determined. This must be investigated through use of the model on these data.

On the other hand, some basic questions concerning the grid model are: the adequacy of the eddy coefficient to describe the turbulent flux, the representation of a concentration field by a finite number of grid elements, the sub-grid variation of concentration, especially near a point source or monitoring station, and the numerical errors from the difference scheme. These questions cannot be resolved quantitatively without careful evaluation of the model with data of good quality. The priority for improvement of these

limitations in the model must also be determined following a thorough investigation with good data. The grid model is a promising approach because of its inherent physical validity, its generality and flexibility. We believe its advantages as a research tool will become more and more apparent as it is systematically improved, feature by feature, in step with improved data quality, and improved knowledge of atmospheric structure.

II. PROGRAM DESCRIPTION

1. Introduction

In part I of this report we described the physical representation of our air quality simulation model (IBMAQ-2) and presented the modeling methologies, input requirements and computational procedures. In this part we shall consider the operational problem of using the computer program based on these equations and assumptions to simulate a concentration field in the St. Louis metropolation area. The notation used in part I is retained in the following discussion unless specified otherwise.

The computer program codes developed under this contract can be divided into two parts. They are all written in FORTRAN IV. The first part is the program for the main diffusion computations (program IBMAQ-2), which consists of one main program and 39 subroutines. The second part is the group of auxiliary programs, which process and prepare input data for the main diffusion model.

The program codes of IBMAQ-2 constitute a new version of our earlier program IBMAQ-1 (Reference 1). The major changes in

this program are the following: a) implementation of improved physical assumptions in the model formulation; b) adaption of the program to operate with data to be obtained from the RAPS project and RAMS stations in St. Louis; c) reconstruction of I/O specifications; and d) streamlining the general structure of the program so that it is easy to modify for future work. It should be pointed out here, due to the delays of the RAPS project, the program code of IBMAQ-2 was completed without testing on the new data. Thus, the I/O specification and certain methodologies employed in this program may need to be revised when such a data set is available.

In section II-2 and II-3, we shall discuss the program IBMAQ-2. The auxiliary programs are briefly described in section II-4. The program codes of IBMAQ-2 include quite comprehensive comment statements, which are necessary for understanding the program logic. The program listing, which is given in Appendix 1, is a self-explanatory document. We believe the user will have no difficulty in understanding it. Therefore, in the following discussion we shall concentrate on an over-view of the program and how to use it.

2. Program IBMAQ-2.---Diffusion Computations

2-A. System requirements

The model program is written in FORTRAN IV. The system requirements depend upon the usage of the model and its operational modes. The following three operational configurations are used in our development and operation of this model in a time sharing system.

2-A-a) Debugging runs:

64k words (one word equal to four bytes) of core are required in this mode along with at least three sequential files or data sets (disk space). The CPU (Central Processing Unit) time is about half of the amount required by a production run. This particular operational mode is to check the execution of I/O statement in the program and to detect any obvious programming errors (e.g. compatibility of passing arguments from one routine to another). The reduction of CPU core requirement is achieved by computing concentration field only at five vertical layers and assuming no vertical variation of wind field.

2-A-b) Testing runs:

75K words of core are required and at least three sequential files or data sets. The CPU time is equivalent to production runs. The concentration fields are computed at 14 vertical layers in the testing run. However, there is no vertical variation of wind field. This operational mode is to check the implementations of modeling methodologies in the program codes.

2-A-c) Production runs:

96K words of core are required for production runs and at least five sequential files or data sets. The CPU time is 2-5 minutes for each 24 hour real time simulations on the IBM 360/195. The precise running time depends upon the meteorological conditions of the simulated days.

The line printer is required for all the above-listed operation configurations. If the job is to be submitted in a batch mode, a card reader is necessary.

The code was developed on an IBM System 360/195 running OS/MVT and TSO. It has been tested on the EPA Research

Triangle Park computer facilities running on a time sharing system. The code runs equally well in either environment.

2-B. General structure of the program

In this section, we shall briefly describe the overall structure of the IBMAQ-2 program.

This model is based upon the numerical solution of a concentration equation, and is, of course, quite different from a Gaussian plume-type model. The pollutant concentration is computed in three spatial dimensions in successive time steps. The procedure is continued to obtain the time evolution of the concentration distribution until the new values of source emissions and/or meteorological variables are read in. In some instances, the steady state solution may be reached before the next input time; in this event it is useless to repeat the computation for the subsequent time steps. In these cases, it is convenient to pass directly to the new values of meteorological and/or source data. Thus, the computational procedure has two nested computational loops--a main loop and a time-step loop. The former one reads in meteorological and source emission data and computes the necessary parameters. The

latter one is nested in the main loop. this time-step loop computes an instantaneous spatially varying concentration field for each small time interval. This time interval is dictated by the numerical stability of the finite-difference scheme.

Fig. II-1 shows the general flow diagram of program IBMAQ-2. The program can be divided into three parts. They are as follows:

2-B-a) Initialization:

This part of the program is executed only once for each run of the program. The CPU storage allocation is first executed, then the model parameters and options are read in, constants are defined and variables and time indices are initialized in this part of the program. It also inputs geographical data of the modeled region and annual source emission data. The names of the subroutines called in this part of the program are: CDTOTP, CONSIN, GEOIN, XYUTMS, XYUTM1, PRINTS, WRITES, and WRITEX. These will be defined in the sequel.

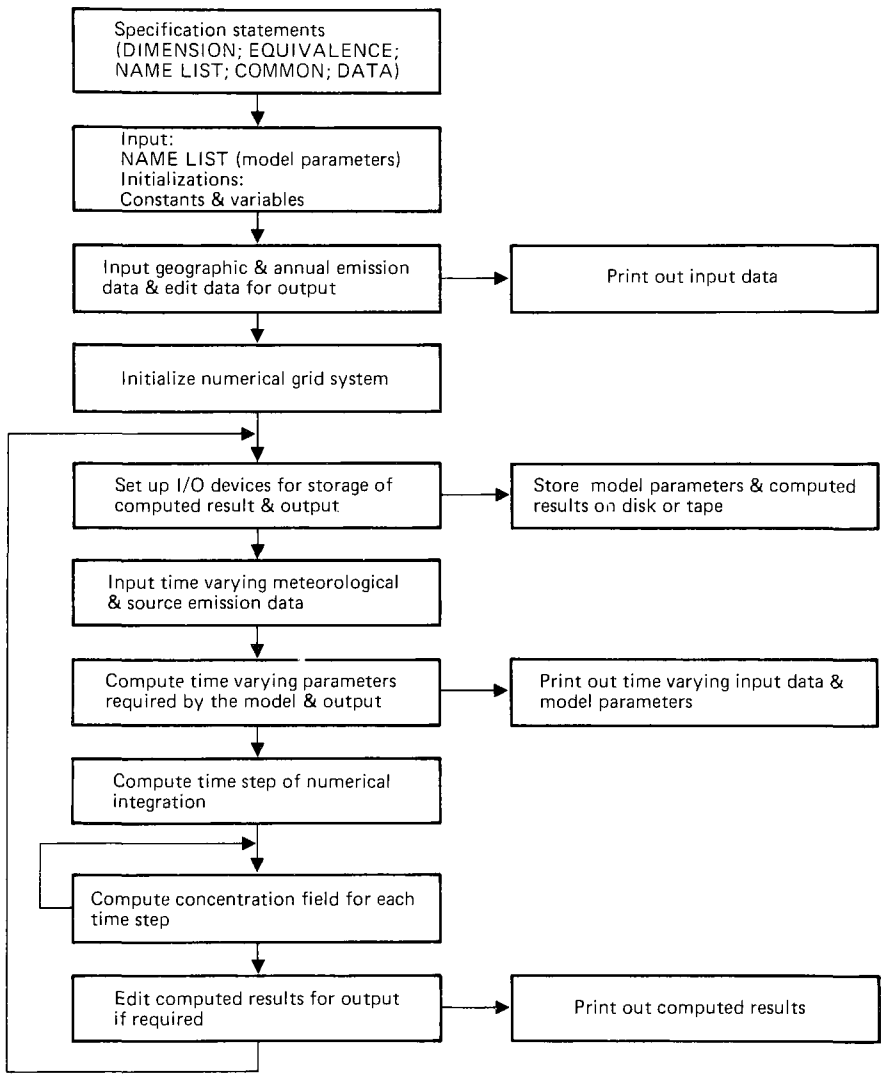

Figure II-1. General Flow Chart of IBMAQ-2

2-B-b) Main loop:

This part of the program is executed every "LPRINT" time interval. This time interval is the smallest time interval over which the hourly average source emission and meteorological data are available and are to be input to the program.

This main loop accomplishes the input of these data and edits them for model use. The meteorological parameters required by the model are also computed in this part of the program. In additon, the variable vertical grid resolution and the numerical time step are determined. The computed average concentration field values at each grid point and RAMS stations are also transmitted as output to a peripheral storage device for future usage. The names of the subroutines used in this part of the program which will be defined later are: OUTAPE, SOUSIN, WINDIN, WINDER, WINDGR, UVINTP, UVZE, WWZF, STABIT, HHCALC, DIMEN1, SHIFTN, CADJUS, AKZCAL, PRINTA, PRINTB, WRITEX, and DTTEST.

2-B-c) Time step loop:

This loop is nested in the main loop. The execution of this part of the program is managed by subroutine AACOMP. In

this loop, the instantaneous concentration field is computed every time step according to the finite-difference approximation of the concentration equation. The hourly average concentration field is also computed. Except for subroutines PRINTC, STNCON, SHIFTN, CCHECK, WRITEX, WRITEZ, ZZGRID and TIMEX, the subroutines used in this part of the program are for the purpose of computing each term of concentration equation. They are: UVFLUX, WWFLUX, XYDIFF, ZZDIFF, SOURCE, and CHEMIC, and along with the previously mentioned subroutines will be described in the next section.

We believe that a program as complex as this model requires should be written in a form so that it is easy for the user to modify any part of it. This ease of modification can extend to the improvement of physical parameterization of the model, to the computational methodologies used, and the I/O specification of the program. Hence, the current program has been constructed in modular form to achieve this objective. The execution of the program is controlled by two routines, namely the MAIN program and the subroutine AACOMP. The flow diagrams of these two routines are given in section II-2-c.

The dimensional arrays used in the computation are all

passed through call arguments and their dimensions are dynamically allocated in the subroutines. If one wishes to change any subroutines or dimension statements, one only has to deal with the calling routine and the referenced subroutine.

Finally, all I/O operations are executed in only a few subroutines. It is very easy to change I/O specifications through the control parameters included in the NAMELIST input. (See section II-3)

2-C. Summary of subroutines and their function

The computer program of this model consists of a main program and a total of 39 subroutines. There are multiple entries among five of these subroutines. For quick reference, Table II-1 lists a brief description of each subroutine. This listing is part of the comment statements appearing in the main program (see Appendix 1). Table II-2 lists the variable arguments passing from call statements to called routine or vice versa. Variables included in the common statements are not listed. (see Table II-3 for variables in common.) Following are the detailed descriptions of each subroutine:

MAIN PROGRAM: CALLED FROM: None

ROUTINE CALLED: AACOMP, AKZCAL, CADJUS, CONSIN
CDTOTP, DIMENS, DIMEN1, HHCALC,
DTTEST, GEOIN, OUTAPE, PRINTS
PRINTA, PRINTB, PRINTC, SHIFTN,
SOUSIN, TIMEX, WINDIN.

I/O PERFORMED: Yes

The main program calls various computational and I/O subroutines. It sets up main computational loops to compute concentration fields. It is a program controlling a general flow of execution of the IBMAQ-2 model. The detailed flow diagram of this routine is shown in Fig. II-2.

NAME	CALLED FROM	FUNCTIONS
AACOMP	MAIN	COMPUTE THE CONCENTRATION FIELDS
AKZCAL	MAIN	COMPUTE EDDY DIFFUSIVITY
CADJUS	MAIN	ADJUST C VALUES DUE TO CHANGE IN GRID DIMEN.
CCHECK	AACOMP	CHECK FOR STEADY STATE CONDITION
CHEMIC	AACOMP	COMPUTE CHEMICAL DECAY
CONSIN	MAIN	SPECIFY MODEL PARAMETERS
*CDTOTP	MAIN	PRINT CARD IMAGE OF NAMELIST INPUT
DIMENS	MAIN	INITIALIZE GRID SYSTEM
*DIMEN1	MAIN	SET VERTICAL GRID SYSTEM
*HHCALC	MAIN	COMPUTE TIME VARYING MIXING HEIGHT
DTTEST	MAIN	TIME STEP FOR NUMERICAL METHOD
GEOIN	MAIN	INPUT GEOGRAPH. AND ANNUAL EMISSION DATA
OUTAPE	MAIN	OUTPUT RESULTS TO TAPE OR DISK
POSITV	(NOT USED)	SET C=0 IF IT IS LESS THAN ZERO
PRINTS	MAIN	PRINT GEOGRAPH. AND ANNUAL EMISSION DATA
*PRINTA	MAIN	PRINT TIME VARYING EMISSION RATES
*PRINTB	MAIN	PRINT TIME VARYING METEOROLOGICAL DATA
*PRINTC	MAIN	PRINT CONCENTRATION FIELDS
SHIFTN	MAIN,AACOMP	SHIFT ARRAY A TO ARRAY B
SOURCE	AACOMP	ADD NEW SOURCE EMISSION INTO THE SYSTEM
SOUSIN	MAIN	INPUT TIME VARYING SOURCE EMISSION RATE
STABIT	WINDIN	ESTIMATE CONTINUOUS STABILITY CLASSES
STNCON	PRINTC	COMPUTE CONC. VALUES AT RAMS STATIONS
TIMEX	MAIN	FIX TIME INDICES
UVZF	WINDIN	COMPUTE VERTICAL WIND PROFILE OF (U,V)
UVFLUX	AACOMP	COMPUTE HORIZONTAL ADVECTION
UVINTP	WINDIN,WINDGR	INTERPOLATE ANALYZED U,V TO NUMERICAL GRID
WWZF	WINDIN	COMPUTE W COMPONENT OF WIND
WINDER	WINDER,UVZF	CONVERT WIND VECTOR TO COMP. OR VICE VERSA
WINDGR	WINDIN	GENERATE SFC. WIND FIELD FROM RAMS DATA
WINDIN	MAIN	READ IN SURFACE WIND FIELD AND RAMS DATA
WRITES	PRINTS	PRINT DATA ARRAY
*WRITEX	PRINTS	PRINT HORIZONTAL FIELD OF ARRAY
*WRITEZ	PRINTC	PRINT VERTICAL CROSS-SECTION OF ARRAY
WWFLUX	AACOMP	COMPUTE VERTICAL ADVECTION
XYDIFF	AACOMP	COMPUTE HORIZONTAL DIFFUSION
XYUTMS	GEOIN	COMPUTE UTM COORDINATE OF NUMERICAL GRID
*XYUTM1	GEOIN,SOURCE	CONVERT (X,Y) FROM UTM TO NUMERICAL GRID
ZZDIFF	AACOMP	COMPUTE VERTICAL DIFFUSION
ZZGRID	SOURCE	CONVERT Z FROM METER TO NUMERICAL GRID UNIT

(NOTE: * DENOTE ENTRY POINT IN LAST STATED SUBROUTINE)

TABLE II-1 SUBROUTINES INCLUDED IN THE PROGRAM IBMAQ-2

```
SUBROUTINE AACOMP  (CP1,C,CC,COLD,U,V,W,ZS,QA,POA,AKZ,AKH,AKA,AKF,UZF,VZF
                   *,WZF,DX,RDX,DXS,DY,RDY,DYS,EK,FK,DZ,RDZ,DZS,Z,ZM,XPUTM
                   *,YPUTM,XP,YP,ZP,ZR,ZPR,IM,JM,KM,KM1,LM,IMJM,IJKM,IJKM1)

SUBROUTINE AKZCAL  (AKZ,U,V,ZO,AKF,AKH,ZM,IMJM,IJKM,KM)

SUBROUTINE CADJUS  (CP1,C,RDZ,IM,JM,KM,IMJM,IJKM,KM1,RH,LHJUS)

SUBROUTINE CCHECK  (CP1,COLD,IJKM,IMJM,ICHECK,DCMIN)

SUBROUTINE CHEMIC  (CP1,C,IM,JM,KM,IMJM,IJKM,AKA)

SUBROUTINE CONSIN  (IM,JM,KM,KM1,IMJM,IJKM,IJKM1)

ENTRY      CDTOTP  (JUNIT1,IUNIT1,IUNIT2)

SUBROUTINE DIMENS  (DX,DY,DZ,RDX,RDY,RDZ,DXS,DYS,DZS,Z,ZM,IM,JM,KM)

ENTRY      DIMEN1  (DZ,RDZ,DZS,Z,ZM,KM,KM1,RH)

ENTRY      HHCALC  (HH,HMIN,HMAX)

SUBROUTINE DTTEST  (U,V,AKH,AKZ,AKF,AKAHR,UZF,VZF,DX,DY,Z,IM,JM,KM,IMJM,
                    IJKM,KM1)

SUBROUTINE GEOIN   (QB,ZS,ZO,POB,XPUTM,YPUTM,XP,YP,ZP,ZR,NP,IUTM,JUTM,DX
                   *,DY,IM,JM,LM,LMAX,XSUTM,YSUTM,XS,YS,IS,JXS,JYS,NS,NPAMS
                   *,KUNITG,JUNIT,QBSUM,POBSUM,QBTOT,POBTOT,ZOMEAN)

SUBROUTINE OUTAPE  (CC,ICAL,IOBS,NSX,IM,JM,IDAYTP,IHRTP,LMAPM)

SUBROUTINE POSITV  (A,IM,JM,KM,IMJM,IJKM)

SUBROUTINE PRINTS  (CP1,CC,C1,COLD,IOBS,ICAL,KOBS,KCAL,ITOBS,U,V,W,U1
                   *,V1,UU,VV,AKZ,UZF,VZF,WZF,AKF,DX,DY,IUTM,JUTM,XSUTM
                   *,YSUTM,XPUTM,YPUTM,ZO,ZS,QB,POB,XP,YP,ZP,ZR,NP,IN,
                   *,JN,KN,LM,IS,XS,YS,JXS,JYS,Z,IM,JM,KM,NS,NSX)

ENTRY      PRINTA

ENTRY      PRINTB  (RH)

ENTRY      PRINTC  (IMC,JMC)

SUBROUTINE SHIFTN  (A,B,IM,JM,KM,IN,JN,KN)

SUBROUTINE SOURCE  (CP1,C,QA,QB,ZS,POA,POB,XPUTM,YPUTM,XP,YP,ZP,ZR,ZPR,U,V
                   *,UZF,VZF,AKF,AKH,AKZ,DX,DY,DZ,Z,EK,FK,IM,JM,KM,KM1,IMJM,LM)

SUBROUTINE SOUSIN  (QB,ZS,ZO,POB,XP,YP,ZP,ZR,IM,JM,LM)
```

Table II-2 ARGUMENTS USED IN EACH SUBROUTINE

```
SUBROUTINE STABIT  (V,ESKY,IHR,STAB,ITRAT)

SUBROUTINE STNCON  (CC,IOBS,ICAL,KOBS,KCAL,ITOBS,NS,NSX,IM,JM,XS,YS,JXS,JYS)

SUBROUTINE TIMEX   (NMONDY)

SUBROUTINE UVZF    (U,V,U1,V1,UZF,VZF,WZF,Z,IM,JM,KM,KN,LX)

SUBROUTINE UVFLUX  (CP1,C,U,UZF,DX,DY,RDX,RDY,Z,EK,FK,IM,JM,KM,IMJM
                   *,IJKM,LX,LY,IJKN)

SUBROUTINE UVINTP  (UU,VV,IN,JN,U,V,IM,JM,DX,DY,DELX)

SUBROUTINE WNZF    (U,V,W,DX,DY,DZ,IM,JM,KM,KN,LWW,JUNIT)

SUBROUTINE WINDER  (U,V,UV,THETA,I)

SUBROUTINE WINDGR  (U1,V1,UU,VV,NEAR,USTN,VSTN,XSUTM,YSUTM,IUTM,JUTM
                   *,DX,DY,IM,JM,IN,JN,NS)

SUBROUTINE WINDIN  (U,V,W,U1,V1,UU,VV,NEAR,USTN,VSTN,UZF,VZF,WZF,XSUTM,YSUTM,
                   *,IUTM,JUTM,Z,DX,DY,DZ,IM,JM,KM,IMJM,IJKN,IN,JN,KN
                   *,IS,NS)

SUBROUTINE WRITES  (Q,IXMAX,IYMAX,ISIZE,JSIZE,IBEG,JBEG,IUTM,JUTM,IFORM
                   *,JUNIT,RATIO,TITLE)

ENTRY      WRITEX  (Q,IXMAX,IYMAX,ISIZE,JSIZE,IFORM,JUNIT,RATIO,TITLE)

ENTRY      WRITEZ  (A,Z,RATIO,IM,JM,KM,IMC,JMC,TITLA)

SUBROUTINE WWFLUX  (CP1,C,W,WZF,Z,DX,DY,DZ,EK,FK,RDX,RDY,RDZ,IM,JM,KM,
                   *,IMJM,IJKM,IJKN)

SUBROUTINE XYDIFF  (CP1,C,AKH,AKZ,AKF,RDX,RDY,DXS,DYS,IM,JM,KM,IMJM,IJKM)

SUBROUTINE XYUTMS  (IUTM,JUTM,IXBEG,IYBEG,IBEG,JBEG,DX,DY,DXA,DYA,IM,JM)

ENTRY      XYUTM1  (XUTM,YUTM,IDIMAX,XD,YD,IDIM,LWAY)

SUBROUTINE ZZDIFF  (CP1,C,AKZ,AKF,RDZ,DZS,ZM,EK,FK,IM,JM,KM,IMJM,IJKM)

SUBROUTINE ZZGRID  (ZA,ZB,Z,IMA,IMB,KM)
```

TABLE II-2 (continued)

```
 DIMENSION

*     CP1(30,40,14),C(30,40,14),U(30,40,7),V(30,40,7),W(30,40,7)
*     CP1(30,40,14),C(30,40,14),U(30,40,1),V(30,40,1),W(30,40,1)
*     CP1(30,40,5),C(30,40,5),U(30,40,1),V(30,40,1),W(30,40,1)
*     U(30,40,7),V(30,40,7),W(30,40,7)
*     U(30,40,1),V(30,40,1),W(30,40,1)
*     ,COLD(30,40),  CC(30,40),  C1(30,40),  U1(30,40),  V1(30,40)
*     ,  QA(30,40),  QB(30,40),  ZS(30,40),  ZO(30,40), AKZ(30,40)
*     ,  UU( 9,13),  VV( 9,13),NEAR( 9,13)
*     ,  DX(30),    RDX(30),   DXS(30),   DY(40),  RDY(40),  DYS(40)
*     ,  DZ(14),    RDZ(14),  DZS(14),    Z(13),   ZM(14),  AKH(14)
*     , AKF(14),    UZF(14),  VZF(14),  WZF(14)
*     , NP(150),    XP(150),  YP(150),  ZP(150),   ZR(150), ZRP(150)
*     ,PQA(150),  PQB(150),  EK(150),  FK(150),  USTN(25), VSTN(25)
*     ,  IS(25),    XS(25),   YS(25),  JXS(25),   JYS(25)
*     ,IOBS(26),  ICAL(26), KOBS(26), KCAL(26), ITOBS(26)
*     ,IUTM(30),JUTM(40),XPUTM(150),YPUTM(150), XSUTM(25),YSUTM(25)
*     , AKA(24), NMONDY(12)

 COMMON    /AADATA/
*    IM1,JM1,KM1,JUNIT,KUNITC,KUNITG,KUNIPT,KUNITS,KUNITW
*   ,IYR,IMO,IDAY,IHR,ITM,ITMHR,ITSEC,ITOTHR,ITSTEP,DT,TM,TSEC
*   ,LPRINT,LTSTOP,LTSOUS,LTWIND
*   ,LWRITE(10),LSOUS(2),LTOP,LWTOP,LPQ,LWT,LWIND,KWIND,LCRUN,LCHEM
*   ,RAMS(6,25),PARM(10),A1(4),AK,HG,HP,HS,QLMIN,DCMIN
*   ,PMAX,PMIN,RIB,ZMAX,ZRPQ,ZRISE,QBTOT,PQBTOT,UQ,PHIFHZ,WZF
 COMMON /CBLOCK/  CP1(30,40,14),C(30,40,14)
 COMMON /CBLOCK/  CP1(30,40,5),C(30,40,5)

 EQUIVALENCE
*       (CP1(1,1,1), C1(1,1))
*      ,(  U(1,1,1),  W(1,1,1))
*      ,(U(1,1,1),U1(1,1)), (V(1,1,1),V1(1,1))
*      , (QA(1,1),QB(1,1)),   (PQA(1), PQB(1))
*      ,   (UZF(1),VZF(1)),     (UZF(1),WZF(1))
*      ,   (UU(1,1),EK(1)),     (VV(1,1),FK(1)), (NEAR(1,1),NP(1))
*      , (USTN(1),EK(120)),  (VSTN(1),FK(120))
```

TABLE II-3 DIMENSION, COMMON, AND EQUIVALENCE STATEMENTS OF MAIN PROGRAM

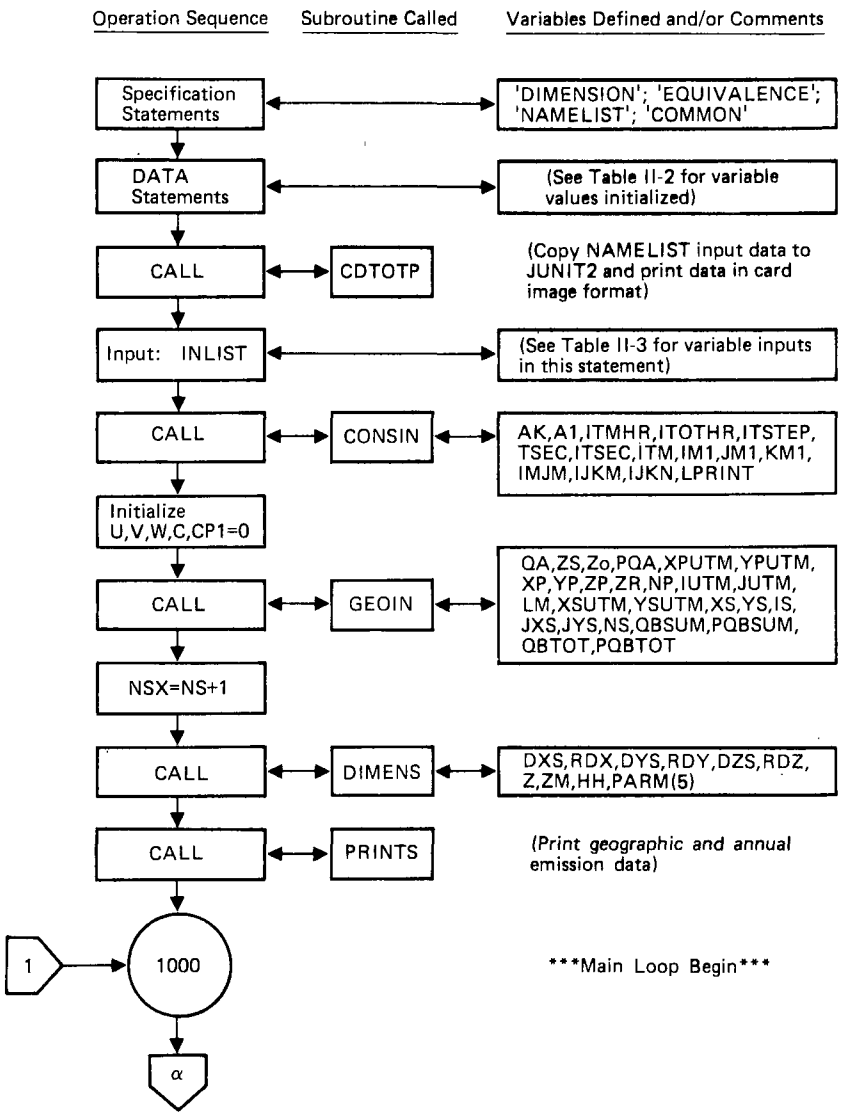

Figure II-2. Detailed Flow Diagram of MAIN Program

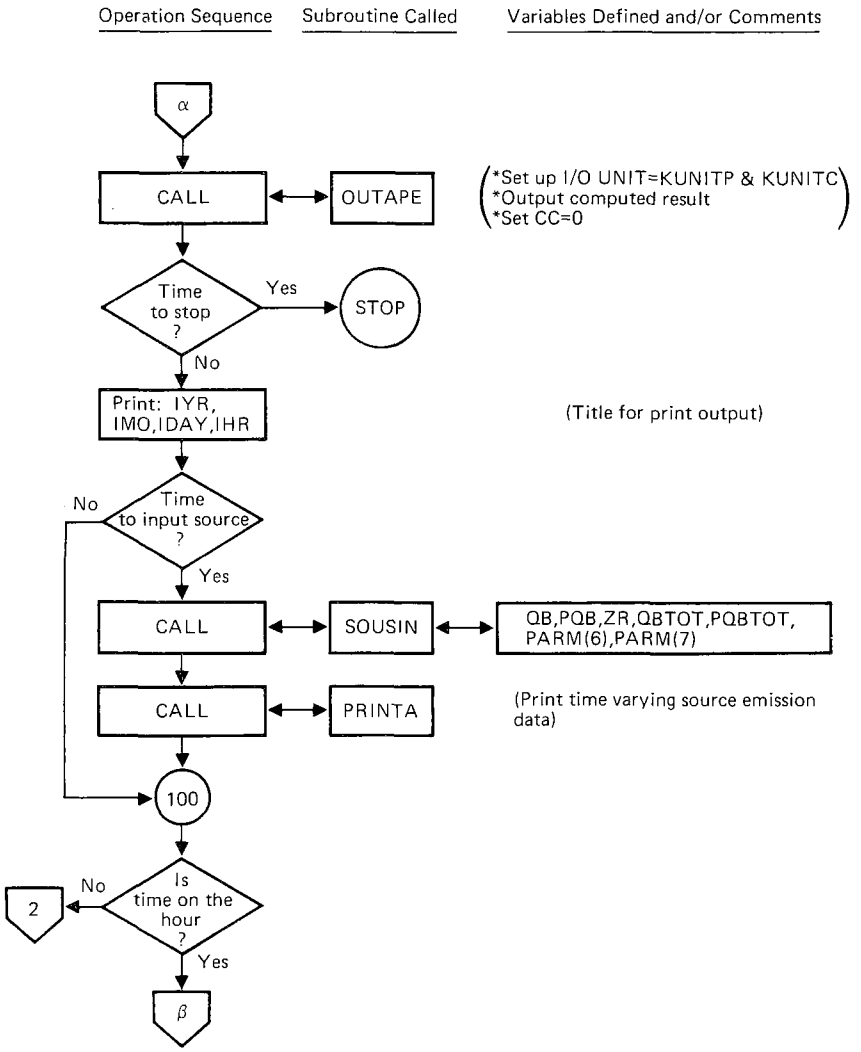

Figure II-2. (continued)

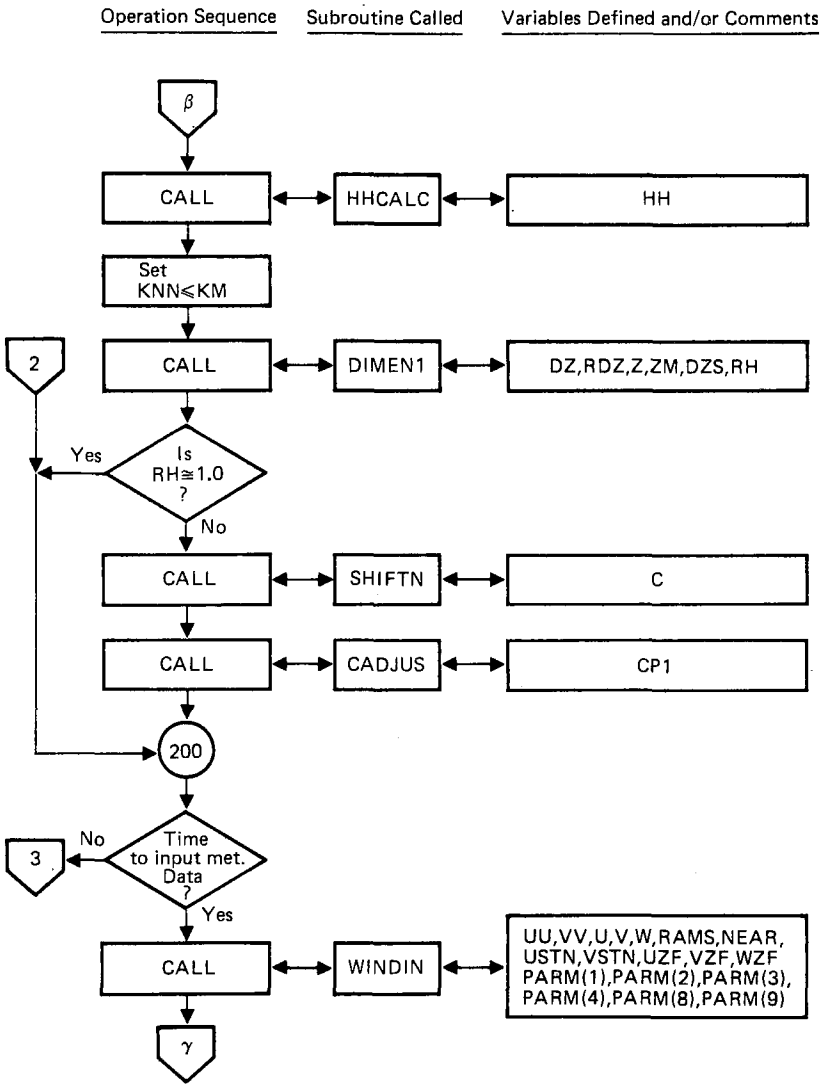

Figure II-2. (continued)

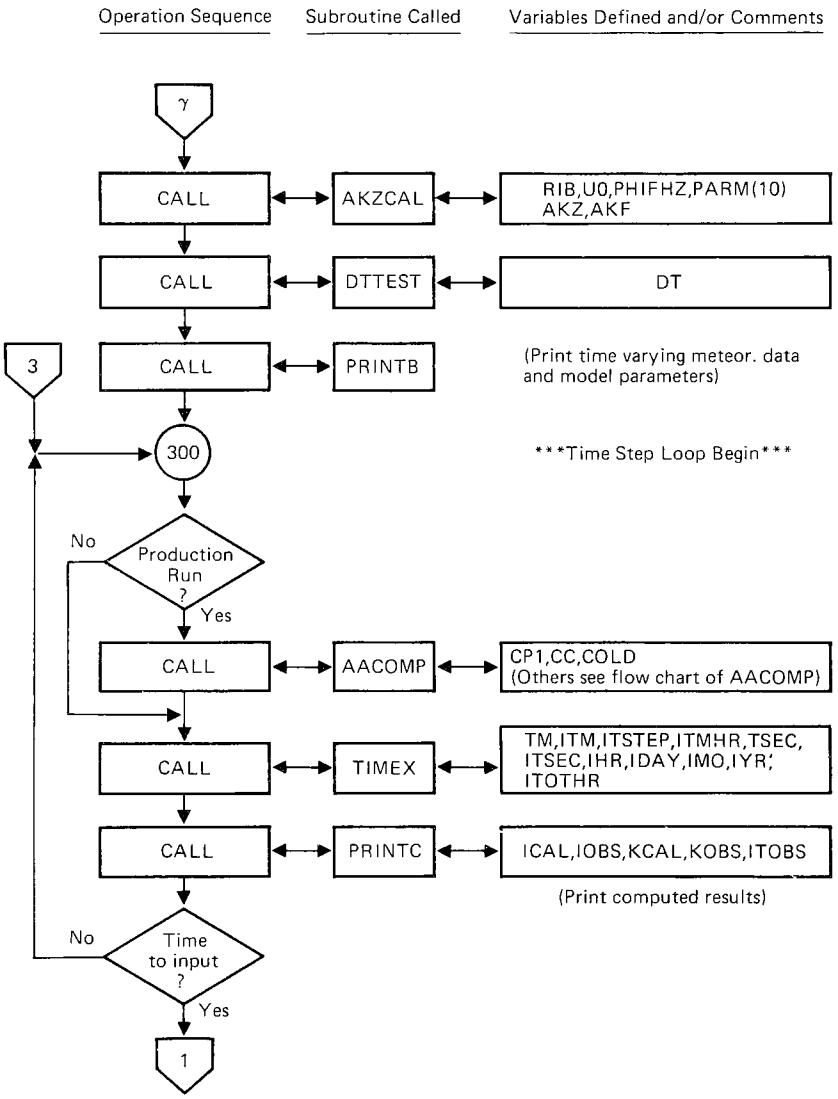

Figure II-2. (continued)

SUBROUTINE AACOMP: CALLED FROM: MAIN
ROUTINE CALLED: CCHECK; CHEMIC, SHIFTN; SOURCE; UVFLUX; WWFLUX; XYDIFF; ZZDIF
I/O PERFORMED: None

This routine is the control program, which supervises the proper execution of the steps for obtaining the numerical solution of the concentration equation. It calls various computational subroutines to compute the concentration field contribution of each term of the equation. It is executed each time step in the numerical integration of the equation. The hourly average concentration field is also computed here. The general flow diagram of this control program is shown in Fig. II-3.

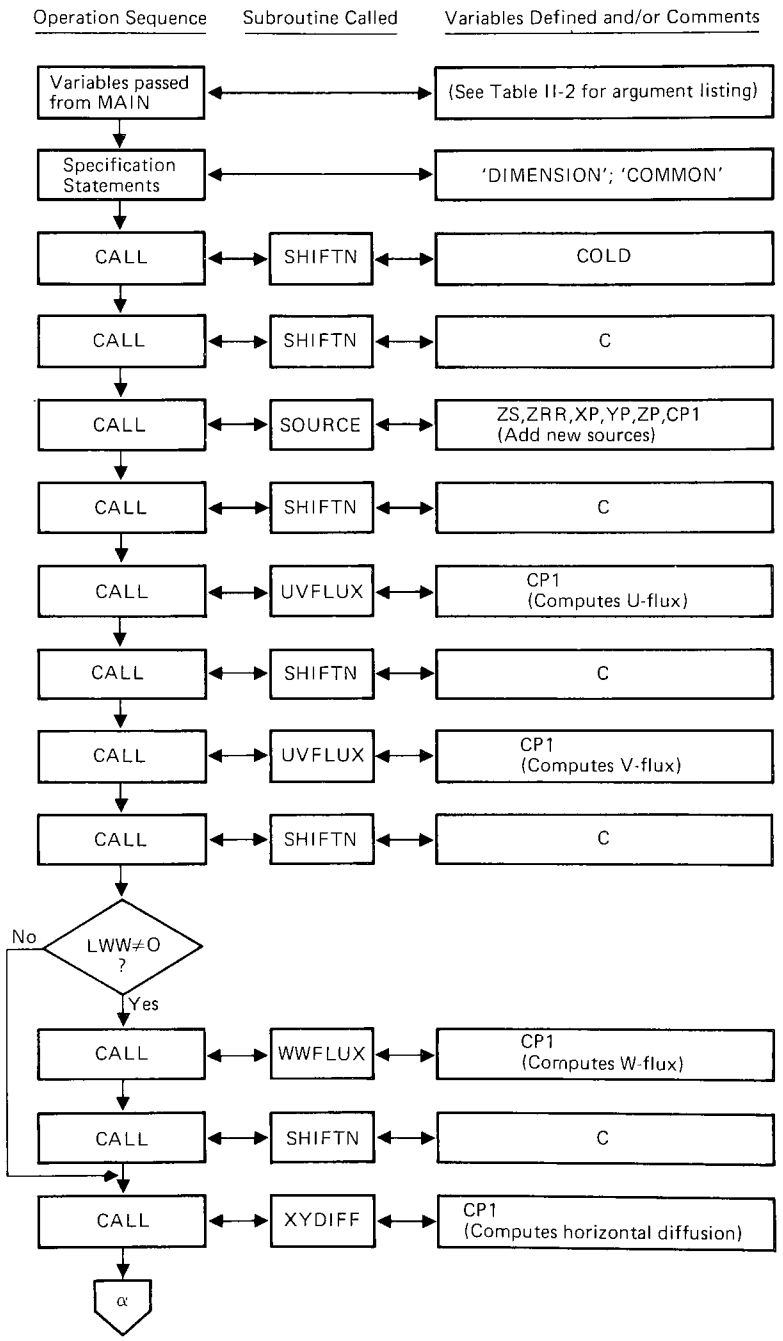

Figure II-3. Detailed Flow Diagram of SUBROUTINE AACOMP

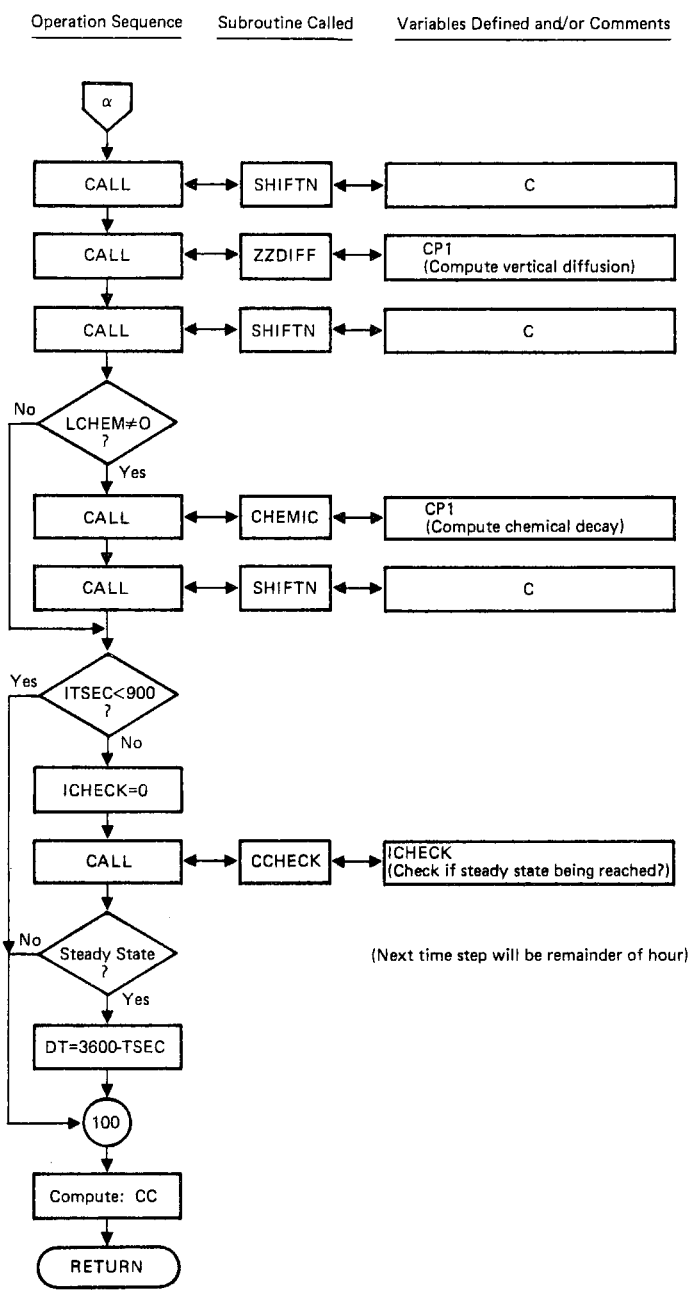

Figure II-3. (continued)

SUBROUTINE AKZCAL: CALLED FROM: MAIN

ROUTINE CALLED: None

I/O PERFORMED: None

This subroutine computes the vertical eddy diffusivity for the surface layer AKZ(I,J) and its vertical variation in a function form AKF(K). This routine is called whenever new meteorological data is input into the model. The routine can be divided into three parts. The first part computes the bulk Richardson number RIB, if upper air measurements are available (only for reference purpose). The second part computes eddy diffusivities for the surface layer from the continuous atmospheric stability class S, and surface routhness Z0(I,J). The equations used in this computation are given in Section I-2-B. Finally, a computation is performed of the vertical variation of eddy diffusivity according to equation (10) given in Section I-2-B.

SUBROUTINE CADJUS: CALLED FROM: MAIN

ROUTINE CALLED: None

I/O PERFORMED: None

This subroutine adjusts the concentration values of upper levels (from grid KNN to KM) after a change in the volume of grid elements due to the variation of mixing height. This routine is executed every one hour of real-time computation, and when the ratio of old time step and new time step grid volume RH is not equal to one. The computation method is given in Section I-2-C, equations 23 and 24.

SUBROUTINE CCHECK: CALLED FROM: AACOMP
ROUTINE CALLED: None
I/O PERFORMED: None

Subroutine CCHECK checks whether the computed concentration field in each time step has reached a steady state solution of the concentration equation. Sets ICHECK=0 if steady state is reached, otherwise sets ICHECK=1.

ENTRY CDTOTP: CALLED FROM: MAIN
ROUTINE CALLED: None
I/O PERFORMED: Yes

This is an entry in subroutine CONSIN. It only executes once in the beginning of the program. It is used to copy card input data to I/O unit = IUNIT2 and to print out input data in card image format.

SUBROUTINE CHEMIC: CALLED FROM: AACOMP
ROUTINE CALLED: None
I/O PERFORMED: None

This subroutine computes chemical decay of SO. It is executed every time step, if ICHEM $\neq$ 0 from NAMELIST input. The equation of computation is given in Section I-2-B.

SUBROUTINE CONSIN: CALLED FROM: MAIN
ROUTINE CALLED: None
I/O PERFORMED: None

In this routine, values of model constants are specified. It only executes once at the beginning of the program.

SUBROUTINE DIMENS: CALLED FROM: MAIN
ROUTINE CALLED: None
I/O PERFORMED: None
MULTIPLE ENTRY: DIMEN1; HHCALC

This subroutine is called once in the beginning of the program. It initializes the necessary parameters for the grid system of the model. It also initializes the mixing height HH at height of planetary-boundary layer.

ENTRY DIMEN1: CALLED FROM: MAIN
ROUTINE CALLED: None
I/O PERFORMED: None

This routine is executed every hour of real time when mixing height is recomputed. It is an entry of subroutine DIMENS

and computes vertical grid system due to changes in the mixing height. The computation of the vertical grid system as function of mixing height is discussed in Section I-2-C.

SUBROUTINE DTTEST: CALLED FROM: MAIN
ROUTINE CALLED: None
I/O PERFORMED: None

This subroutine computes and checks the time step for the numerical integration of the concentration equation. The numerical stability criteria for horizontal advection, horizontal diffusion and chemical reaction are all included. See Section I-2-C for detailed stability criteria.

SUBROUTINE GEOIN: CALLED FROM: MAIN
ROUTINE CALLED: XYUTMS; XYUTM1
I/O PERFORMED: Yes

This subroutine reads in geographical and annual emission

data. It executes once at the beginning of the program. The input variables are A) Origin of numerical grid in UTM coordinate; B) UTM coordinates of RAMS stations XSUTM(L),YSUTM(L); C) Surface roughness parameter Z0(I,J); D) Effective emission height of area sources ZS(I,J); E) UTM coordinate of point sources and their stack heights, XPUTM(L), YPUTM(L) and ZP(L); F) Annual averaged area source emission rates QB(I,J) and their sum QBTOT; G) Annual average point source emission rates PQB(L) and their sum PQBTOT; and H) Normalized plume rise on each point source ZR(L). By calling subroutines XYUTMS and XYUTM1, this subroutine also: A) Fixes UTM coordinates for all numerical grid points; B) Converts UTM location of RAMS station to numerical grid. Methods of preparing these input data are given in Section II-4, and input requirements are discussed in Section II-3-B.

ENTRY HHCALC: CALLED FROM: MAIN
ROUTINE CALLED: None
I/O PERFORMED: None

This is also an entry of subroutine DIMENS. It computes the mixing height for every hour of real time. Current

programmed methods are discussed in Section I-2-B. This routine is subject to modification or revision when more information about mixing height or vertical stratification of boundary layer atmosphere in the St. Louis area is available.

SUBROUTINE OUTAPE: CALLED FROM: MAIN
ROUTINE CALLED: None
I/O PERFORMED: Yes

This subroutine outputs the computed results on two I/O units = KUNITP and KUNITC. The detail output specification is given in Section II-3-D. This routine is executed in two ways. During the initialization of the program (ITM=0), it sets up I/O units KUNITP and KUNITC and checks whether there are previously computed results stored in these I/O units. If the answer is yes, it sets LWARM=1, and gets these I/O units ready for additional writes. Otherwise, it sets LWARM=0 and returns to main program. In the subsequent execution, it is only called every LPRINT interval of real time to output the averaged concentration values into these two I/O units according to the output specification.

SUBROUTINE POSITV

This subroutine sets variable A(I,J,K) = 0, if it is a negative value. Currently, it is not used in the model. It is included in the program for the possibility of using other finite difference methods which may result in negative values of concentration due to numerical or truncation error.

SUBROUTINE PRINTS:	CALLED FROM:	MAIN
	ROUTINE CALLED:	WRITEX, WRITEZ
	I/O PERFORMED:	Yes
	MULTIPLE ENTRY:	PRINTA, PRINTB, PRINTC

This subroutine prints out geographical and annual emission data according to output specification (Section II-3-C). It also calls subroutine WRITES to initialize the dummy arguments needed in entry WRITEX and WRITEZ. It only executes one time in the program.

ENTRY PRINTA: CALLED FROM: MAIN

ROUTINE CALLED: WRITEX

I/O PERFORMED: Yes

This subroutine is an entry in subroutine PRINTS. It prints out time varying emission rates of area and point sources. It is executed every LTSOUS interval. See Section II-3-C for output specification.

ENTRY PRINTB: CALLED FROM: MAIN

ROUTINE CALLED: WRITEX

I/O PERFORMED: Yes

This subroutine is an entry in subroutine PRINTS. It prints out time varying meteorological data, RAMS stations data, and model parameters. It is executed every LTWIND interval. See Section II-3-C for output specification.

ENTRY PRINTC: CALLED FROM: MAIN

ROUTINE CALL: WRITEX, WRITEZ, STNCON

I/O PERFORMED: Yes

This subroutine is also an entry in the subroutine PRINTS. It prints out computed results according to output specification (see Section II-3-C). This routine is called every time step. However, it is executed in two ways. For every time step, it prints out instantaneous concentration values at RAMS stations and returns to the main program at the beginning of the time step loop. For every LPRINT interval and ICRUN≠0, it prints out: A) Instantaneous surface concentration field, C1,(I,J), B) Two vertical cross sections of instantaneous concentration for I=IMC and J=JMC; C) Averaged surface concentration field CC(I,J) for LPRINT interval, D) Averaged concentration values at RAMS stations, and C) 24-hour average concentration values at RAMS stations.

SUBROUTINE SHIFTN: CALLED FROM: MAIN; AACOMP

ROUTINE CALL: None

I/O PERFORMED: None

This subroutine shifts array A(I,J,K) to B(I,J,K). Its execution is determined by the numerical method employed in the model. See Fig. II-2 and II-3 for current usage of this routine.

SUBROUTINE SOURCE: CALLED FROM: AACOMP

ROUTINE CALL: ZZGRID, XYUTM1

I/O PERFORMED: None

This subroutine adds new source emission into the system. It is executed every time step. The program can be divided into two parts: add area sources and add point sources. The logical path which determines the execution of each part is specified by LSOUS(1) and LSOUS(2). The method by which the new sources are added into the system is discussed in Section I-2-F. The effective stack heights of point sources are computed in this routine for each LPRINT interval.

SUBROUTINE SOUSIN: CALLED FROM: MAIN
ROUTINE CALL: None
I/O PERFORMED: Yes

This subroutine reads in time-varying source emission data QB(I,J) and PQB(L). It is executed every LTSOUS interval. See Section II-3-B for input specification.

SUBROUTINE STABIT: CALLED FROM: WINDIN
ROUTINE CALL: None
I/O PERFORMED: None

This subroutine estimates a continuous atmospheric stability class as function of average wind speed, solar insolation, and sky condition (cloud cover). It is executed every LTWIND interval or upon the input of new meteorological data. More data and further study are necessary to generalize this subroutine. A method of analysis applied in this routine is discussed in Section I-2-B.

SUBROUTINE STNCON: CALLED FROM: PRINTC

ROUTINE CALL: None

I/O PERFORMED: None

This subroutine stores concentration values measured at RAMS stations on array IOBS(L) and computes simulated concentration values at stations on array ICAL(L) by bilinear interpolation of CC(I,J). It also computes 24-hour-average concentration at stations KOBS(L) and KCAL(L) for observed and computed values, respectively. In addition, the average values of each array CAL(L), IOBS(L), KCAL(L) and KOBS(L) for L=1, NS are calculated. These values represent the spatial average concentration and they are stored on same array with index of NSX. NS is the total number of RAMS station and NSX=NS+1. This routine is executed every LPRINT interval.

SUBROUTINE TIMEX: CALLED FROM: MAIN

ROUTINE CALL: None

I/O PERFORMED: None

This subroutine fixes the time indices for both simulation time and real time. It is executed every time step.

SUBROUTINE UVZF: CALLED FROM: WINDIN
ROUTINE CALL: WINDER
I/O PERFORMED: None

This subroutine computes vertical variation of horizontal wind components U and V. Three methods are included in this routine. The choice of method of computation is controlled by LWIND, which is defined in NAMELIST input. These three methods are discussed in Section I-2-D. This routine is executed upon the input of new meteorological data.

SUBROUTINE UVFLUX: CALL ROUTINE: AACOMP
ROUTINE CALLED: None
I/O PERFORMED: None

This subroutine computes horizontal advection terms in the concentration equation. It is executed every time step. The current version of the program is the second-order central finite difference scheme with flux correction. It has been discussed in detail in Section I-2-C. The program works for both X-direction and Y-direction advection by interchanging the actual arguments in call statements. The actual arguments listed in Table II-2 for this subroutine is to compute x-direction advection. For computing y-direction advection, the actual arguments in the CALL statement is (CP1, C, U, UZF, DY, DX, RDY, RDX, Z, EK, FK, JM, IM, KM, IMJM, IJKM, LY, LX, IJKN).

SUBROUTINE UVINTP: CALLED FROM: WINDIN, WINDGR
ROUTINE CALL: None
I/O PERFORMED: None

This subroutine obtains the surface wind field at all numerical grid points by bilinearly interpolating analyzed wind fields over a wind analysis grid system, which has a grid size of DELX. (It is assumed that DELX>DX, DY). This routine is executed whenever there is an input of new wind

data.

SUBROUTINE WWZF: CALLED FROM: WINDIN
ROUTINE CALL: None
I/O PERFORMED: None

This subroutine computes the vertical component of wind W(I,J,K). The control parameter LWW supervises the execution of this subroutine. For LWW=0, it assumes W(I,J,K)=0.0. For LWW=1, a continuity equation is used to compute W(I,J,K). For LWW=2, after obtaining W(I,J,K), a nine-point averaging scheme is used to smooth the W field. This routine is executed after each new input of meteorological data.

SUBROUTINE WINDER: CALLED FROM: WINDER, WWZF
ROUTINE CALLED: None
I/O PERFORMED: None

This subroutine converts wind vector (given wind direction

and speed) to wind components in X and Y directions or vice versa.

SUBROUTINE WINDER: CALLED FROM: WINDIN
ROUTINE CALL: WINDER, UVINTP
I/O PERFORMED: Yes

This subroutine generates surface wind field from observed wind data at RAMS stations. Two methods are included in this program. The first method assumes a spatially uniform wind field which is assigned a value from a wind observation at a station nearest to the center of the city. The second method employs a weighted interpolation scheme to obtain a wind field on the wind analysis grid, UU(I,J), VV(I,J) which has a grid size of DELX. Then subroutine UVINTP is called to obtain U(I,J), V(I,J) at all numerical grid points. The interpolation scheme is discussed in Section I-2-D.

SUBROUTINE WINDIN: CALLED FROM: MAIN

ROUTINE CALL: WINDER, WINDER, UVINTP, STABIT, UVZF, WWZF

I/O PERFORMED: Yes

This subroutine reads in meteorological data and data observed at RAMS stations. Thereafter, various subroutines are called to generate a three-dimensional wind field at numerical grid points. It also calls subroutine STABIT to obtain a continuous atmospheric stability class. It is executed every LTWIND interval. The input specification is discussed in Section II-3-B.

SUBROUTINE WRITES: CALLED FROM: PRINTS

ROUTINE CALL: None

I/O PERFORMED: None

MULTIPLE ENTRY: WRITEX, WRITEZ

This dummy subroutine is executed once in the beginning of the program to initialize the dimension and data statements needed in the entries WRITEX and WRITEZ.

ENTRY WRITEX: CALLED FROM: PRINTS, PRINTA, PRINTC

ROUTINE CALL: None

I/O PERFORMED: Yes

This subroutine is an entry in subroutine WRITES. It prints out array Q(I,J) under the title 'TITLE'. A variable format is used in the WRITE statements. Parameter IFORM determines the number of columns to be printed on each line and controls a page layout.

ENTRY WRITEZ: CALLED FROM: PRINTC

ROUTINE CALL: None

I/O PERFORMED: Yes

This subroutine also is an entry in subroutine WRITES. It prints out two vertical cross sections of array A at J=JMC and I=IMC.

SUBROUTINE WWFLUX: CALLED FROM: AACOMP

ROUTINE CALL: None

I/O PERFORMED: None

This subroutine computes the vertical advection term in the concentration equation. The same numerical scheme as used in subroutine UVFLUX is applied in this routine. It is executed every time step. See Section I-2-C for a detailed discussion.

SUBROUTINE XYDIFF: CALLED FROM: AACOMP

ROUTINE CALL: None

I/O PERFORMED: None

This subroutine computes the horizontal diffusion terms in the concentration equation. It is executed every time step. The second-order central finite difference scheme is used. See Section I-2-C for detailed discussion.

SUBROUTINE XYUTMS: CALLED FROM: GEOIN

ROUTINE CALL: None

I/O PERFORMED: None

MULTIPLE ENTRY: XYUTM1

This subroutine computes UTM coordinates for all numerical grid points. It is executed once at the beginning of the program.

ENTRY XYUTM1: CALLED FROM: GEOIN, SOURCE

ROUTINE CALL: None

I/O PERFORMED: None

This subroutine converts point (XUTM,YUTM) in UTM coordinates to point (XD,YD) in coordinates based on numerical grid system which has an origin of (0,0). It is an entry in subroutine XYUTMS.

SUBROUTINE ZZDIFF: CALLED FROM: AACOMP
ROUTINE CALLED: None
I/O PERFORMED: None

This subroutine computes the vertical diffusion term in the concentration equation. It is executed every time step. An implicit second-order central finite difference scheme with variable grid sizes and variable eddy diffusivities is used. See Section II-2-C for detailed discussion.

SUBROUTINE ZZGRID: CALLED FROM: SOURCE
ROUTINE CALLED: None
I/O PERFORMED: None

This subroutine converts height ZA in units of meters into numerical grid unit ZB.

2-D. VARIABLES USED IN THE PROGRAM

The most important variables and constants used in the program are listed in this section. They are arranged in alphabetical order. This listing includes the array size, at which part of the program that array been defined, the unit used and definition of each variable.

NAME	ARRAY SIZE	WHERE DEFINED	UNIT	DEFINITION
AK		CONSIN		Von Karman constant.
AKA(N)	24	INLIST	sec^{-1}	Chemical reaction rate constants for hour N of a day.
AKF(K)	KM	AKZCAL		Function determines the vertical variation of AKZ.
AKH(K)	KM	INLIST	m^2/sec	Normalized horizontal eddy diffusivity over layer K.
AKZ(I,J)	IMJM	AKZCAL	m^2/sec	Surface vertical eddy diffusivity at grid point (I,J).
A1(N)	4	CONSIN		Four constants in in Businger's formula.
C(I,J,K)	IJKM	AACOMP	ug/m^3	Last computed concentration values at grid point (I,J,K).
CC(I,J)	IMJM	AACOMP	ug/m^3	Average concentration at grid point (I,J) over LPRINT time interval.
COLD(I,J)	IMJM	AACOMP	ug/m^3	Surface concentration at grid point (I,J) for previous time step.
CP1(I,J,K)	IJKM	AACOMP	ug/m^3	New computed concentration value at grid point (I,J,K).
C1(I,J)	IMJM	AACOMP	ug/m^3	Surface concentration layer of CP1.

DCMIN		INLIst	ug/m^3	Value of criterion for checking convergence of concentration field.
DT		DTTEST	sec	Time step in numerical integration.
DX(I)	IM	INLIST	m	Grid interval size in X direction.
DXS(I)	IM	DIMENS	m^2	DX(I) squared.
DY(J)	JM	INLIST	m	Grid size in Y direction.
DYS(J)	JM	DIMENS	m^2	DY(J) squared.
DZ(K)	KM	DIMEN1	m	Vertical grid interval size.
DZS(K)	KM	DIMEN1	m^2	DZ(K) squared.
EK,PK(N)	LM			Temporary storage array.
HFZ		AKZCAL		Integral of non-dimensional wind shear.
HG		INLIST	m	Thickness of planetary boundary layer.
HH		HHCALC	m	Height of mixing layer.
HMAX		INLIST	m	Maximum height of mixing layer during a day.
HMIN		INLIST	m	Minimum height of mixing layer during a day
HP		INLIST	m	Height of upper wind measurement.
HS		INLIST	m	Effective height of surface wind.
ICAL(N)	NSX	STNCON	ug/m^3	Computed average concentration value at monitoring station N; N=NSX is spatial average of ICAL(N), N=1,NS.
IDAY		TIMEX		Day of the month.
IDAYTP		INLIST		Starting day for which the computed and observed concentration value are stored on I/O UNIT=KUNITP and KUNITC.
IHR		TIMEX		Time of the day.
IHRTP		INLIST		Starting hour of IDAYTP.
IJKM		CONSIN		IM*JM*KM.

IJKN		CONSIN		IM*JM*KN.
IM		INLIST		Number of grid points in X direction.
IMC		INLIST		Grid point in x direction where a Y-Z cross section of concentration field to be printed.
IMJM		CONSIN		IM*JM.
IMO		TIMEX		Month of the year.
IM1		CONSIN		IM-1.
IN		INLIST		Number of wind grid points in X direction for which the analyzed wind field is stored.
IOBS(N)	NSX	STNCON	ug/m^3	Observed average concentration at monitoring station N; N=NSC is spatial average of IOBS(N), N=1,NS.
IS(N)	NS	GEOIN		Identification number of monitoring station N.
ITM		TIMEX		Equals TM, simulated time in seconds (integer).
ITOTHR		TIMEX	Hour	Total real time being simulated in a run.
ITSEC		TIMEX	Sec	Simulation time starting from each one hour interval (integer, ITSEC=TSEC).
ITSTEP		TIMEX		Number of time steps being simulated.
ITOBS(N)	NSX	STNCON		Number of observed datum values at monitoring station N during a 24-hour period.
IUNIT		MAIN		An I/O unit for card input (=IUNIT2).
IUNIT1		MAIN		I/O unit for card reader.
IUNIT2		MAIN		I/O unit for temporary storage unit.
IUTM(I)	IM	XYUTMS	m	UTM coordinate of numerical grid point in X direction.
IYR		TIMEX		Year of the centry.
JM		INLIST		Number of grid points in Y direction.
JMC		INLIST		Grid point in y direction where a X-Z

				cross section of concentration field to be printed.
JM1		CONSIN		JM-1.
JN		INLIST		Same as IN, except in Y direction.
JUNIT		INLIST		I/O unit for line printer.
JXS(N)	NS	GEOIN		X coordinate of monitoring station N in grid units.
JYS(N)	NS	GEOIN		Y coordinate of monitoring station N in grid units.
KCAL(N)	NSX	STNCON	ug/m^3	24-hour average of ICAL(N).
KM		INLIST		Number of grid points in vertical direction.
KM1		CONSIN		KM-1.
KN		INLIST		Number of levels at which 3-dimensional wind field is computed.
KNN		INLIST		Number of fixed grid intervals in vertical direction.
KOBS(N)	NSX	STNCON	ug/m^3	24-hour average of IOBS(N).
KUNITC		INLIST		I/O unit for storing computed and observed average concentration (ICAL,IOBS).
KUNITG		INLIST		Input unit for geographical and annual emission data.
KUNITP		INLIST		I/O unit for storing computed surface concentration field.
KUNITS		INLIST		Input unit for the varying source emission data.
KUNITW		INLIST		Input unit for time-varying meteorological data (RAMS) and surface wind field (UU,VV).
KWIND		INLIST		Control flag for the choice of obtaining surface wind field.
				=1, Input the preprocessed objective analyzed wind field (U1,V1);

			=2, Input the subjective analyzed wind field (UU,VV);
			=3, Input RAMS data, spatially uniform wind field is assumed;
			=4, Input RAMS data, variable wind field is generated.
LCHEM	INLIST		Control flag for computing chemical reaction.
			=0, Chemical decay of pollutant is not computed;
			=1, Compute chemical decay.
LCRUN	INLIST		Control flag for a run.
			=0, I/O test run;
			=1, actual run.
LHJUS	INLIST		Control flag for adjusting concentration values due to the change in the volume of grid cells.
			=0, keep total mass constant;
			=1, keep mass constant, if RH <1, otherwise, mass is not constant;
			=2, keep mass constant, if RH >1, otherwise mass is not constant,
			=3, mass is not constant.
LM	GEOIN		Total number of point sources.
LPRINT	CONSIN	sec	Minimum value of LTSOUS and LTWIND. Time average concentration field CC is computed over this time interval. This parameter is also used for controlling the logic path of executing the main program and certain I/O operations.
LPQ	INLIST		Control flag for modeling point sources.
			=1, source is added at one grid point only with downwind distance of U*min(T1,T2);

				=2, source is added at four neighboring grid points;
				=3, same as =1 but with downwind distance of V/DT;
				=4, same as =2 but with downwind distance of V/DT.
LSOUS(M)	2	INLIST		Control flags for adding area (M=1) and point (M=2) source into the system.
				=0, 'M' source is not considered;
				=1, 'M' source is injected.
LTOP		INLIST		Control flag for choice of upper boundary condition for vertical diffusion computations.
				=0, sets C=0 at the boundary.
				=1, reflecting boundary.
LTSTOP		INLIST	Hour	Maximum hours of real time to be simulated in a run.
LTSOUS		INLIST	Sec	Time interval of the time-varying source emission data that is to be input.
LTWIND		INLIST	Sec	Time interval of the time varying meteorological data is to be input.
LWARM		OUTAPE		A parameter indicating the status of I/O UNIT = KUNITC and KUNITP.
				=0 I/O units are initiated in this run;
				=1 I/O units contain results from previous runs.
LWIND		INLIST		Control flag for choice of computing vertical variation of horizontal wind components (U,V).
				=1, upper wind above height HP is same as wind at HP, wind below is computed by power law;
				=2, no vertical change in wind direction, wind speed is computed by power law;

				=3, vertical change in wind direction is assumed linearly proportional to the height.
LWRITE(N)	10	INLIST		Control flag for output options (see Section II-B-C).
LWTOP		INLIST		Control flag for choice of upper boundary condition for vertical advection computations. =0, no vertical flux crosses the boundary; =1, flux is allowed to cross the boundary.
LWW		INLIST		Control flag for choice of computing vertical wind component W(I,J,K). =0, set W(I,J,K)=0; =1, W(I,J,K) is computed by continuity equation; =2, after computing W(I,J,K) by continuity equation, it is smoothed again by 9-point average.
NEAR(I,J)	IN,JN	WINDER		The nearest RAMS station to wind grid point (I,J) has observed wind data.
NMONDY(N)	12	MAIN		Number of days in Nth month of a year.
NP(L)	LM	GEOIN		Point source identification number (refer to the NEDS data set).
NS		INLIST		Total number of monitoring stations.
NSX		MAIN		NS+1.
OLMIN		INLIST		Minimum value of Monin-Obukhov length.
P ARM(N)	10	-		Array to store various meteorological and source parameters.
'N=1'	-	WINDIN	m/sec	Mean wind speed.
'N=2'	-	WINDIN	deg.	Wind direction measured at center of the city.
'N=3'	-	WINDIN	°C	1st-level temperature measured at center of the city.

'N=4'	-	WINDIN		Continuous atmospheric stability class (=S).
'N=5'	-	MAIN	m	=HH, mixing height.
'N=6'	-	SOUSIN	g/sec	= QBTOT, total area source emission rate.
'N=7'	-	SOUSIN	g/sec	=PQBTOT, total point source emission rate.
'N=8'	-	WINDIN	°C	2nd-level temperature measured at center of the city.
'N=9'	-	WINDIN		Radiation or sky condition.
'N=10'	-	AKZCAL		=OL, Manin-Obukhov length.
PHIFHZ		AKZCAL		Non-dimensional temperature gradient.
PMAX		INLIST		Maximum value of exponent in wind profile power law.
PMIN		INLIST		Minimum value of exponent in wind profile power law.
PQA(L)	LM	SOUSIN	g/sec	Emission rate of point source L.
PQB(L)	LM	SOUSIN	g/sec	Emission rate of point source L at current time plus LTSOUS time interval (Not used in the current program).
PQBSUM		SOUSIN	g/sec	Total point source emission rate used in the model.
PQBTOT		SOUSIN	g/sec	Total point source emission rate.
QA(I,J)	IMJM	SOUSIN	g/sec/ km^2	Area source strength at grid point (I,J) at current time plus LTSOUS time interval (not used in the current program).
QB(I,J)	IMJM	SOUSIN	g/sec/ km^2	Area source strength at grid point (I,J).
QBSUM		GEOIN	g/sec	Total area source emission within the computational region or total source emission used in the model (only used when model runs on annual emission data).
QBTOT		SOUSIN	g/sec	Total area source emission rate.

RAMS(N)	6	WINDIN		RAMS station data.
'N=1'	-		m/sec	Surface wind speed.
'N=2'	-		deg.	Surface wind direction.
'N-3'	-		°C	1st-level temperature.
'N=4'	-		°C	2nd-level temperature.
'N=5'	-		ug/m³	SO_2 concentration.
'N=6'	-			Radiation or sky condition.
RDX(I)	IM	DIMENS		DX(I)/DX(I-1), I=2, IM.
RDY(J)	JM	DIMENS		DY(J)/DY(J-1), J=2, JM.
RDZ(K)	KM	DIMEN1		DZ(K)/DZ(K-1), K=2, KM.
RH		DIMEN1		Ratio of old and new vertical grid size at upper level.
RIB		AKZCAL		Bulk Richardson number.
TM		TIMEX	sec	Simulated time in seconds (floating point number).
TSEC		TIMEX	sec	Simulated time starting from each one-hour interval (floating point number).
U(I,J,K)	IJKN	WINDIN	m/sec	Wind component in X direction at grid point (I,J,K).
USTN(N)	NS	WINDER	m/sec	Surface wind component in X direction at monitoring station.
UU(I,J)	IN,JN	WINDIN	m/sec	Surface wind component in X direction at wind grid point (I,J).
UO		AKZCAL	m/sec	Surface friction velocity.
U1(I,J)	IMJM	WINDIN	m/sec	Surface wind component in X direction at grid point (I,J).
UZF(K)	TM	UVZF		Function determining the vertical variation of wind component in X direction.
V(I,J,K)	IJKN	WINDIN	m/sec	Wind component in Y direction at grid point (I,J,K).

VSTN(N)	NS	WINDGR	m/sec	Surface wind component in Y direction at monitoring station N.
VV(I,J)	IM,JM	WINDIN	m/sec	Surface wind component in Y direction at wind grid point (I,J).
V1(I,J)	IMJM	WINDIN	m/sec	Surface wind component in Y direction at grid point (I,J).
VZF(K)	KM	UVZF		Function determining the vertical variation of wind component in Y direction.
W(I,J,K)	IJKM	WWZF	m/sec	Wind component in Z direction at grid point (I,J,K).
WZF(K)	KM	WWZF		Function determining the vertical variation of wind component in Z direction.
XP(L)	LM	GEOIN		X coordinate of point source L in numerical grid units.
XPUTM(L)	LM	GEOIN	km	UTM coordinate of point source L in X direction.
XS(N)	NS	GEOIN		X coordinate of RAMS station N in numerical grid unit.
XSUTM(N)	NS	GEOIN	km	UTM coordinate of RAMS station N in X direction.
YP(L)	LM	GEOIN		Y coordinate of point source L in numerical grid units.
YPUTM(L)	LM	GEOIN	km	UTM coordinate of point source L in Y direction.
YS(N)	NS	GEOIN		Y coordinate of RAMS station N in numerical grid units.
YSUTM(N)	NS	GEOIN	km	UTM coordinate of RAMS station N in Y direction.
Z(K)	KM	DIMEN1	m	Height of vertical grid point K.
ZM(K)	KM	DIMEN1	m	Height of points in the middle of vertical grid element.
ZMAX		INLIST	m	Maximum mixing height used in the model.
ZP(N)	NS	GEOIN	m	Physical stack height of point source N.

ZPR(N)	NS	SOURCE		Effective stack height of point source N in numerical grid units.
ZR(N)	NS	SOUSIN		Normalize plume rise of point source N.
ZRPQ		INLIST		Constant used to get plume rise from its emission rate (if plume rise is not supplied).
ZRISE		INLIST		Parameter for adjusting plume rise.
ZS(I,J)	IMJM	GEOIN	m	Effective emission height of area source at grid point (I,J).
ZO(I,J)	IMJM	GEOIN	m	Surface roughness length at grid point (I,J).
ZOMEAN		INLIST	m	The uniform value of surface roughness for entire region. If ZOMEAN=0., then original ZO(I,J) is used.

3. Computational Procedures

The model requires three input data files and two output data files. The current program provides various options in I/O operations. The users can exercise these options through the parameters in included in the NAMELIST input and Job Control Language (JCL) specifications. In this section, we shall describe the specifications and requirements of the I/O devices for the model and the JCL set-up to run the program. Table II-4 lists the I/O units used in this program. The third column of the table indicates that I/O unit is for input (I) or for output(O). The fourth column indicates in which subroutine that I/O operations are executed.

UNIT	DSNAME	I/O	ROUTINE	VARIABLES
IUNIT		I	MAIN	'NAMELIST' (IUNIT=IUNIT2)
IUNIT1		I	CDTOTP	(UNIT FOR CARD READER)
IUNIT2		I/O	CDTOTP	(SCRATCH STORAGE UNIT)
JUNIT		O	(ALL)	(UNIT FOR LINE PRINTER)
JUNIT1		O	CDTOTP	(UNIT FOR LINE PRINTER)
KUNITG	EPAGE02	I	GEOIN	XRAMS,ZS,ZO,QB,PQB,...
KUNITS	EPASOUS	I	SOUSIN	KHR,KMO,KDAY,KYR,QB,PQB
KUNITW	WINDDATA	I	WINDIN	KYR,KMO,KDAY,KHR,U1,V1,RAMS
KUNITW	WINDDATB	I	WINDIN	KYR,KMO,KDAY,KHR,UU,VV,RAMS
KUNITW	EPARAMS	I	WINDIN	KYR,KMO,KDAY,KHR,RAMS
KUNITC	EPASTNO1	O	OUTAPE	IYR,IMO,IDAY,IHR,PARM,ICAL,IOBS
KUNITP	EPACONC1	O	OUTAPE	IYR,IMO,IDAY,IHR,PARM,CC, ICAL,IOBS

Table II-4 I/O Units Used in the Program

3-A. Parameter specification

All the necessary parameters for the model are initialized by means of input NAMELIST/INLIST/. Some of the secondary parameters and values of constants are specified in subroutine CONSIN. Initialization of variable arrays and certain constants are specified in DATA statements in various subroutines when it is necessary. The numerical grid system is initialized when subroutine DIMENS is called and executed.

Except for NAMELIST input, all other initializations of the model parameters are default processes and shall be consistent with the model formulation and programming logic. Therefore, in the following discussion we shall only deal with NAMELIST input.

The parameters included in the NAMELIST/INLIST/ and their sample values are given in Table II-5. The definition of each variable is given in Section II-2-D.

For better perspective, let us discuss these parameters in various groups according to their functions in the program.

```
&INLIST
     IM=30,  JM=40,  KM=14,  IN=9, JN=13,  KN=1,  KNN=10,  NS=25,
     LM=150,
     IMC=15, JMC=19,
     DX=5*2000.,20*1000.,5*2000.,DY=10*2000.,20*1000.,10*2000.,
     DZ=5*20.,9*25.,TM=0.0, DT=120.,AKA=24*1.0E-4,AKH=0.,13*10.,
     HS=10., HP=140., HG-1000., ZMAX=1000.,HMIN=300.,HMAX=600.,
     ZRPQ=0.6,ZRISE=1.0,PMAX=0.5,PMIN=0.15,DCMIN=2.0,OLMIN=30.,
     IHR=0,IDAY=1,IMO= 2,IYR=75, LTSTOP=8,IHRTP=1,IDAYTP=1
     JUNIT=6,KUNITG=13,KUNITS=14,KUNITW=15,KUNITC=16,KUNITP=17,
     LCRUN=1,LHJUS=0,LCHEM=1,LWW=0,LTOP=1,LWTOP=1,LSOUS=1,1,
     LWIND=2,KWIND=4,LPQ=1,LTSOUS=3600,LTWIND=3600,ZOMEAN=0.0,
     LWRITE=1,1,1,1,2,2,2,2,0,0,
&END
```

Table II-5. Example of NAMELIST/INLIST/to INPUT DATA

3-A-a) Parameters specifying grid system:

IM,JM,KM,KNN,IN,JN,KN,LM,NS,DX,DY,DZ.

DX, DY and DZ specify non-uniform grid size for a numerical method in the x,y and z directions respectively. The choice of DX and DY shall correspond to the area source inventory grid. The dimensions of DX, DY, DZ are IM,JM,KM, respectively. Therefore, they shall have IM values for DX and so forth. IM,JM, KM,IN,JN,KN,LM,NS are also used for dynamic allocation of storage when various subroutines are called. Hence, the values specified for these parameters shall not exceed the number used in the DIMENSION statement in the MAIN program. As mentioned in section II-2-A, this program can run on three operational configurations, namely, debug, test, and production run. To choose one particular operational mode, the following rules shall be followed. For the debug run, set KM=5, and KN=1; for the test run, set KM=14 and, KN=1; and for the production run, set KM=14 and KN=7. In addition, the DIMENSION specification in MAIN program for three dimensional arrays, namely, CP1, C, U, V, W, shall be changed accordingly. (The program provides three cards for this purpose. The user only needs to select one card and keep the other two as comment cards.)

3-A-b) Parameters for time indices:

TM,DT,IHR,IDAY,IMO,IYR,IDAYTP,IHRTP,LTSTOP.

TM shall be set equal to zero. DT is the initial guess of

the time step for numerical integration. It will be recomputed in the execution of the program. IHR,IDAY,IMO,IYR specify the starting real time for which the model computation is to be performed. LTSTOP determines the number of hours to be simulated in a run. It is assumed that the necessary input data for time-varying source emission and meteorological data are available through the time span of simulation. (See section II-3-B). IDAYTP and IHRTP specify the starting day and the hour for which the computed concentrations have been stored on I/O units KUNITC and/or KUNITP. (see section II-3-D).

3-A-c) Physical parameters:

AKH,AKA,HS,HG,ZMAX,HMIN,HMAX,ZRPQ,ZRISE,PMAX,PMIN,
DCMIN, OLMIN, ZOMEAN

This group of the parameters deal with physical assumptions currently employed in the program. The specification of these values is confined to the context of the current model formulation, and within this formulation they have reasonable physical meaning. We suggest that unless one is completely familiar with the model and its programming logic, caution should be observed in changing these values from those given in Table II-4.

3-A-d) Parameters for I/O operation:

LTSOUS,LTWIND,IMC,JMC,LWRITE.

LWRITE control the output options, and will be described in section II-3-C and section II-3-D. IMC,JMC shall have values less than IM,JM respectively. These two numbers decide where vertical cross-sections of concentration field are to be printed out. LTSOUS and LTWIND specify at what time interval the time-varying source emission and meteorological data were prepared. The units for these two parameters are in seconds. However, they shall be chosen in the multiple of 3600 seconds with minimum values of 3600 seconds.

3-A-e) Number for I/O unit:

JUNIT,JUNITC,KUNITG,KUNITP,KUNITS, KUNITW.

These numbers specify various I/O units to be used in the program. The values given to these parameters shall be consistent with JCL specifications. More detailed description is given in section II-3-E.

3-A-f) Parameters for selection of modelling options:

LCRUN, LHJUS, LCHEM, LWW, LTOP, LWTOP, LSOUS, LPQ, KWIND, LWIND.

The values given to these parameters shall be in accordance with the users need and shall be confined to the context of the logic used in the program. Each value given to a

parameter has a special meaning in the computational method. Hence, they must be defined carefully. The variables described in section II-2-D offer a quick reference.

3-B. Input specifications and requirements

In addition to the NAMELIST input described in the previous section, the model requires three sets of input data. They are: a) geographical and annual emission data, b) time-varying source emission data (if available), and c) time-varying meteorological data.

3-B-a) Geographical and annual emission data.

These data are input through subroutine GEOIN. The I/O unit is KUNITG. They are prepared by auxiliary programs (see section II-4). Since this data set is prepared in card-input format, the following discussion is based on an 80-column card format. The listing of this input data set is given in Appendix 3.

This data set shall consist of eight (8) data groups. They should be arranged in the following sequence.

(i) Region specification

IXBEG, IYBEG,IBEG,JBEG: Format = (4I5).

These four numbers appear in one card. IXBEG and IYBEG specify the UTM coordinates of the southwestern corner of the area source inventory map. IBEG and JBEG are the x and y distances (in kilometers) from point (IXBEG, IYBEG). Point (IXBEG+IBEG, IYBEG+JBEG) is the origin of the numerical grid system.

(ii) RAMS station locations

NS	Format = (I5)
(FMTDS(N),N=1,10)	Format = (10A4)
(IS(L), XSUTM(L), YSUTM(L), L=1,NS)	Format = (FMTDS)

Note that variable format is used to read in data of RAMS station identification and locations. FMTDS specify the format statement by which the following data are to be read in. The same method is applied to input the remainder of the data in KUNITG.

(iii) Surface roughness parameters

(FMTDS(N),N=1,10)	Format = (10A4)
((ZO(I,J),I=1,IM),J=1,JM)	Format = (FMTDS)

(iv) Effective emission heights of error sources

(FMTDS(N),N=1,10)	Format = (10A4)
((ZS(I,J),I=1,IM),J=1,JM)	Format = (FMTDS)

(v) Point source locations and physical stack heights

LMAX	Format = (I5)
(FMTDS(N),N=1,10)	Format = (10A4)
(NP(L),XPUTM(L),YPUTM(L),L=1,LMAX)	Format = (FMTDS)

(vi) Annual average emission rates of area source

(FMTDS(N),N=1,10)	Format = (10A4)
((QB(I,J),I=1,IM),J=1,JM)	Format = (FMTDS)
QBTOT	Format = (F10.1)

(vii) Annual average emission rate of point sources

(FMTDS(N),N=1,10)	Format = (10A4)

(PQB(U),L=1,LMAX) Format = (FMTDS)

PQBTOT Format = (F10.1)

(viii) Normalized plume rise for point sources

FMTDS(N),N=1,10 Format = (10A4)

(ZB(L),L=1,LMAX) Format = (FMTDS)

3-B-b) Time- varying source emission data

If time-varying source emission data are available, the model will receive it through subroutine SOUSIN. It will carry out its computations based on these data. Otherwise, the annual average emission data will be used. These time-varying source emission data are input every LTSOUS seconds, which is specified by NAMELIST input. Consequently, the data shall be prepared for every LTSOUS time interval and cover the time span over which the model computation is to be performed, i.e. (ITOTHR*3600/LTSOUS) sets of these data. These data shall be prepared in advance of model computation and stored on I/O unit = KUNITS. For every LTSOUS time interval, the data are arranged as follows:

KYR,KMO,KDAY,KHR((QB(I,J),I=1,IM),J=1,JM),(PQB(L),

L=1,LM),(ZR(U),L=1,LM), QBTOT,PQBTOT.

Unformatted read statement is used to input this data set. Therefore, it is necessary to prepare these data in KUNITS based on unformatted write statement. KYR,KMO,KDAY,KHR define the ending time of each averaged emission rate data.

3-B-c) Meteorological data

Meteorological data are input through subroutine WINDIN every LTWIND second of real time. Similarily to time varying source emission data, the unformatted write and read is used in the I/O processes. Data shall also be prepared in advance of the model computation and stored on I/O unit = KUNITW. It shall at a minimum cover the entire time period for which model computation is to be performed, i.e. (ITOTHR*3600/LTWIND) sets of these data.

There are four options in the model for constructing surface wind fields. These options are controlled by parameter KWIND. Thus, the meteorological data should be prepared consistent with the choice of options.

KWIND=1: KYR,KMO,KDAY,KHR,((U1(I,J),I=1,IM),J=1,JM)

((V1(I,J),I=1,IM),J=1,JM),((RAMS(M,N),M=1,6),N=1,NS)

KWIND=2: KYR,KMO,KDAY,KHR,((UU(I,J),I=1,IN),J=1,JN),
((VV(I,J),I=1,IN),J=1,JN),((RAMS(M,N),M=1,6),N=1,NS)

KWIND=3,4: KYR,KMO,KDAY,KHR,((RAMS(M,N),M=1,6),N=1,NS)

3-C. Output specifications

For each computation run, the NAMELIST input is automatically printed out in its original image. This is executed in subroutine CDTOTP. For every pass through the main computational loop in MAIN program, the real time of the simulated period is printed out. It serves as a title heading for other output.

All other print outputs of the model computations are executed in subroutine PRINTS (including entry point PRINTA,PRINTB and PRINTC). The storage of computational results on tape or disk is performed in subroutine OUTAPE. We shall discuss the storage of computed results in the next section. In the following discussion, we shall only deal with print output. Its I/O unit is JUNIT.

Depending on the mode of each computational run, this program provides to the users the selection of which variables are to be printed out. When the surface field and vertical cross-section are needed, subroutine WRITES and WRITEZ are automatically called to perform such duties. The choice of print output is controlled by parameter LWRITE(N) where the maximum value of N is ten. These ten integer values of LWRITE shall be specified by the user in the NAMELIST input. In table II-6 the options of printing each variable is listed. The subroutine names listed on the first column of table II-6 indicate that where the output operations are executed. The 3rd column of the table specifies the condition that the value of LWRITE is needed in order to output or print out variables listed in the 4th column. In general, the highlights of Table II-6 are as follows:

a) If LWRITE(N)=0, for all N, there will be no output performed.

b) Each element of LWRITE control a group of variables to be printed out. The function of each

LWRITE(M) = CONTROL FLAG FOR OUTPUT

ROUTINE	M	COND.	VARIABLES TO BE OUTPUT
PRINTS	1	.GE. 1	IS,XSUTM,YSUTM,XS,YS,JXS,JYS(L),L=1,MS
			(ZO(I,J),ZS(I,J),QB(I,J),QBTOT,QBSUM
			MP,XPUTM,YPUTM,PQB,XP,YP,ZP,ZR(L),L=1,LM
			PQBTOT,PQBSUM
PRINTA	2	.GE. 1	QBTOT,PQBTOT,QBSUM,PQBSUM
		= 2,4	QB(I,J)
		= 3,4	PQB(L)
PRINTB	3	.GE. 1	RAMS(M,L)
		= 2	UU(I,J),VV(I,J)
	4	.GE. 2	U1(I,J),V1(I,J)
			+W(I,J,1), (IF LWW=1)
		= 3	U(I,J,K),V(I,J,K)
			+W(I,J,K), (IF LWW=1)
		.NE. 0	Z(K),RH
		.GE. 1	UZF(K),VZF(K)
			+WZF(K), (IF LWW=1)
	5	.GE. 1	AKF(K)
		= 2	AKZ(I,J), FOR J=JM/2
		= 3	AKZ(I,J)
	6	.GE. 1	PARM(L),DT
		= 2	UO,PHIFHZ,HFZ,RIB
PRINTC	7	= 2,4	CP1(JXS,JYS)
		.GE. 1	CP1(IMC,J,K),CP1(I,JMC,K)
		.GE. 3	CP1(I,J,1)
			CP1(I,J,K), (IF IHR=0)
	8	.GE. 1	ICAL(L),IOBS(L)
			+ KCAL(L),KOBS(L), (IF IHR=0)
		= 2	CC(I,J)
OUTAPE	9	.GE. 1	IYR,IMO,IDAY,IHR,PARM(M),ICAL(L),IOBS(L)
			-- ON I/O UNIT=KUNITC
	10	.GE. 1	IYR,IMO,IDAY,IHR,PARM(M),CC(I,J),ICAL(L),
			& IOBS(L) -- ON I/O UNIT = KUNITP

Table II-6 Output Operations Controlled by LWRITE(M)

element of LWRITE can be summarized as:

LWRITE(1)	:	Geographical and annual average emission data;
LWRITE(2)	:	Time- varying source emission data
LWRITE(3)	:	RAMS station data and subjective analyzed wind field (if KWIND=2)
LWRITE(4)	:	3-D wind field at grid points and vertical grid system (vertical component only print when LWW≠0)
LWRITE(5)	:	Eddy diffusivities
LWRITE(6)	:	Time step and meteorological parameters
LWRITE(7)	:	Instantaneous concentration fields
LWRITE(8)	:	Average concentration fields
LWRITE(9)	:	Storing computed results on I/O unit=KUNITC
LWRITE(10)	:	Storing computed results on I/O unit=KUNITP

c) The largest value which can be assigned to each element of LWRITE varies from one to four. When these largest values are used, it will result in a large volume of print output.

d) The optimum print output for a production run is:

LWRITE=1,1,1,1,2,2,2,2,1,1.

This will result in three pages of output per each LPRINT interval of simulation.

A sample of print outputs is given in appendix 4.

3-D. Storage of Results

Frequently the user will wish to store the computational

results on a disk or a tape. Such storage will provide a data base for further analysis of the model performance or for other usages, e.g., graphic display and climatological study.

The storage of computed results is executed by subroutine OUTAPE. The control parameters are LWRITE(9) and LWRITE(10). They must be set greater than or equal to one, if the user wishes to exercise this option. The I/O units are KUNITC and KUNITP.

The variables to be stored on KUNITC are:
ITR,IMO,IDAY,IHR,(PARM(N),N=1,10),
(ICAL(N),N=1,NSX),(IOBS(N),N=1,NSX).
On KUNITP, they are:
ITR,IMO,IDAY,IHR,(PARM(N),N=1,10),((CC(I,J),I=1,IM),J=1,
JM),(ICAL(N),N=1,NSX), (IOBS(N),N=1,NSX).
Unformatted write statements are used for both output executions.

The data stored on KUNITC and KUNITP are in sequential data sets. The user can choose to store each set of computed results sequentially with previously computed results (if they are in the same month and year). However, the time

index shall be in chronological order. In addition, the starting time (day and hour) that data were stored on these I/O unit should be specified in the NAMELIST input. They are IDAYTP and IHRTP. The following example illustrates how it works:

Example 1:

LWRITE(9)=1, LWRITE(10)=0, IHR=0, IDAY=3, IHRTP=1, IDAITP=2.

The program will write its results on I/O unit = KUNITC following data for the 24th hour of the second day. If such data cannot be found, then the run will be terminated due to EOF or Error on I/O unit =KUNITC.

Example 2:

LWRITE(9)=1,LWRITE(10)=0,IHR=0,IDAY=1,IHRTP=1,IDAYTP=1

The program will assume that the I/O unit=KUNITC does not contain any previously computed results. It will start its output execution from the beginning of the allocated space on KUNITC.

3-E. JCL Specification

To run the program, the user is required to prepare the input data according to the above described input specifications. He is also required to specify the JCL cards. One of the most important considerations in preparing the job deck for running the program is that the parameters specified in the NAMELIST input must be consistent with JCL specification, with the operational mode of the run, and with the intended modeling options. In this section, we shall briefly illustrate these factors. We shall assume that all the necessary input data described in section II-3-B are created, catalogued and stored on the peripheral storage device. The DSNAME for each data set is:

a) Geographical and Annual emission data
   DSN=JCS4165.EPAGEO2.DATA
b) Time-varying emission data
   DSN=JCS4165.EPASOUS.DATA
c) Time-varying meteorological data
   DSN=JCS4165.EPARAMS.DATA

There are various ways of running the program. The simplest way is to use all the source decks and go through the compiling, linkediting and executing steps. An example of the job set-up is given in Table II-7. In this example, it is assumed that the source program of IBMAQ-2 has been previously copied to a data set named JCS4165.IBMAQ2.FORT, stored on a direct access device and catalogued. If the source program is to be submitted on the card reader, the

```
//EPA35A     JOB (JCS4165,'L=9,G=EPA'),SHIR,MSGLEVEL=1,CLASS=E,TIME=2
/*ROUTE  PRINT EXPRESS
//AA    EXEC  FWHLX,REGION.X=384K
//*C.SYSPRINT DD DUMMY,SYSOUT=S
//C.SYSIN   DD  DSN=JCS4165.IBMAQ2.FORT,DISP=SHR
//L.SYSLMOD  DD UNIT=DISK
//L.SYSUT1 DD UNIT=DISK
/*
//X.FT12F001 DD UNIT=SYSDA,SPACE=(TRK,(1,1))
//X.FT13F001 DD DSN=JCS4165.EPAGE02.DATA,DISP=SHR
//X.FT14F001 DD DSN=JCS4165.EPASOUS.DATA.DISP=SHR
//X.FT15F001 DD DSN=JCS4165.EPARAMS.DATA,DISP=SHR
//X.FT16F001 DD DSN=JCS4165.EPASTNO1.DATA,DISP=SHR
//X.FT17F001 DD DSN=JCS4165.EPACONC1.DATA,DISP=SHR
//X.SYSIN   DD  *
 &INLIST
      IM=30,JM=40,KM=14,IN=9,JN=13,KN=1,KNN=10,NS=25,LM=150,
      IMC=19,JMC=15,
      DX=5*2000.,20*1000.,5*2000.,DY=10*2000.,20*1000.,10*2000.,
      DZ=5*20.,9*25.,TM=0.0,DT=120.,AKA=24*1.0E-4,AKH=0.,13*10.,
      HS=10.,HP=140.,HG=1000.,ZMAX=1000.,HMIN=300.,HMAX=600.,
      ZRPQ=0.6,ZRISE=1.0,PMAX=0.5,PMIN=0.15,DCMIN=2.0,OLMIN=30.,
      IHR=0,IDAY=1,IMO= 2,IYR=75,LTSTOP=8,IHRTP=1,IDAYTP=1.
      JUNIT=6,KUNITG=13,KUNITS=14,KUNITW=15,KUNITC=16,KUNITP=17,
      LCRUN=1,LHJUS=0,LCHEM=1,LWW=0,LTOP=1,LWTOP=1,LSOUS=1,1,
      LWIND=2,KWIND=4,LPQ=1,LTSOUS=3600,LTWIND=3600,ZOMEAN=0.0,
      LWRITE=1,1,1,1,2,2,2,2,0,0,
 &END
/*
```

Table II-7 Sample of JCL, Example 1

```
//EPA35A     JOB (JCS4165,'L=9,G=EPA'),SHIR,MSGLEVEL=1,CLASS=E,TIME=2
/*ROUTE  PRINT EXPRESS
//AA    EXEC  FWHLX,REGION.X=384K
//*C.SYSPRINT DD DUMMY,SYSOUT=S
//C.SYSIN DD *
        .
        .
        . (SOURCE DECK)
        .
        .
/*
//L.SYSLMOD  DD UNIT=DISK
//L.SYSUT1 DD UNIT=DISK
//X.FT12F001 DD UNIT=SYSDA,SPACE=(TRK,(1,1))
//X.FT13F001 DD DSN=JCS4165.EPAGE02.DATA,DISP=SHR
//X FT14F001 DD DSN=JCS4165.EPASOUS.DATA,DISP=SHR
//X.FT15F001 DD DSN=JCS4165.EPARAMS.DATA,DISP=SHR
//X.FT16F001 DD DSN=JCS4165.EPASTN01.DATA,DISP=SHR
//X.FT17F001 DD DSN=JCS4165.EPACONC1.DATA,DISP=SHR
//X.SYSIN   DD   *
 &INLIST
      IM=30, JM=40, KM=14, IN=9,JN=13,KN=1,KNN=10,NS=25,LM=150,
      IMC=19,JMC=15,
      DX=5*2000.,20*1000.,5*2000.,DY=10*2000.,20*1000.,10*2000.,
      DZ=5*20.,9*25.,TM=0.0, DT=120.,AKA=24*1.0E-4,AKH=0.,13*10.,
      HS=10., HP=140., HG=1000., ZMAX=1000.,HMIN=300.,HMAX=600.,
      ZRPO=0.6,ZRISE=1.0,PMAX=0.5,PMIN=0.15,DCMIN=2.0,OLMIN=30.,
      IHR=0,IDAY=1,IMO= 2,IYR=75, LTSTOP=8,IHRTP=1,IDAYTP=1,
      JUNIT=6,KUNITG=13,KUNITS=14,KUNITW=15,KUNITC=16,KUNITP=17,
      LCRUN=1,LHJUS=0,LCHEM=1,LWW=0,LTOP=1,LWTOP=1,LSOUS=1,1,
      LWIND=2,KWIND=4,LPQ=1,LTSOUS=3600,LTWIND=3600,ZOMEAN=0.0,
      LWRITE=1,1,1,1,2,2,2,2,0,0,
 &END
/*
```

Table II-8 Sample of JCL, Example 2.

JCL set-up is given in Table II-8. It is noted that in both examples, JCL specification of the I/O unit for geographical and annual emission data is 13; time-varying source emission data is 14, time-varying meteorological data is 15, and storage of computed results is specified by 16 and 17. All these I/O units in JCL specifications are consistent with NAMELIST input parameters of KUNITG=13, KUNITS=14, KUNITW=15, KUNITC=16 and KUNITP=17 respectively. I/O unit =12 is for scratch storage.

4. Auxiliary Program--Input Data Preparation

In this section we shall briefly describe the auxiliary program which processes and analyzes geographical and annual average emission data for the model input. The input specifications were described in Section II-3-B, above.

For this study, we obtained the following data sets:

1) Annual average area source emission data of SO_ for the St. Louis area: This data set consists of 2049 punched cards. Each card represents an area source. The area source grid is non-uniform and consists of square elements ranging from one to ten kilometers in size. It

covers an area of 200x140 kilometer squares. This data set was provided by EPA.

2) NEDS point source data for the St. Louis area: This set consists of about 4700 cards. There are 175 plants and factories included in this source inventory. Many of them have multiple stacks within a plant. The structure and format of this data set is described in "Guide for compiling a Comprehensive Emission Inventory", published by EPA (Reference 9).

3) UTM conversion table and program: This data set and program is provided by EPA. It is to be used for converting a location in longitude and latitude units to a UTM coordinate system. It also can be used for converting one zone of UTM as an extension of the adjacent zone.

4) RAMS station locations: Twenty-five RAMS station locations in longitude and latitude units are provided by EPA in printed form.

5) Topographical and building information: These data were obtained by us as a few pages of handwritten notes. (Reference 10). It consists of information related to average building height, height of ground surface above the bottom of Miss. River, and the estimated surface

roughness. A nested grid system is used for these data. The origin of the grid is placed at the intersection of highways 67 and 40. These data is obtained from Dr. Fred M. Vukovich of Research Triangle Institute, Research Triangle Park, N.C.

6) St. Louis Maps: They are published by U.S. Geological Survey and by various oil companies.

It is obvious that the above-described data are not compatible with model input specifications. To convert these data sets into the form required for model usage is quite a time-consuming task. Our experience has indicated that the systematic analysis of input data is as important as the model computation. Therefore, the analysis procedures described in this section may be useful in the further model development.

The first objective of processing these data is to select a unified coordinate system, the computational region of the model, and its grid system. Although, we try to be as objective as possible, some of the work still involves extensive subjectivity. In this respect, the computer programs can only systematically screen the data, tabulate it and display it in map forms, and the investigator must

make the decisions.

The selection of a coordinate system is straightforward. All the data should be based on the UTM coordinate system. Consequentially, the numerical grid system in the model computation should also be related to this coordinate system. However, the selection of the computational region of the model and its detailed grid system requires careful consideration. The accuracy of model computations and the requirements of computer capability for performing these computations are closely related to the characteristics of the modeled region and its computational mesh. The factors that need to be considered are as follows:

1) The computational region shall be sufficiently large so that we can minimize the numerical error in the central region (where we are most concerned) due to the specified inflow boundary condition.

2) The computational region shall include the major area-source and point-source emission in the area. This will make the computed concentration field consistent with the total pollutant mass emitted.

3) The computational region shall encompass all the RAMS stations (if possible). This will permit utilization of

the data obtained from the RAMS stations.

4) The numerical grid resolution shall be compatible with the area source emission inventory grid. It is desirable that numerical computations shall be based on the finest mesh size available in the area source emission inventory. Thus, the accuracy of numerical computations will be compatible with the given input data.

5) In addition to the above-mentioned criteria, we should keep in mind the computer capability for performing the computation involving a large region to be covered, and utilizing a fine grid resolution. The CPU core storage and CPU time required to run a job may outweight other factors. Our most important concern in this work was that the model be operable on EPA's computer facilities in a reasonable amount of CPU time.

It is obvious that the selection of the computational region of the model and its grid system shall be performed concurrently with other data analysis. Based on the criteria described above, we arrived at the following design features:

1) The computational region employed is 40x60 km centered

at RAMS station 101 (center of St. Louis city). This total area is about the same as in our earlier model and includes all the major area sources from St. Louis, E. St. Louis, Alton city and Granite City and the major point sources located at Alton and Merames. A total of 21 RAMS stations are within this region.

2) The smallest grid element of the area source inventory is 1x1 km . It is clear that the model computational grid must have the same resolution.

3) With 14 levels in the vertical grid adopted , the 30x40 element horizontal grid is the maximum resolution acceptable by most computer facilities. (Note that increasing the number of grid cells also means increasing the required CPU time for computation).

4) A non-uniform numerical grid is adopted in order to cover the 40x60 km area with a 30x40 element grid system. We call this non-uniform system a "stretched" grid. The center of the computational region is a 20x20 grid of one kilometer squares. This is compatible with the finest area-source resolution. In the outer area, the grid elements are stretched, and become 2x1, 1x2, and 2x2 km in size.

In addition to the above analysis, the St. Louis map was

digitized. This is for graphic display purposes. Now, let us briefly discuss our analysis procedure and the function of each auxiliary program.

4-A. Area Source data

1) Objective

- To make the best use of NEDS data for the model and obtain the information for determining the computational region and the numerical grid system.

2) Pertinent factors:

- Geographical distribution of area sources and their emission strengths.
- Grid resolution used in the area source inventory.
- Area source distribution as related to location of RAMS stations.
- Computational requirements of the model.

3) Analysis procedures:

- Screen the original data set for error and consistency check.
- Convert the original data to a uniform grid

of 1x1 km size and compute total emission rate from all sources.

- o Print data in map form for checking their distribution.
- o Choose 40x60 grid elements and check the sub-total emission rates. (This is iterated several times).
- o Convert 40x60 grid system to 30x40 stretched system which is compatible to the computational (numerical) grid.
- o Convert emission rate to density units.
- o Estimate approximate effective emission height or each area source from current data and from 1964-1965 data.
- o Check emission data with 1964-1965 monthly emission data.

4-B. Point source data

1) Objective

- o Select significant point sources from NEDS data.
- o Combine small stack emission.
- o Estimate plume rise from available stack parameters.
- o Subjectively fill in the missing information

in the original data.

2) Pertinent factors

- o Geographical distribution of point sources.
- o Relative location to RAMS stations.
- o Computational requirements of the model.
- o Retain the stack identification parameter for reference.

3) Analysis procedure

- o Tabulate and screen NEDS data (we found many error and missing cards).
- o Subjectively edit original data set. (Mostly fill in missing cards or place cards in proper order).
- o Select stacks with SO_2 emission and compute their total emission.
- o Estimate UTM coordinate for selected source.
- o Map source locations on area source grid and computational grid for checking their distribution.
- o Select necessary stack parameters from original data set.
- o Compute plume rise for each stack based on available stack parameters (various formulas

were used).

- o Combine small stacks together to reduce total number of point sources.
- o Estimate values for all the missing data.
- o Sort and arrange point-source sequence within the computational region and compute the sub-total emission rate.
- o Check emission data with 1964-1965 data.

4) Comment

This is most difficult data analysis the authors have ever been called upon to perform. It is obvious that a better source inventory is required, if a model validation is to be considered.

4-C. Surface parameter data

a) Objective

- o Estimate surface roughness parameters.
- o Estimate effective emission height of area sources.

b) Pertinent Factor

- o The effect of results on the final

diffusion computation.

c) Analysis procedure

- o Screen and tabulate F.M. Vukovich data,
- o Convert F.M. Vukovich data from highway coordinate to UTM coordinate.
- o Convert F.M. Vukovich data from nested grid to numerical grid.
- o Estimate values for vacant region (when nested grid is converted to stretched grid, a few strips of the region are without data).
- o Estimate silhouette area ratio of each grid element.
- o Estimate surface roughness parameters based on Lettau's formula.
- o Estimate effective emission height of area sources.
- o Compare with 1964-1965 data.

4-D. RAMS Station location data

The task required for this data set is to convert station location in longitude and latitude to UTM coordinates and to compute station locations in terms of the grid unit used by

the model.

4-E. Validity check of all the data

The above-analyzed data are combined together in order to meet the input specifications of the model. The model computation was performed based on this geographical and annual emission data. The 1965 meteorological data was used in these computations. The computed results were checked with our previous model results and observed data at ten monitorforg stations in Feb. 1965. This was done to check the consistency of the current data set with respect to model formulation. No validation analysis was attempted.

4-F. Function of each auxiliary program

As mentioned previously, the objective of these auxiliary programs is to prepare the data for model input. The final result of data analysis is to create a data set "EPAGE02.DATA." This data set is read into the model by I/O unit=KUNITG. The schematic diagram shown in Figure II-4 describes how this data set is created by these auxiliary programs. In this diagram, XXXXX.F designates a FORTRAN program and XXXXX.D is a input or output data. The listing of these auxiliary programs are given in Appendix 2.

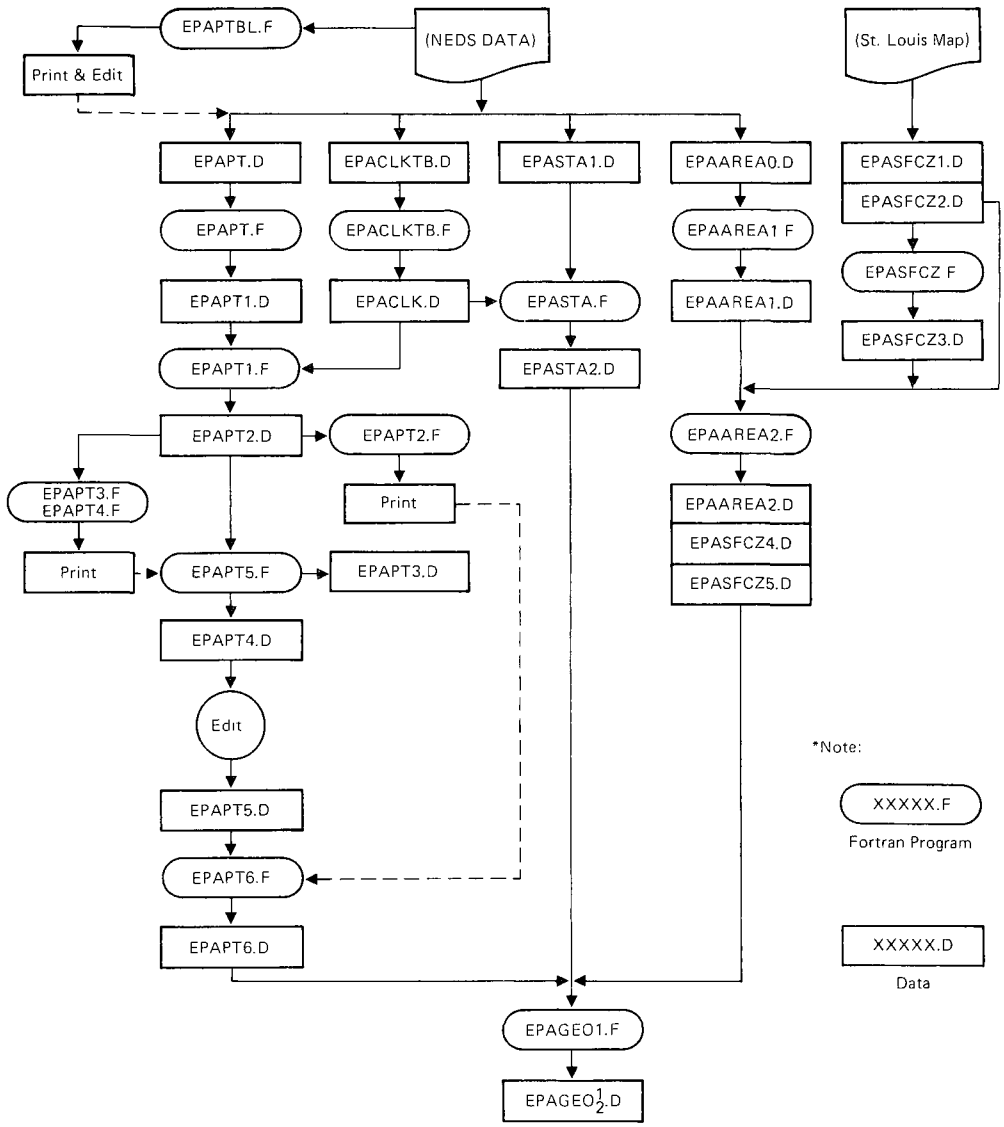

Figure II-4. Schematic Diagram of Processing NEDS & Geographical Data

1) Program : EPAPTBL.FORT
Input : NEDS point source data
Output : Print only
Function : a) Tabulate NEDS point source data.
b) Identify missing or misplaced cards in data set.
c) The result of this information is used to edit (subjectively) original data.

2) Program : EPAPT.FORT
Input : EPAPT.DATA (edited NEDS point source data)
Output : EPAPT1.DATA
Function : a) Tabulate data.
b) Create new data set EPAPT1 DATA, which eliminate stacks with zero SO2 emission and only contains selected stack parameters.

3) Program : EPACLKTB.FORT (EPA-provided program)
Input : EPACLKTB.DATA
Output : EPACLK.DATA
Function : Copy UTM conversion table from sequential data set to a direct-access device.

4) Program : EPAPT1.FORT
Input : EPAPT1.DATA
EPACLK.DATA
Output : EPAPT2.DATA
Function : a) Convert UTM coordinate of stacks in zone 16 as extension of zone 15.
b) compute total emission rates from all point source in tons/year.

5) Program : EPAPT2.FORT
Input : EPAPT2.DATA
Output : Print only
Function : Compute plume rise from each stack by various formulae.
Comments : Current program included five formulae. They are:
a) Moses and Carson (Reference 11).
b) Modified Csanady (Reference 12).
c) CONCAWE (Reference 13).
d) Modified CONCAWE#1 (Reference 12).
e) Modified CONCAWE#2 (Reference 12).

6) Program : EPAPT3.FORT
EPAPT4.FORT
Input : EPAPT2.DATA
Output : Print only

Function : a) Map point source onto 1x1 km2 grid for whole region in units of tons/year and gm/sec.
b) Map point source location onto numerical grid.
c) Compute point source emission per each numerical grid element.
d) List point sources located outside the region.
e) Compute total point source emission in the map region and its ratio to original total emission rate.
f) Computes total number of point source in the map region.

Comment : The information resulting from this program is used to:
a) select computational region.
b) help in writing program "EPAPTS.FORT.

7) Program : EPAPT5.FORT
Input : EPAPT2.DATA
Output : EPAPT3.DATA
EPAPT4.DATA

Function : a) Combines small-source emission stacks within a plant to a large stack.
b) Compute normalized plume rise by modified CONCAWE#1 Formulae.
c) Create new data EPAPT3,DATA, which has same format as input data set EPAPT2.DATA.
d) Create new data EPAPT4.DATA, which contains only x,y,z location of the stack, SO2 emission rate and normalized plume rise. However, the stacks for which data are missing are identified.

Comment : a) EPAPT4.DATA is used to create EPAPT5.DATA, by terminal input to fill in all the missing data.
b) The criteria for combining stacks together are:
- o all stacks must be within a plant.
- o stack emission rate shall be less than 150 tons/year.
- o if combined emission rate of small stacks is greater than 150 tons/year, then treat as an independent stack.
- o if it is less than 150 tons/year, then it is combined to other stack which has emission greater than 150 tons/year.
- o weighted average method is used to computed average physical stack height and plume rise for combined stack. The weighting factor is the emission rate.

8) Program : EPAPT6.FORT
Input : EPAPT5.DATA
Output : EPAPT6.DATA
Function : a) Arranges and prints point source sequence in a particular order for analysis purpose. This program provides four methods of ordering point source sequence. These methods are according to source strength; x,y locations; regions, and the distance to the center of computational region.
b) Creates EPAPT6.DATA, which eliminates sources outside the computational region and arranges point source sequence in a particular order.
Comment : Format for EPAPT6.DATA is put on the first card of the data set.

9) Program : EPASTA.FORT
Input : EPACLK.DATA
: EPASTA1.DATA (RAMS station location in Latitude and Longtitude).
Output : EPASTA2.DATA
Function : a) Converts RAMS station location in Latitude and Longtitude to UTM coordinate.
b) Compute UTM coordinate of RAMS station location in zone 16 as extension of zone 15.
Comment : This program is provided by EPA.

10) Program : EPAAREA1.FORT
Input : EPAAREA0.DATA
Output : EPAAREA1.DATA
Function : a) Maps NEDS area source data from non-uniform grid size to 1x1 km grid.
b) Create EPAAREA1.DATA.

11) Program : EPASFCZ.FORT
Input : EPASFCZ1.DATA
EPASFCZ2.DATA
Output : EPASFCZ3.DATA
Function : Reads in total height and terrain height to calculate average building height for each grid element and stores the data in EPASFCZ3.

12) Program : EPAAREA2.FORT
Input : EPAAREA1.DATA
EPASFCZ2.DATA
EPASFCZ3.DATA

Output : EPAAREA2.DATA
EPASFCZ3.DATA
EPASFC25.DATA

Function : a) Reads in area sources in 200x140 uniform grid elements from EPAAREA1, and chooses 40x60 desired area sources, and converts 40x60 to 30x40 area sources corresponding to computational non-uniform grid elements.
b) Reads in terrain height and building height data in Bukhovich's highway coordinates, and converts them to UTM coordinates.
c) Fills up the undefined area by interpolation and extrapolation, and converts data from his nested grid system to uniform grid.
d) Convert the data from uniform grid to stretched grid for desired region.
e) Combines the terrain height, building height, and area sources to estimate the surface roughness.

13) Program : EPAGEO1.FORT
Input : EPAPT6.DATA
EPASTA2.DATA
EPAAREA2.DATA
EPASFCZ4.DATA
EPASFCZ5.DATA
Output : EPAGEO2.DATA
Function : Creates EPAGEO2.DATA, which meets the input specification of model requirement for geographical and annual average emission data (see section II-3-B)

14) Program : EPAGEOIN.FORT
Input : EPAGEO2.DATA
Output : print only
Function : Prints out EPAGEO2.DATA in map form for checking purposes.

15) Program : EPAMAP.FORT
Input : EPAMAP2.DATA
Output : print only
Function : prints out St. Louis map on line printer.
Comment : EPAMAP2.DATA is a data set which contains a digitized information of St. Louis map.

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16. ABSTRACT

An advanced generalized urban air quality model (IBMAQ-2) is developed based on the theory utilized in an existing model (IBMAQ-1) as prescribed in Ref. 1. The model, based on numerical integration of the concentration equation, computes temporal and three-dimensional spatial concentration distributions resulting from specified urban point and area sources by using NEDS (National Emission Data System) and simulated RAMS (Regional Air Monitoring System) data. The UTM (Universal Transverse Metric) coordinates are used in all geographical, source emission, and monitoring data. A new method to incorporate point sources into the grid computation is developed by using a Lagrange trajectory method. Many model options are provided which enable users to study conveniently the significant effects which these options have on the final concentration distributions.

The program description is included to provide a guide for users. The program is constructed in a modular form which allows users to change or improve each component conveniently. The input auxiliary model, which processes geographical, source emission, and monitoring data, is also included.

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