EPA-600/7-78-066
April 1978

A REVIEW OF REGIONAL-SCALE AIR QUALITY MODELS FOR LONG DISTANCE DISPERSION MODELING IN THE FOUR CORNERS AREA

John A. Nuber, Arthur Bass,
Michael T. Mills, and Charles S. Morris
Environmental Research and Technology, Inc.
696 Virginia Road
Concord, MA 01742

NOAA Contract No. 03-6-02-35254

Project Officer

Herbert J. Viebrock
Meteorology Laboratory
National Oceanic and Atmospheric Administration
Research Triangle Park, NC 27711

OFFICE OF RESEARCH AND DEVELOPMENT
ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, DC 20460

DISCLAIMER

Publication of this report does not signify that the contents necessarily reflect the views and policies of the U.S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

Contents

ABSTRACT

A review of available long-range air quality transport and diffusion models has been prepared under NOAA contract 03-6-022-35254, to select, modify and apply such a model for the simulation of air quality impact associated with emissions from new energy resource development in the Four Corners area of the Western United States. Primary emphasis has been placed upon the review of models that are presently operational and currently available for use and adaptation.

A REVIEW OF REGIONAL-SCALE AIR QUALITY MODELS FOR LONG DISTANCE DISPERSION MODELING IN THE FOUR CORNERS REGION

1. INTRODUCTION

This document presents a review (ca. April 1977) of available air quality simulation models that are appropriate to long-range transport (e.g., 100-1000 km) of atmospheric pollutants. This review has been prepared as part of a contractual effort by Environmental Research & Technology, Inc. under NOAA contract 03-6-022-35254 to select, modify and apply long-range atmospheric transport and diffusion models suitable to the simulation of air quality impact associated with emissions from new energy resource development (power generation, coal gasification, oil shale processing) in the Four Corners Area of the Western United States. In this effort, primary emphasis has been placed upon the review of models that are already operational, and that are, in principle, currently available for use and adaptation outside the originating organization. A number of additional constraints were used to select models for review. These included the relative ease and costs of modification for use in the Four Corners area, the computer implementation restrictions, the computational, data and technical resources required for program utilization, the flexibility for multiple-scenario exercise to address both short-term and long-term ambient air quality issues, etc.

This report is certainly not exhaustive; it does not include, for example, some very recent advances in particle-in-cell modeling methods. It does represent a conscientious effort, within limited resources, to assess the current operational status and availability of long-range transport models, and their potential suitability for application to the Four Corners Area under the specific requirements of the study contract.

To facilitate the description and intercomparison of the various models, a 'model characteristics' outline form of presentation has been used, somewhat similar to that used in the Argonne National Laboratories "Description of Air Quality Models and Abstracts of Reference Materials" prepared for the February, 1977 Specialists Conference on the EPA Modeling Guidelines. The characteristics used to describe the models fall into three major divisions, e.g., (a) functional criteria, (b) usage criteria, and (c) operational criteria. Each of these general divisions is subdivided further.

The remainder of this introductory section presents an overview of the two main types of models considered, e.g., grid models and trajectory models. In succeeding sections each of these models is in turn abstracted and outlined by characteristics.

Models suitable for regional scale air quality simulation studies can be divided into two general groups:

- o grid models which numerically integrate the species continuity equation, and
- o trajectory models which numerically integrate the horizontal advective terms and treat the diffusive terms by algebraic technique.

Grid models have the potential to provide for accurate simulation of nonlinear chemistry, horizontal advection, vertical diffusion, wet and dry removal, and deposition processes. They are inherently well suited to accomodate space and time variations in meteorology and emission inventories. In addition, for several grid models, there is a substantial body of validating literature. (For discussion of the advantages and disadvantages of grid models, see, for example, Sheih [1], Sheih and Moroz [2], Shir and Shieh [3], and Liu and Durran [4].)

There are several well-known problems inherent in grid models. Chief among these is the phenomenon called numerical pseudo-diffusion. (see Molenkamp [5], Shieh [6], and Egan and Mahoney [7]). Most common numerical approaches exhibit this phenomenon to some degree, but techniques have been developed (Egan and Mahoney [7], Boris and Book [8], and Long and Pepper [29]) to overcome this difficulty.

Given that numerical pseudo-diffusion can be minimized or eliminated, another inherent problem with grid models lies in their ability to properly treat subgrid-scale phenomenon. As discussed in Sheih [1], the typical grid scale for a regional model is of the order of 10 kilometers. Thus, emission sources are modeled as, typically, 100 square kilometer area sources. This is appropriate for distributed emission sources, but for point sources this modeling procedure leads to premature dilution of several orders of magnitude, and there is a corresponding tendency to underestimate concentrations in the near vicinity of point sources.

Beyond these problems, the criteria for numerical stability of the integration techniques often require time steps which are small compared to the computational costs of each time step. While for short-term simulations (up to, say, 24 hours) the total cost may not be excessive, the cost of projecting seasonal or annual averages, assuming the model can do so, rapidly becomes prohibitive. Because of these problems, several groups have developed trajectory models which numerically treat horizontal advection (the dominant phenomenon on the regional scale) and treat the diffusive phenomena by a variety of well-known analytic approximations. These trajectory models avoid the problems associated with numerical pseudo-diffusion, are inherently capable of dealing with subgrid-scale phenomena, and generally cost relatively little for each The interence from [6] is that time step so that long-term simulations are feasible. (See Sheih [1], [6], or Start and Wendell [9].)

However, trajectory models generally assume that the total concentration field of a pollutant is obtained by superposition of the concentration fields for each source. This linear superposition principle precludes an accurate treatment of nonlinear chemistry. This limitation is a problem in terms of the ability to incorporate future developments in the modeling of nonlinear chemistry. Trajectory models also tend to require large computer storage, although they are computationally cheaper than grid models. Finally, while several groups have done validation studies using trajectory models for long-term averages, little has been done in the area of short-term averages.

Recently, Sheih [1] has proposed a model which uses the trajectory approach until such time as the concentration field has grown to grid-scale dimensions and then treats further diffusion and advection by a grid mode. This interesting hybrid of a trajectory and grid model could well prove the most accurate approach to regional scale modeling. But, as a developmental model, it has not yet been subjected to extensive validation.

TRAJECTORY MODELS

One class of trajectory models uses the particle-in-cell (PIC) approach to model regional dispersion of pollutants. Originally developed by Harlow for fluid dynamical problems, this approach was modified by Sklarew et al. [10] to apply to air pollution simulations. In this approach, it is assumed that pollutant concentrations can be adequately represented by particles of various "weights". Dispersion is represented by the movement of individual particles throughout the grid system, while the "weight" of each particle is altered as chemical reactions occur. Eliassen and Saltbones [11] use this PIC approach to model $SO2$ and $SO4$ transport over Europe. In their model dry deposition is included through the deposition velocity approach. Topography is not modeled explicitly, as is generally true for the trajectory models discussed in this section, but could be implicitly included through specification of the wind field and spatial variation of the mixing depth. Eliassen and Saltbones generalize this one-layer model to a two-layer model [12] capable of exhibiting a vertical concentration gradient, but with associated computational cost penalties.

The major practical drawback of these PIC models lies in the large number of particles that must be tracked to achieve realistic simulations. Large numbers of particles imply both large storage requirements and long execution times (See [4] for further discussions.)

Another class of trajectory models simulate source emissions as time series of puffs or plume segments. The concentration distribution within each puff is assumed to be Gaussian, with standard deviations taken to be power-law functions of travel distance. Trajectory-puff models have been developed by Lamb [13], Roberts et al. [14], and others. Recently, Start and Wendell [9] have developed a trajectory-puff model, MESODIF, to study dispersion effects on regional scales. The initial version of their model does not consider plume rise, spatially variable stability and mixing heights, topography, wet or dry removal processes, linear sulfur chemistry, nor does it allow for multisource configurations. Extensions to include topography, multiple sources, and modifications to the time history of Gaussian diffusion coefficients are not difficult. Perhaps the most attractive feature of MESODIF is its relative simplicity, which allows for easy installation, modification, checkout, and quality control. Moreover, MESODIF requires only modest storage and computational time. It also lends itself readily to effective graphical visualizations of trajectories and concentration fields.

One critical assumption in the MESODIF model is the inclusion of a horizontally isotropic Gaussian diffusion. Thus, puffs are allowed to diffuse both in the crosswind and longitudinal directions at equal rates. Heffter et al. avoided this assumption with a plume segment model. This model assumes the emission source to be a sequence of slices diffusing vertically and crosswind by the Gaussian formula. The model was modified by Meyers and Cederwall [17] at Brookhaven National Laboratory to include both linear sulfur chemistry and removal processes. Wendell et. al [15], and Hales et. al [30] have also used the plume segment approach in their model. This conceptual improvement as well as their capability for displaying plume trajectories make them attractive alternatives to MESODIF.

More sophisticated trajectory models have been developed by Sheih and Moroz [2] and Sheih [6]. In their most sophisticated model, the plume from a continuous source is treated as a series of puffs; each puff is represented by a set of six tracer particles, which determine its size, shape, and location. At each time step, the particles are moved to take into account advection, eddy diffusion, wind shear, and buoyancy entrainment. The concentration distribution of each puff is determined by fitting an ellipsoid to the cluster of particles, with the lengths of the principal axes taken to be standard deviations of a Gaussian distribution. Since a copy of Sheih's model program code is not available for evaluation at this time, its operational requirements cannot be accurately assesses at present. The inference from [6] is that the model may be expensive in time and storage requirements; moreover, it has yet to be demonstrated that the additional complexity offers significant advantages in the accuracy of concentration predictions for an air quality model appropriate to the Four Corners Area.

GRID MODELS

In the grid model discussed in this section, time and space derivatives are replaced by finite difference expressions. Inherent in many finite difference approximations is a type of numerical error called pseudo-diffusion. This numerical diffusion is typically much larger than atmospheric turbulent diffusion. (For more detailed discussion, see [5] or [6].) It is, therefore, very important to use finite difference techniques which minimize or eliminate numerical diffusion.

In the model developed by Shir and Shieh [18] to study SO2 transport in the St. Louis region, the horizontal advection terms are approximated by an explicit, second-order, centered finite difference technique, while the vertical diffusion term is integrated by an implicit Crank-Nicholson method. A similar scheme is used in the model developed by SAI [19]. Both of these techniques are afflicted with numerical pseudo-diffusion which seriously limit duration of simulations (see, for example, Liu and Seinfeld [20]). The SAI model is, additionally, extremely costly to run. It is presently being upgraded to eliminate numerical diffusion by use of the SHASTA method of Boris and Book [8]. As of this date, however, the new version of their model has not been released.

Another model using the SHASTA method is the LIRAQ model developed at Lawrence Livermore Laboratory [21]. This model, numerically integrates a vertically averaged concentration equation and can treat reactive chemical species. The LIRAQ model has only recently been developed and remains to be validated. It would require extensive modifications for application to the Four Corners Area. It is not capable of implementation except on a CDC-7600 system.

An alternate method for eliminating numerical diffusion was developed by Egan and Mahoney [7]. This second-moment method not only eliminates the pseudo-diffusion but can be modified to allow consideration of subgrid-scale sources. The Egan-Mahoney method was used by Rao et al. ([22], [23]) to develop a regional-scale advective-diffusive model for the Sulfate Regional Experiment (SURE). This model, SULFA3D, has the flexibility to incorporate vertically variable inputs such as wind and turbulent diffusivity profiles, and observed mixing depth data. Further, linear chemical transformation and removal processes can be modeled as indicated in [22] or [23].

ACKNOWLEDGMENTS

This study was performed for NOAA under an interagency agreement with the Office of Energy, Minerals and Industry, Office of Research and Developmen t, EPA. We acknowledge with thanks the guidance and helpful suggestions of Herbert J. Viebrock, Meteorology Laboratory (EPA/NOAA) -ARL, and Dr. John Bowen, (EPA/EMSL)-Las Vegas.

REFERENCES FOR INTRODUCTION

1. C. M. Sheih, "A Puff-Grid Model for Predicting Pollutant Transport Over an Urban Area", (1976) to appear in APCA.

2. C. M. Sheih and W. V. Moroz, "A Lagrangian Puff Diffusion Model for the Prediction of Pollutant Concentration Over Urban Areas", Proc. Third International Clean Air Congress, B43-B52, (1973).

3. C. C. Shir and L. J. Shieh, "A Generalized Urban Air Pollution Model and Its Application to the Study of SO2 Distributions in the St. Louis Metropolitan Area", JAM, Vol. 13, pp. 185-224, (1974).

4. M. K. Liu and D. Durran, "On the Modeling of Transport and Diffusion of Air Pollutants Over Long Distances", SAI Interim Report ER76-55, EPA Contract 68-01-3591, (1976).

5. C. R. Molenkamp, "Accuracy of Finite-Difference Methods Applied to the Advection Equation", JAM Vol. 7, pp. 160-167, (1968).

6. C. M. Sheih, "A Lagrangian Puff Diffusion Model with Wind Shear and Dynamic Plume Rise", (1973), submitted to Atmos. Env.

7. B. A. Egan and J. R. Mahoney, "Numerical Modeling of Advection and Diffusion of Urban Area Source Pollutants", JAM, Vol. 11, pp. 312- 322, (1972).

8. J. P. Boris and D. L. Book, "Flux-Corrected Transport 1: SHASTA, A Fluid Transport Algorithm That Works", J. Comp. Physics, Vol. 11, pp. 38-69, (1973).

9. G. E. Start and L. L. Wendell, "Regional Effluent Dispersion Calculations Considering Spatial and Temporal Meteorological Variables", NOAA Tech. Memo. ERL-ARL-44, (1974).

10. R. C. Sklarew, A. J. Fabrick, and J. E. Prager, "A Particle-In-Cell Method for the Numerical Solution of the Atmospheric Diffusion Equation, and Applications to Air Pollution Problems -- Final Report", EPA Contract Number 68-02-0006, (1971).

11. A. Eliassen and J. Saltbones, "Sulfur Transport and Dry Deposition Over Europe Described By A Simple Lagrangian Dispersion Model", Norwegian Institute For Air Research, (1976).

12. A. Eliassen and J. Saltbones, "A Two-Layer Dispersion Model: Description and a Few Results", Norwegian Institute for Air Research, (1975).

13. R. G. Lamb, "An Air Pollution Model of Los Angeles", (1969), Master's Thesis, UCLA.

14. J. J. Roberts, E. S. Croke, and A. S. Kennedy, "An Urban Atmospheric Dispersion Model", Proc. of Symposium on Multiple-Source Urban Diffusion Models, Air Poll. Conf. Off.

Publication No. AP-86, 6.1-6.72, (1970).

15. L. L. Wendell, D. G. Powell, and R. L. Drake, "A Regional Scale Model For Computing Deposition and Ground Level Air Concentration of SO2 and Sulfates from Elevated and Ground Sources", *Proceedings of the Third Symposium on Atmospheric* Turbulence and Air Quality, pp. 318-324, (1976).

16. J. L. Heffter, A. D. Taylor, G. J. Ferber, "A Regional-Continental Scale Transport, Diffusion, and Deposition Model", NOAA Technical Memorandum ERL AR-50, (1975).

17. R. E. Meyers and R. T. Cederwall, "Fossil Pollutant Transport Model Development", BNL RESP Annual Report, BNL 50478, pp. 46-61, (1975).

18. C. C. Shir and L. J. Sheih, "A Generalized Urban Air Pollution Model and Its Application to the Study of the SO2 Distribution in the St. Louis Metropolitan Area", JAM, Vol. 13, pp. 185-204, (1974).

19. S. D. Reynolds, P. M. Roth, and J. H. Seinfeld, "Mathematical Modeling of Photochemical Air Pollution -I: Formulation of the Model", Atmos. Env. Vol. 7, pp. 1033-1061, (1973).

20. M. K. Liu and J. H. Seinfeld, "On the Validity of Grid and Trajectory Models of Urban Air Pollution", Atmos. Env., Vol. 9, pp. 555-574, (1975).

21. M. C. MacCracken and G. D. Sauter, ed., "Development of an Air Pollution model for the San Francisco Bay Area", Final Report to NSF, UCRL-51920, Lawrence Livermore Lab., Livermore, CA (1975).

22. K. S. Rao, I. Thomson, and B. A. Egan, "Regional Transport Model of Atmospheric Sulfates", 69th Annual Meeting of the Air Pollution Control Association, Portland, Oregon, (1976).

23. G. M. Hidy, E. Y. Tong, and P. K. Mueller, "Design of the Sulfate Regional Experiment (SURE)", EPRI-EC-125, Vol. 1, Electric Power Research Institute, Palo Alto, California (1976).

24. M. H. Dickerson, "MASCON-A Mass Consistent Atmospheric Flux Model for Regions With Complex Terrain", submitted to JAM, (1976).

25. Y. Sasaki, "An Objective Analysis Based on the Variational Method", J. Meteor. Soc. Japan, Vol. 36, pp. 77-78, (1958).

26. Y. Saski, "Some Basic Formalisms in Numerical Variational Analysis", Mon. Wea. Rev, Vol. 98, pp. 875-883, (1970).

27. Y. Sasaki, "Numerical Variational Analysis Formulated Under the constraints Determined by Longwave Equation and Low-Pass Filter", Mon. Wea. Rev., Vol. 98, pp. 884-898, (1970).

28. C. Y. Liu and W. R. Goodin, "An Iterative Algorithm for Objective Wind Field Analysis", Mon. Wea. Rev., Vol. 104, pp. 784-792, (1975).

29. P. E. Long and D. W. Pepper, "A Comparison of Six Numerical Schemes for Calculating the Advection of Atmospheric Pollution", Proc. Third Symposium on Atmospheric Turbulence and Air Quality, (1976).

30. Hales, J. M., Powell, D. C., and T. D. Fox, "STRAM-An Air Pollution Model Incorporating Non-Linear Chemistry, Variable Trajectories and Plume Segment Diffusion". EPA-450/3-77-012, (1977).

2. SAI 1973 MODEL

This model performs a numerical integration of the species conservation equation. A fractional steps technique is used to subdivide the governing equation into three independent steps in the 3 spatial directions. The horizontal dimensions are solved explicitly using a mass conservative finite difference scheme devised by Price, Varga, and Warren [1966], while the vertical direction is solved implicitly using a Crank-Nicholson algorithm. The kinetic mechanism is embedded in the vertical integration.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? No.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? No.
SPATIAL EXTRAPOLATION TECHNIQUE? None.
(Input wind field at each grid point.)
INPUT TIME INTERVAL? Hourly.
DIVERGENCE FREE? No.
SMOOTHING? Manually.
ADJUSTED FOR MIXING LID? Implicit.

MIXING LID:

INPUT SPATIAL REQUIREMENT? At each grid point.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity
INPUT SPATIAL REQUIREMENT? Horizontal K spatially uniform. Vertical K at grid points.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.

OTHER METEOROLOGICAL DATA? Radiation Intensity.

EMISSIONS:

SOURCE INVENTORY: Species concentrations, ground level cells.

ELEVATED SOURCES? No.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN? Implicit through windfield and mixing lid. Explicitly treated in transport equations.

WIND FIELD ADJUSTED FOR TERRAIN? Yes.
MIXING LID ADJUSTED FOR TERRAIN? Yes.
VARIABLE RECEPTOR HEIGHTS? No.
VARIABLE SOURCE HEIGHTS? No.

TRANSPORT:

ADVECTIVE METHOD?
DIFFUSIVE METHOD?

Both advection and diffusion are modeled by numerical integration of the species mass conservation equation. The 4 dimensional equations are integrated by the method of fractional steps described by Yanenko [1971]. The horizontal integrations use an explicit second order method developed by Price et al. [1966]. The vertical integration uses an implicit Crank-Nicolson method to avert stability problems that might arise in the treatment of diffusion when the grid spacing is small due to a shallow mixing lid.

HORIZONTAL DIFFUSION? Yes.

VERTICAL DIFFUSION? Yes.

PSEUDO-DIFFUSION? Yes, dominating results after 24 hours.

SPATIAL RESOLUTION AND EXTENT OF MESH?

25 by 25 by 5 grid with approximate horizontal resolution of 2 miles.

RESOLUTION AND EXTENT OF TIME INCREMENT?

Four minute time increment, with 24 hour time extent.

BOUNDARY CONDITIONS?

Boundary conditions are imposed on the vertical and horizontal sides of the 3 dimensional modeling region. At the surface, the mass flux of each species is specified. At the mixing lid, the boundary condition states that the normal component of the mass flux is continuous across the boundary when material is transported into the modeling region from above the inversion base. When material is transported in the other direction, the flux is set equal to 0 to reflect the abrupt change in stability associated with an inversion layer.

On the horizontal sides, the boundary conditions express the continuity of mass flux when flow is directed into the region. For flow out of the region, the diffusive component of the total flux is set equal to 0.

INITIAL CONDITIONS?

Initial conditions are specified by giving the species concentrations for each grid cell. The surface cells are assigned values based on the source inventory, and these concentrations are assumed to be vertically uniform.

NUMBER OF VERTICAL LAYERS? 5

BACKGROUND DATA? Within the modeled region, all sources included in the source inventory. There is no provision to include transport of material into the region from exterior sources.

SPECIES:

MULTIPLE SPECIES? Yes.

WHICH REACTIVE SPECIES? NOx Ox HNOx COx HOx ROx HC

WHICH NON-REACTIVE SPECIES? None.

DEPOSITION? Yes.
WET? No.
DRY? Yes.
DECAY? No.
CHEMISTRY? Yes.
LINEAR? No.
NONLINEAR? Yes.
WHAT CHEMICAL SYSTEM?
31 steps for the NOx-HC-O3 system.
Seinfeld et al [1971], Hecht and Seinfeld [1972].

COMPUTED DATA:

AVERAGING PERIODS? Short term only (run duration)
LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.
1 HOUR? Yes.
3 HOUR? Yes (run duration).
24 HOUR? Yes (run duration).

VALIDATION HISTORY?
The SAI model has been validated by comparing predicted results with data taken in the Los Angeles Basin in September, 1969, and favorable agreement has been obtained.

APPLICABLE TO FOUR CORNERS REGION?
As a short-range (urban scale) photochemical smog model for the Los Angeles air basin, the validation studies have little applicability to the regional Four Corners problem, with its significantly different chemistry.

INCORPORATION OF OBSERVED DATA? No.
CALIBRATION POTENTIAL? Dependent on existence of observed data for each species in the Four Corners Region.

USAGE CRITERIA:

USER'S MANUAL? Yes.
AVAILABILITY OF THE MODEL? In the public domain.
EASE OF MODIFYING MODEL? Very difficult unless intimately familiar with code.
EASE OF USING MODEL? Requires skilled interpretation.
VOLUME OF DATA REQUIRING MANUAL PREPARATION?
There is a large volume of input data required for each model run. The data includes the gridded windfield for each model hour, the inversion lid heights, the turbulent diffusivities and emission rate for each species, for each grid point and hour.

In addition, there is a large labor investment in preparing an exhaustive source inventory for each species to accurately assess the initial species concentration in each grid cell.

EASE OF MODEL INSTALLATION ON UNIVAC? Has been implemented.
EASE OF MODEL MAINTENANCE? Difficult.
OUTPUT INTERPRETATION REQUIREMENTS? No unusual requirements.

OPERATION:

CORE REQUIREMENTS? Less than 128K.
COMPUTATIONAL TIME REQUIREMENTS? A 10 hour simulation for non-reactive hydrocarbons takes 2 min.,reactive 26.5 min.
INPUT DATA PREPARATION TIME REQUIREMENTS? Substantial.

REFERENCES FOR SAI 1973 MODEL:

M.K. Liu, D. C. Whitney, J. H. Seinfeld, P. M. Roth, 1976, "Continued Research in Mesoscale Air Pollution Simulation Modeling", EPA 600/4-76-016

S. D. Reynolds, P.M. Roth, and John Seinfeld , 1974, "Mathematical Modeling of Photochemical Air Pollution - III Evaluation of the Model", Atmos. Env. Vol. 8 pp 563-596

S. D. Reynolds, P.M. Roth, and John Seinfeld , 1974, "Mathematical Modeling of Photochemical Air Pollution - II A Model and Inventory of Pollutant Emissions" Atmos. Env. Vol 8 pp 97-130

S. D. Reynolds, P.M. Roth, and John Seinfeld , 1973, "Mathematical Modeling of Photochemical Air Pollution - I Formulation of the Model" Atmos. Env. Vol 7,pp 1033-1061

Hecht T.A. and Seinfeld J.H., 1972, "Development and Validation of a Generalized Mechanism for Photochemical Smog", Environ. Sci. Technol. Vol 6,p 47

Seinfeld J. H.,Hecht T. A. and Roth P.M., 1971, "A Kinetic Mechanism for Atmospheric Photochemical Reactions", Report 71SAI-9, Systems Applications, Inc.

Yanenko,N N, 1971, "Method of Fractional Steps: The Solution of Problems of Mathematical Physics in Several Variables",Eng. Trans. by M. Holt, Springer-Verlag,N.Y.,N.Y.

3. SAI 1976 MODEL

The SAI 1976 model is the result of efforts to upgrade the 1973 model (see Section 2). These efforts are purported to have resulted in

> The implementation of improved treatments of atmospheric transport and chemical reaction processes,

> The development of microscale modeling capabilities,

> The parameterization and incorporation of pollutant uptake processes,

> The refinement of numerical integration procedures, and

> The development of aerosol modeling capabilities.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Yes.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? No.
SPATIAL EXTRAPOLATION TECHNIQUE? None.
(Input wind field at each grid point.)
INPUT TIME INTERVAL? Hourly.
DIVERGENCE FREE? No.
SMOOTHING? Manually.
ADJUSTED FOR MIXING LID? Implicit.

MIXING LID:

INPUT SPATIAL REQUIREMENT? At each grid point.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? Horizontal K spatially uniform. Vertical K at grid points.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.

OTHER METEOROLOGICAL DATA? Radiation Intensity.

EMISSIONS:

SOURCE INVENTORY: Species concentrations, ground level cells.

ELEVATED SOURCES? No.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN? Implicit through windfield and mixing lid. Explicitly treated in transport equations.

WIND FIELD ADJUSTED FOR TERRAIN? Yes.
MIXING LID ADJUSTED FOR TERRAIN? Yes.
VARIABLE RECEPTOR HEIGHTS? No.
VARIABLE SOURCE HEIGHTS? No.

TRANSPORT:

ADVECTIVE METHOD?
DIFFUSIVE METHOD?

Both advection and diffusion are modeled by numerical integration of the species mass conservation equation. The 4 dimensional equations are integrated by the method of fractional steps described by Yanenko [1971]. The horizontal integrations use the SHASTA method of Boris and Book [1973] to minimize pseudo-diffusion. The vertical integration uses an implicit Crank-Nicolson method to avert stability problems that might arise in the treatment of diffusion when the grid spacing is small due to a shallow mixing lid.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.

PSEUDO-DIFFUSION? Kept minimal.
SPATIAL RESOLUTION AND EXTENT OF MESH?
25 by 25 by 10 grid with approximate resolution of 2 miles.
RESOLUTION AND EXTENT OF TIME INCREMENT?
Four minute time increment, with 24 hour time extent.

BOUNDARY CONDITIONS?

Boundary conditions are imposed on the vertical and horizontal sides of the 3 dimensional modeling region. At the surface, the mass flux of each species is specified. At the mixing lid, the boundary condition states that the normal component of the mass flux is continous across the boundary when material is transported into the modeling region from above the inversion base. When material is transported in the other direction, the flux is set equal to 0 to reflect the abrubt change in stability associated with an inversion layer.

On the horizontal sides, the boundary conditions express the continuity of mass flux when flow is directed into the region. For flow out of the region, the diffusive component of the total flux is set equal to 0.

INITIAL CONDITIONS?

Initial conditions are specified by giving the species concentrations for each grid cell. The surface cells are assigned values based on the source inventory, and these concentrations are assumed to be vertically uniform.

NUMBER OF VERTICAL LAYERS? 10

BACKGROUND DATA? Within the modeled region, all sources included in the source inventory. There is no provision to include transport of material into the region from exterior sources.

SPECIES:

MULTIPLE SPECIES? Yes.

WHICH REACTIVE SPECIES? NOx Ox HNOx COx HxOx ROx HC paraffins,olefins,aromatics,aldehydes,PAN, SO2, total aerosol mass concentration.

WHICH NON-REACTIVE SPECIES? None.

DEPOSITION? Yes.

WET? No.

DRY? Yes.

DECAY? No.

CHEMISTRY? Yes.

LINEAR? No

NONLINEAR? Yes.

WHAT CHEMICAL SYSTEM?

Whitten and Hogo [1976].

COMPUTED DATA:

AVERAGES? Short term only (run duration).

LONG TERM(ANNUAL)? No.

SHORT TERM? Yes.

1 HOUR? Yes
3 HOUR? Yes (run duration).
24 HOUR? Yes (run duration).

VALIDATION HISTORY?
None to date.

INCORPORATION OF OBSERVED DATA? No.
CALIBRATION POTENTIAL? Dependent on existence of observed data for each species in the Four Corners Region.

USAGE CRITERIA:

AVAILABILITY OF THE MODEL? Model exists in a developmental state at this time.
EASE OF MODIFYING MODEL? Cannot be ascertained at this time.
EASE OF USING MODEL? Cannot be ascertained at this time.
VOLUME OF DATA REQUIRING MANUAL PREPARATION?

There is a large volume of input data required for each model run. The data includes the gridded windfield for each model hour, the inversion lid heights, the turbulent diffusivities and emission rate for each species, for each grid point and hour.

In addition, there is a large labor investment in preparing an exhaustive source inventory for each species to accurately assess the initial species concentration in each grid cell.

EASE OF MODEL INSTALLATION ON UNIVAC? Cannot now be ascertained .
EASE OF MODEL MAINTENANCE? Cannot now be ascertained .
OUTPUT INTERPRETATION REQUIREMENTS? Cannot now be ascertained .

OPERATION:

CORE REQUIREMENTS? Cannot now be ascertained.
ON LINE STORAGE REQUIREMENTS? Cannot now be ascertained.
COMPUTATIONAL TIME REQUIREMENTS? Cannot now be ascertained.
INPUT DATA PREPARATION TIME REQUIREMENTS? Substantial.
OTHER HARD WARE REQUIREMENTS? Cannot now be ascertained.

REFERENCES FOR SAI 1976 MODEL:

All references for the SAI 1973 model, plus

Reynolds et al., 1976, "Continued Development and Validation of a Second Generation Photochemical Air Quality Simulation Model: Volume I --Refinements in the Treatment of Meteorology, Chemistry, Pollutant Removal Processes, and Numerical Analysis", Final Report EPA Contract 68-02-2216

G.Z. Whitten and H. Hogo, 1976, "Mathematical Modeling of Simulated Photochemical Smog",Final Report, EPA Contract 68-02-0580

M.K. Liu and Dale Durran, 1973, "On the Modeling of Transport and Diffusion of Air Pollutants Over Long Distances" Interim Report ER76-55, EPA Contract 68-01-3591

J.P. Boris and D.L.Book, 1973, "Flux Corrected Transport --I "SHASTA, A Fluid Transport Algorithm That Works", J.Comp.Phys. Vol 11, pp38-69

4. PIC NEXUS/P

NEXUS/P is one example of many particle-in-cell models. The particle-in-cell models simulate pollutant emissions by particles each of which accounts for a definite amount of pollutant. They are advected in a Lagrangianly manner by a pseudo-velocity contrived from local diffusion and advection velocity. The pollutant concentration in each grid cell is given by the total number of particles in the cell.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD: Particle in cell models can be used with almost any routine which generates a suitable gridded wind field.

VERTICAL RESOLUTION? No.
SINGLE STATION? No.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE? Yes.
INPUT TIME INTERVAL? Hourly.
DIVERGENCE FREE? No.
SMOOTHING? Yes.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Spatially uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant in time.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? Every cell.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT Hourly?

OTHER METEOROLOGICAL DATA? None.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? No.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? No?

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN?

IMPLICIT or EXPLICIT? Implicit.
WIND FIELD ADJUSTED FOR TERRAIN? External to model.
MIXING LID ADJUSTED FOR TERRAIN? External to model.
VARIABLE RECEPTOR HEIGHTS? No.
VARIABLE SOURCE HEIGHTS? No.

TRANSPORT:

ADVECTIVE METHOD?
DIFFUSIVE METHOD?

Particles are advected in a Lagrangianly manner by a pseudo-velocity contrived from local diffusion and the advection velocity.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.

PSEUDO-DIFFUSION? No.
SPATIAL RESOLUTION AND EXTENT OF MESH? 22x21 cells, resolution of 2 miles.
RESOLUTION AND EXTENT OF TIME INCREMENT? Five minutes is typical.
BOUNDARY CONDITIONS? Impervious barrier at the ground with transmittive sides and top. Inversion between 3rd and 4th

layers limits upward diffusion. Particles which penetrate past the middle of the fourth layer are eliminated.

INITIAL CONDITIONS?
Initial vertical profile of the pollutant concentration is assumed to be reduced by one half every 100 meters.

NUMBER OF VERTICAL LAYERS? 4.
BACKGROUND DATA? Yes, supplied by user.

SPECIES:

MULTIPLE SPECIES? Yes.

WHICH REACTIVE SPECIES? NO, NO2, O3, HC, and HNO2 with O, RO2, and OH in pseudo-equilibrium.
WHICH NON-REACTIVE SPECIES? None.
DEPOSITION? No.
DECAY? None.
CHEMISTRY? Yes.
LINEAR? No.
NON-LINEAR? Yes.
WHAT CHEMICAL SYSTEM? After Eschenroeder and Martinez.

COMPUTED DATA:

AVERAGES? No, instantaneous concentrations.
LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? No.

VALIDATION HISTORY? See Sklarew et al. [1971].
APPLICABLE TO FOUR CORNERS REGION?
NEXUS/P is not applicable in its present form. However, a particle in cell model could be designed for the region.

INCORPORATION OF OBSERVED DATA? Possible.
CALIBRATION POTENTIAL? Good if observed data are available.

USAGE CRITERIA:

USER'S MANUAL? No.
AVAILABILITY OF THE MODEL? In public domain.
EASE OF MODIFYING MODEL? ???
EASE OF USING MODEL? ???

VOLUME OF DATA REQUIRING MANUAL PREPARATION?
Source emissions, mean winds, and diffusivities specified for each cell throughout the grid during the time period being simulated.

ERROR DIAGNOSTICS? ???
EASE OF MODEL INSTALLATION ON UNIVAC? Easy
EASE OF MODEL MAINTENANCE? ???
OUTPUT INTERPRETATION REQUIREMENTS? ???

OPERATION:

CORE REQUIREMENTS? 230K for 2000 cells, 10000 particles and 5 species.

ON LINE STORAGE REQUIREMENTS? ???
COMPUTATIONAL TIME REQUIREMENTS? Extremely expensive: a 16 hour simulation takes 1.5 hours on a UNIVAC 1108.

INPUT DATA PREPARATION TIME REQUIREMENTS? Depends on the given simulation.

OTHER HARDWARE REQUIREMENTS? ???

REFERENCES FOR NEXUS/P MODEL:

Sklarew,R.C.,1970, 'A New Approach:The Grid Model of Urban Air Pollution', APCA Paper No. 70-79 (june 1970), Systems, Science and Software, La Jolla, Calif.

Sklarew, R.C. ,1970, 'Preliminary Report of the S3 Urban Air Pollution Model Simulation of Carbon Monoxide in Los Angeles',Systems, Science, and Software Inc, La Jolla, Calif. p 2

Sklarew, R. C., A. J. Fabrick, and J. E. Prager, 1971: A Particle-In-Cell Method for Numerical Solution of the Atmospheric Diffusion Equation and Applications to Air Pollution Problems (Volume 1). Systems, Science, and Software, La Jolla, California.

Eschenroeder, A. Q. and Martinez,J.R., 1972, 'Mathematical Modeling of Photochemical Smog', General Research Corporation, Santa Barbara, Calif.

5. SULFA3D MODEL

SULFA3D is a quasi-Lagrangian model with linear chemistry based on the Egan-Mahoney method of moments. The model accounts for advective transport in the horizontal by the mean wind, and for vertical diffusion. The air masses are advected and dispersed each time step in the Lagrangian sense, and immediately afterwards a mass decomposition to a stationary Eulerian grid is performed. To accomplish the turbulent diffusion calculations, the model has three air layers, each of uniform depth over the grid region, in the vertical. For each grid cell in the horizontal, emissions can be introduced into one of the three layers depending on the effective release height for elevated point sources. All ground-level point and area source emissions are introduced into the lowest layer next to the ground. Thus, this model is particularly suited to investigate, for example, the effects of tall stacks in reducing the ambient concentration levels of SO2 and SO4.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Yes.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE? None.
INPUT TIME INTERVAL? Every 12 hours.
TEMPORAL INTERPOLATION TECHNIQUE? Not at present.
DIVERGENCE FREE? Depends on specification of wind field.
SMOOTHING? Manual.
ADJUSTED FOR MIXING LID? Yes.

MIXING LID: Uniform lid.

INPUT SPATIAL REQUIREMENT? Spatially uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? None.
TEMPORAL INTERPOLATION? Temporally uniform.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Vertical diffusivity only.
INPUT SPATIAL REQUIREMENT? Three discrete values of K are specified at the centers of the three vertical layers.

SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Temporally uniform.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? No.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN?

IMPLICIT OR EXPLICIT? Implicit (terrain following coordinate system.)
WIND FIELD ADJUSTED FOR TERRAIN? External to model.
MIXING LID ADJUSTED FOR TERRAIN? External to model.
VARIABLE SOURCE HEIGHTS? Yes.

TRANSPORT:

ADVECTIVE METHOD?

The masses are advected and dispersed each time step in the Lagrangian sense, and immediately afterwards a mass decomposition to the stationary Eulerian grid is preformed.

DIFFUSIVE METHOD?

The conservation of mass tracer equation is solved using the Egan-Mahoney numerical method. Details and discussion of this method can be found in Egan and Mahoney [1972a,b] and Pedersen-Prahm [1974].

HORIZONTAL DIFFUSION? No.
VERTICAL DIFFUSION? Yes, explicit.

PSEUDO-DIFFUSION? Minimal.
SPATIAL RESOLUTION AND EXTENT OF MESH? Default:

26x17x3 with 80 km resolution. Variable vertical resolution.

RESOLUTION AND EXTENT OF TIME INCREMENT?

Time increment determined by the linear advective and diffusive stability criteria:

U*(delta t/delta x) < 1

K*(delta t/H**2) < 0.5

BOUNDARY CONDITIONS?

Upper boundary: complete reflection.
Lower boundary: complete or partial reflection.

INITIAL CONDITIONS? User specified.
NUMBER OF VERTICAL LAYERS? 3.
BACKGROUND DATA? Yes, user specified.

SPECIES:

MULTIPLE SPECIES?

WHICH REACTIVE SPECIES? SO2, SO4 only
WHICH NON-REACTIVE SPECIES? None, but could be modified readily for any passive species.

DEPOSITION? Yes.

WET? Yes (with assumed precipitation rate).
DRY? Yes.

DECAY? No.
CHEMISTRY?

LINEAR? Yes.
NON-LINEAR? No.
WHAT CHEMICAL SYSTEM? Simple linear transformation of SO2 to SO4.

COMPUTED DATA:

AVERAGES?

LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.

1 HOUR? Yes, if 1 hour run duration.
3 HOUR? Yes, if 3 hour run duration.
24 HOUR? Yes if 24 hour run duration.

VALIDATION HISTORY?

SULFA3D has been extensively exercised in the Northeastern U.S., New York City, and Los Angeles area.

APPLICABLE TO FOUR CORNERS REGION? Yes, with modifications.
INCORPORATION OF OBSERVED DATA? Can be modified to include observed data.
CALIBRATION POTENTIAL? Good.

USAGE CRITERIA:

USER'S MANUAL? No.
AVAILABILITY OF THE MODEL? Not presently in public domain but it is releasable.
EASE OF MODIFYING MODEL? Model written in highly modular fashion - readily modified.
EASE OF USING MODEL? Good, with documentation which is not generally available at present.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? SO2 emission rates must be specified in each cell. Background concentrations of SO2 and SO4 must be specified. Wind field data must be determined (once every 12 hours).

ERROR DIAGNOSTICS? Minimal.
EASE OF MODEL INSTALLATION ON UNIVAC? Easily implemented.
EASE OF MODEL MAINTENANCE? Easily maintained.
OUTPUT INTERPRETATION REQUIREMENTS? Requires some meteorological and sulfur chemistry background.

OPERATION:

CORE REQUIREMENTS? Moderate to high - a function of resolution. 350K on IBM 360.
ON LINE STORAGE REQUIREMENTS? Moderate - a function of resolution.
COMPUTATIONAL TIME REQUIREMENTS? 5 - 15 minutes on IBM 360. A function of the resolution.
INPUT DATA PREPARATION TIME REQUIREMENTS? Substantial - 3 - 4 man-weeks of work.
OTHER HARD WARE REQUIREMENTS? None.

REFERENCES FOR SULFA3D MODEL:

Design of the Sulfate Regional Experiment (SURE). prepared by Environmental Research and Technology, Inc. for Electric Power Research Institute. 1976. EPRI document EC-125.

Egan,B.A. "Numerical Modeling of Urban Air Pollution Transport Phenomena",Ph.D. Dissertation,Harvard School of Public Health,(1971)

Egan,B.A. and J. R. Mahoney, "Applications of a Numerical Air Pollution Transport Model to Dispersion in The Atmospheric Boundry Layer", J. Appl. Meteor. Vol 11, No. 7 pp 312-322 (1972)

Egan,B.A. and J.R. Mahoney, "Applications of a Numerical Air Pollution Transport Model To Dispersion in The Atmospheric Boundry

Layer",J.Appl. Meteor. Vol 11,No. 7, pp 1023-1039 (1972)

Pedersen, L. B. and Prahm, L. P., "A Method for Numerical Solution of the Advection Equation", Tellus Vol 26,No. 5, pp 594-602 (1974)

6. LIRAQ-1 MODEL

LIRAQ is a very large regional-scale air quality simulation model developed by Lawrence Livermore Laboratory to predict the spatial and temporal variations in the concentrations of the most significant photochemically reactive and non-reactive air pollutants throughout the San Francisco Bay Area. LIRAQ-1 is the non-reactive version. It takes into explicit account the complex topography, meteorology, and source inventory of the Bay Area. LIRAQ-1 is implementable at present only on a CDC-7600 and specifically implemented only at the Lawrence Livermore Laboratory and the Lawrence Berkeley Laboratory.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:
LIRAQ uses the mass consistent wind fields generated by the MASCON program (Dickerson,1973; Sherman,1975)

VERTICAL RESOLUTION? No, vertical wind profile assumed; model uses vertically integrated layer.

GRIDDED INPUT? Yes.

SPATIAL EXTRAPOLATION TECHNIQUE? Missing data is interpolated or extrapolated manually on the basis of expert meteorological judgement or prior experience.

INPUT TIME INTERVAL? Every three hours.
DIVERGENCE FREE? Yes.
ADJUSTED FOR MIXING LID? Yes, explicitly.

MIXING LID:

INPUT SPATIAL REQUIREMENT?
For as many grid points as are available or are needed to define the meteorological structure.

SPATIAL EXTRAPOLATION? Same as wind field.
INPUT TEMPORAL REQUIREMENT? Every three hours.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? None, K is calculated internally.
SPATIAL EXTRAPOLATION? ???
INPUT TEMPORAL REQUIREMENT? None.

OTHER METEOROLOGICAL DATA? Yes, but external to program.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN?

IMPLICIT OR EXPLICIT? Explicit in the wind field.
WIND FIELD ADJUSTED FOR TERRAIN? Yes.
MIXING LID ADJUSTED FOR TERRAIN? Yes.
VARIABLE RECEPTOR HEIGHTS? Yes.
VARIABLE SOURCE HEIGHTS? Yes,but of little benefit since since sources are vertically averaged in a layer.

TRANSPORT:

ADVECTIVE METHOD?

LIRAQ-1 uses the SHASTA method of Boris and Book [1973] to minimize psuedo-diffusion in the horizontal advection. This method takes into account the integrated mass flux and variable inversion height properties.

DIFFUSIVE METHOD?
LIRAQ-1 uses the eddy diffusion velocity scheme of Sklarew et al. for horizontal diffusion.

HORIZONTAL DIFFUSION? Yes, explicitly.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? Yes, but minimized.
SPATIAL RESOLUTION AND EXTENT OF MESH?
45x50 grid - 1, 2, or 5 km resolution.
RESOLUTION AND EXTENT OF TIME INCREMENT? On the order of one to five minutes.
BOUNDARY CONDITIONS?
CO, NO, HC1, and HC2 fluxes are specified at each of the four horizontal boundaries and above the inversion. These are assumed to be uniform in time.

INITIAL CONDITIONS? Station data, where available, is used to initialize the concentration field.
NUMBER OF VERTICAL LAYERS? 1.
BACKGROUND DATA? Yes.

SPECIES:

MULTIPLE SPECIES?
WHICH REACTIVE SPECIES? None.
WHICH NON-REACTIVE SPECIES? CO,NO,HC1,HC2.
DEPOSITION?
WET? No.
DRY? Yes.
DECAY? Yes.
CHEMISTRY? No.

COMPUTED DATA:

AVERAGES? No, only short-term concentrations.
LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.
1 HOUR? Run time dependent.
3 HOUR? Run time dependent.
24 HOUR? Run time dependent.

VALIDATION HISTORY? Limited validation history. (See MacCracken and Sauter, 1975.)

APPLICABLE TO FOUR CORNERS REGION? No, only the San Francisco Bay area. However, in principle could be modified in principle for the Four Corners region.

INCORPORATION OF OBSERVED DATA?
Initial conditions include station data to initialize the concentration field, but not real time data.

CALIBRATION POTENTIAL? Dependent on existence of observed data for each species in the Four Corners Region.

USAGE CRITERIA:

USER'S MANUAL? Yes.

AVAILABILITY OF THE MODEL? In public domain, but only implemented on the LBL and LLL systems.

EASE OF MODIFYING MODEL? Not assessable at this time.

EASE OF USING MODEL? Problem formulation language makes model usage quite simple; results require skilled interpretation.

VOLUME OF DATA REQUIRING MANUAL PREPARATION?
Meteorology - Substantial labor may be needed to generate the wind field from MASCON. The data required are the average inversion height, surface wind speed, and wind direction, and/or the mean layer wind speed and wind direction for every three hours. MASCON is limited to a grid size of 65x65 with a resolution of 1, 2, or 5 km.

Topography - Topographic heights averaged over 1 km cells of a Universal Transverse grid for the entire computational region.

Source emission inventory - In general a substantial amount of work is required. The following sources are considered:

- mobile
- population-distributed
- airport
- major ground sources - ground-based and elevated

ERROR DIAGNOSTICS? Some, in problem formulation.

EASE OF MODEL INSTALLATION ON UNIVAC? Impossible at present-program architecture requires a CDC 7600.

EASE OF MODEL MAINTENANCE? Good.

OUTPUT INTERPRETATION REQUIREMENTS? Substantial.

OPERATION:

CORE REQUIREMENTS? Substantial, requires all the core available to a CDC 7600.
ON LINE STORAGE REQUIREMENTS? High.
COMPUTATIONAL TIME REQUIREMENTS? One hour for 24 hour simulation.
INPUT DATA PREPARATION TIME REQUIREMENTS? Substantial (see above).

REFERENCES FOR LIRAQ-1 MODEL:

Boris, J. P., and D. L. Book, 1973: Flux Corrected Transport - I, SHASTA, a Fluid Transport Algorithm that Works. J. Comp. Phys., Vol. 11, 38 - 69.

Bass, A., A. Q. Eschenroeder, and B. A. Egan, 1977: The Livermore Regional Air Quality Model (LIRAQ): A Technical Review and Market Analysis. Docement P-2348-1, Environmental Research & Technology, Inc., Concord, Mass.

MacCracken, M. C. (ed.), 1975: User's Guide to the LIRAQ Model: An Air Pollution Model for the San Francisco Bay Area, Report UCRL-S1983, Lawerance Livermore Laboratory, Livermore, CA.

MacCracken, M. C., and G. D. Sauter (editors), 1975: Development of an Air Pollution Model for the San Francisco Bay Area. Volume 1, Report UCRL-S1920, Vol. 1; Volume 2. Appendices, Report UCRL-S1920, Vol. 2, Lawrence Livermore Laboratory, Livermore, CA.

Dickerson, M. H., 1976: "MASCON- A Mass Consistent Atmospheric Flux Model for Regions with Complex Terrain", Preprint UCRL-79157, Rev. 2, Lawrence Livermore Laboratory, Livermore, CA.

Sherman, C. A., 1975: "A Mass-Consistent Model for Wind Fields over Complex Terrain",Preprint UCRL-76171, Rev. 1, Lowrence Livermore Laboratory, Livermore, CA.

7. LIRAQ-2 MODEL

LIRAQ is a very large regional-scale air quality simulation model developed by Lawrence Livermore Laboratories and the BAAPCD to predict the spatial and temporal variations in the concentrations of the most significant photochemically reactive and non-reactive air pollutants throughout the San Francisco Bay Area. LIRAQ-2 is the reactive version. It takes into explicit account the complex topography meteorology, and source inventory of the Bay Area. LIRAQ-2 is implementable at present only on a CDC-7600 and specifically at the Lawrence Livermore Laboratory and the Lawrence Berkeley Laboratory.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

LIRAQ uses the mass consistent wind fields generated by the program MASCON (Dickerson,1976; Sherman,1975)

VERTICAL RESOLUTION? No, vertical wind profile assumed, model uses vertically integrated layer.

GRIDDED INPUT? Yes

SPATIAL EXTRAPOLATION TECHNIQUE? Missing data is interpolated or extrapolated manually on the basis of expert meteorological judgement or prior experience.

INPUT TIME INTERVAL? Every three hours.
DIVERGENCE FREE? Yes.
SMOOTHING? ???
ADJUSTED FOR MIXING LID? Yes, explicitly.

MIXING LID:

INPUT SPATIAL REQUIREMENT? For as many grid points as are available or are needed to define the meteorological structure.

SPATIAL EXTRAPOLATION? Same as wind field.
INPUT TEMPORAL REQUIREMENT? Every three hours.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? None, K is calculated internally.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? None.

OTHER METEOROLOGICAL DATA?

Radiative and other data as required by the photochemical system.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN?

IMPLICIT OR EXPLICIT? Explicit in wind field.
WIND FIELD ADJUSTED FOR TERRAIN? Yes.
MIXING LID ADJUSTED FOR TERRAIN? Yes.
VARIABLE RECEPTOR HEIGHTS? Yes.
VARIABLE SOURCE HEIGHTS? Yes?

TRANSPORT:

ADVECTIVE METHOD?
DIFFUSIVE METHOD?

Because of the nature of the stiff differential equations involved in the photochemical system, the time stepping is done using a modified Gear method. This method makes it impossible to use current pseudo-diffusion suppressing techniques for the spatial integrations. The spatial integrations are done by a backward or upstream 1st order diffence scheme which may become dominated by pseudo-diffusive errors.

HORIZONTAL DIFFUSION? Yes, explicitly.

VERTICAL DIFFUSION? Yes.

PSEUDO-DIFFUSION? Substantial.

SPATIAL RESOLUTION AND EXTENT OF MESH?

20x20 grid - 1, 2, or 5 km resolution.

RESOLUTION AND EXTENT OF TIME INCREMENT?

60 to several hundred seconds.

BOUNDARY CONDITIONS?

Specification of species fluxes or concentrations at the lateral and vertical boundries. These are assumed to be uniform in time.

INITIAL CONDITIONS? Station data is used to initialize the concentration field.

NUMBER OF VERTICAL LAYERS? 1.

BACKGROUND DATA? Yes.

SPECIES:

MULTIPLE SPECIES?

WHICH REACTIVE SPECIES?

Up to 15 chemically reactive species plus four species which are assumed to be in instantaneous equilibrium. The 15 chemically reactive species are: alkene-like hydrocarbons, alkane-like hydrocarbons, aldehyde-like hydrocarbons, nitrous acid, nitric acid, hydrogen peroxide, nitric oxide, nitrogen dioxide, nitrogen pentoxide, ozone, alkyl nitrites, alkyperoxyl radicals, hydroperoxyl free radicals and carbon monoxide.

DEPOSITION?

WET? No.

DRY? Yes.

DECAY? Yes.

CHEMISTRY? Yes.

LINEAR? No.

NON-LINEAR? Yes.

WHAT CHEMICAL SYSTEM? After Hecht et al. [1974] with different reaction times.

COMPUTED DATA:

AVERAGES? No, only short-term concentrations.

LONG TERM(ANNUAL)? No.

SHORT TERM? Yes.

1 HOUR? Run-time dependent.

3 HOUR? Run-time dependent.

24 HOUR? Run-time dependent.

VALIDATION HISTORY? Very limited validation history.

MacCracken, M. C., and G. D. Sauter(editors), 1975: Development of an Air Pollution for the San Francisco Bay Area. Volume 1, Report UCRL-S1920, Vol. 1; Volume 2. Appendices, Report UCRL-S1920, Vol. 2, Lawrence Livermore Laboratory, Livermore, CA.

APPLICABLE TO FOUR CORNERS REGION? No, only the San Francisco Bay area. However, in principle could be modified for the Four Corners region.

INCORPORATION OF OBSERVED DATA? Initial conditions include station data to initialize the concentration field, but not real time data.

CALIBRATION POTENTIAL? Dependent on existence of observed data for each species in the Four Corners Region.

USAGE CRITERIA:

USER'S MANUAL? Yes.

AVAILABILITY OF THE MODEL? In public domain, but presently only on the Berkeley LBL system.

EASE OF MODIFYING MODEL? Not assessable at this time.

EASE OF USING MODEL? Problem formulation language makes model usage quite simple; results require skilled interpretation.

VOLUME OF DATA REQUIRING MANUAL PREPARATION?

Meteorology - Substantial labor may be needed to generate the wind field from MASCON. The data required are the average inversion height, surface wind speed, and wind direction, and/or the mean layer wind speed and wind direction for evevy three hours. MASCON is limited to a grid size of 65x65 with a resolution of 1, 2, or 5 km.

Topography - Topographic heights averaged over 1 km cells of a Universal Transverse grid for for the entire computational region.

Source emission inventory - A substantial amount of work is required. The following sources are considered:

- mobile
- population-distributed
- airport
- major ground sources - ground-based and elevated

ERROR DIAGNOSTICS? Some in the problem formulation.

EASE OF MODEL INSTALLATION ON UNIVAC? Impossible at present: program architecture requires a CDC-7600.

EASE OF MODEL MAINTENANCE? Good.
OUTPUT INTERPRETATION REQUIREMENTS? Substantial.

OPERATION:

CORE REQUIREMENTS? Substantial, requires all the core available to a CDC 7600.
ON LINE STORAGE REQUIREMENTS? Very high.
COMPUTATIONAL TIME REQUIREMENTS? One hour for 24 hour simulation.
INPUT DATA PREPARATION TIME REQUIREMENTS? Substantial (see above).

REFERENCES:

Boris, J. P., and D. L. Book, 1973: Flux Corrected Transport - I, SHASTA, a Fluid Transport Algorithm that Works. J. Comp. Phys., Vol. 11, 38 - 69.

Bass, A., A. Q. Eschenroeder, and B. A. Egan, 1977: The Livermore Regional Air Quality Model (LIRAQ): A Technical Review and Market Analysis. Document P-2348-1, Environmental Research & Technology, Inc., Concord, Mass.

MacCracken, M. C. (ed.), 1975: User's Guide to the LIRAQ Model: An Air Pollution Model for the San Francisco Bay Area, Report UCRL-S1983, Lawerance Livermore Laboratory, Livermore, CA.

MacCracken, M. C., and G. D. Sauter (editors), 1975: San Francisco Bay Area. Volume 1, Report UCRL-S1920, Vol. 1; Volume 2. Appendices, Report UCRL-S1920, Vol. 2, Lawrence Livermore Laboratory, Livermore, CA.

Hecht, T. A., J. H. Seinfeld, and M. C. Dodge, 1974: Further Development of a Generalized Kinetic Mechanism for Photochemical Smog. J. Environ. Sci. Technol. Vol. 8, 327.

Dickerson,M.H., 1976:"MASCON - A Mass Consistent Atmospheric Flux Model for Regions with Complex Terrain",Preprint UCRL-761577, Rev. 2, Lawrence Livermore Lab.,Livermore,Ca.

Sherman, C.A.,1975: "A Mass Consistent Model for Wind Fields over Complex Terrain",Preprint UCRL-76171 Rev. 1,Lawrence Livermore Lab.,Livermore,CA.

8. SHIR-SHIEH MODEL

This a generalized urban air pollution model based on numerical integration of the conservation of species equation. The model computes the temporal and three-dimensional spatial distributions resulting from specified multiple point and area sources . Special treatments of the finite difference scheme to accomodate the large variations of concentrations are incorporated.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION?
Vertical wind speeds are interpolated by a power law. Wind direction is assumed vertically uniform.

SINGLE STATION? Yes.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE?
The initial wind field is derived by assigning the wind vector from the closest station. This initial wind field is "smoothed" by a 1/r**2 inverse weighting.

INPUT TIME INTERVAL? Hourly
TEMPORAL INTERPOLATION TECHNIQUE? None.
DIVERGENCE FREE? No.
SMOOTHING? Yes.
ADJUSTED FOR MIXING LID? No.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform in space.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY?
Vertical diffusivity calculated from a continuous stability class based on Turner's method. Horizontal diffusivity is constant.

INPUT SPATIAL REQUIREMENT? Each grid point.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? Sky cover.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD?
DIFFUSIVE METHOD?
A second-order, centered finite-difference scheme is used to integrate the advection and horizontal terms and the Crank-Nicholson method is used for the vertical diffusion term.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? Yes.
SPATIAL RESOLUTION AND EXTENT OF MESH? 30 by 40 by 14 3 dimensional grid with 5000 ft spacing.
RESOLUTION AND EXTENT OF TIME INCREMENT?
The time increment is on the order of 2000 seconds.

Extent of integration is 24 hours.

BOUNDARY CONDITIONS?
Boundary surfaces above and below assumed impermeable to SO2. Continuity of flow across vertical sufaces.

INITIAL CONDITIONS?
Initial concentrations set equal to 0.

NUMBER OF VERTICAL LAYERS? 14.
BACKGROUND DATA? No.

SPECIES:

MULTIPLE SPECIES? No.
WHICH REACTIVE SPECIES? Only SO2.
WHICH NON-REACTIVE SPECIES? None.
DEPOSITION? No.
DECAY? Yes.
CHEMISTRY? Yes.
LINEAR? Yes.
NON-LINEAR? No.
WHAT CHEMICAL SYSTEM? Linear decay of SO2.

COMPUTED DATA:

AVERAGES? Yes.
LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.
1 HOUR? Yes.
3 HOUR? Yes.
24 HOUR? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? No.

VALIDATION HISTORY?
CC Shir and L.J. Shieh, "A Generalized Urban Air Pollution Model and Its Application to the Study of SO2 Distributions in the St. Louis Metropolitan Area.",J.A.M. Vol 13, pp 185-204 (1974)

APPLICABLE TO FOUR CORNERS REGION?
Given its limitations, it would be applicable in principle for short averaging times if modified.
CALIBRATION POTENTIAL? Not known at this time.

USAGE CRITERIA:

USER'S MANUAL? Not presently known.

AVAILABILITY OF THE MODEL? Developmental and probably not user oriented.
EASE OF MODIFYING MODEL? Not presently known.
EASE OF USING MODEL? Not presently known.
VOLUME OF DATA REQUIRING MANUAL PREPARATION?
Source emission inventory must be large. Hourly meteorological input requirements are small.

ERROR DIAGNOSTICS? Not presently known.
EASE OF MODEL INSTALLATION ON UNIVAC? Not presently known.
EASE OF MODEL MAINTENANCE? Not presently known.
OUTPUT INTERPRETATION REQUIREMENTS? A large volume of output requires substantial labor to reduce and interpret.
OPERATION:

CORE REQUIREMENTS? Not presently known.
ON LINE STORAGE REQUIREMENTS? Not presently known.
COMPUTATIONAL TIME REQUIREMENTS?
A 24 hour simulation requires 3 to 5 minutes on IBM 360.

INPUT DATA PREPARATION TIME REQUIREMENTS? Substantial.
OTHER HARD WARE REQUIREMENTS? Not presently known.

REFERENCES FOR SHIR-SHIEH MODEL:

C.C. Shir and L.J.Shieh,1974: "A Generalized Urban Air Pollution Model and Its Application to the Study of SO2 Distributions in the St. Louis Metropolitan Area", J.A.M. Vol 13, pp 185-204

Shir, C. C. ,1973:"A preliminary numerical study of atmospheric turbulent flows in the idealized planetary boundary layer",J.Atmos.Sci, Vol 30, pp 1327-1339

Shir, C. C., 1972:"A numerical computation of air flow over a sudden change in surface roughness",J. Atmos. Sci. Vol 29, pp 304-310

Shir, C. C., 1972:"Numerical investigation of the atmospheric dispersion of stack effluents.",IBM J. Res. Devel. Vol 16, pp 172-179

Shieh,L.J., P.K.Halpern, B. A. Clemens, H.H. Wang, and F.F.Abraham,1972: "Air Quality Diffusion Model: Application to New York City",IBM J.Res. Devel., Vol 16, pp 162-170

Shir, C. C.,1970:"A pilot study in numerical techniques for predicting air pollutant distribution downwind from a stack",J. Atmos. Env. Vol 4 pp 387-407

9. MESODIF MODEL

MESODIF (for mesoscale diffusion) uses an objective regional trajectory analysis scheme combined with a Gaussian diffusion model to simulate regional scale dispersion effects.

The trajectory analysis scheme uses wind data from a network of tower mounted wind sensors to consider the effects of spatial variability of horizontal wind flow near the surface, incorporates time changes in rates of diffusion, and an upper level lid to bound vertical mixing.

Continuous emissions sources are modeled as a sequence of instantaneous puffs which diffuse in the vertical and horizontal by a Gaussian formula for an instantaneous release. At each time step the puffs are advected by the time field and sampled at each of the receptors. The Gaussian dispersion coefficients are functions of the distance from the source.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? None.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE?
1/r**2 extrapolation to grid points, linear interpolation from grid points to puff points.
INPUT TIME INTERVAL? Hourly.
TEMPORAL INTERPOLATION TECHNIQUE? Linear.
DIVERGENCE FREE? No.
SMOOTHING? No.
ADJUSTED FOR MIXING LID? No, but could be modified.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform in space.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.
TEMPORAL INTERPOLATION? Persistence.

TURBULENCE DATA: Stability Class

INPUT SPATIAL REQUIREMENT? Uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly.
TEMPORAL INTERPOLATION? Persistence.

OTHER METEOROLOGICAL DATA? None.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? No.
AREA SOURCES? No.
MULTIPLE SOURCE SITES? No. .
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD?
Simple Euler integration.
DIFFUSIVE METHOD?
MESODIF models the emission releases as a series of puffs. At each time step, the puff centers are advected by the local wind field. Then the concentrations are diffused by the Gaussian law, with vertical and horizontal standard deviations calculated from the total distance traveled and the current stability, as well as from the accumulated sigmas acquired thus far.
HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? None.
SPATIAL RESOLUTION AND EXTENT OF MESH?
MESODIF has a 26 by 32 grid, with user specified x and y grid spacing.
RESOLUTION AND EXTENT OF TIME INCREMENT?
Puffs may be released at various user specified interval, and advected at user specified interval.
BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? None.
BACKGROUND DATA? No.

SPECIES:

MULTIPLE SPECIES? No.
WHICH REACTIVE SPECIES? None.
WHICH NON-REACTIVE SPECIES? Any passive species (eg. SO2, TSP, etc).
DEPOSITION? No.
DECAY? No.
CHEMISTRY? No.

COMPUTED DATA:

AVERAGES? Yes. (Non-overlapping)
LONG TERM(ANNUAL)? Yes.
SHORT TERM? Yes.
1 HOUR? Yes.
3 HOUR? Yes.
24 HOUR? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? Can be modified to print instantaneous plume as superposition of puff streak trajectories, an important advantage in variable flow situations.

VALIDATION HISTORY?
"Regional Effluent Dispersion Calculations Considering Spatial and Temporal Meteorological Variations", G.E. Start and L.L. Wendell
NOAA Technical Memorandum ERL ARL-44 (1974)

APPLICABLE TO FOUR CORNERS REGION?
The model is, with the necessary modifications, applicable to the Four Corners region.
INCORPORATION OF OBSERVED DATA? No.
CALIBRATION POTENTIAL? Good, given adequate observed data.

USAGE CRITERIA:

USER'S MANUAL? Yes, but not user oriented.
AVAILABILITY OF THE MODEL? In the public domain.
EASE OF MODIFYING MODEL? Relatively short code facilitates incorporation of improvements.
EASE OF USING MODEL? Relatively easy, given meteorological data.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Small.
ERROR DIAGNOSTICS? Minimal.
EASE OF MODEL INSTALLATION ON UNIVAC? Relatively easy.
EASE OF MODEL MAINTENANCE? Relatively easy.
OUTPUT INTERPRETATION REQUIREMENTS? Average.

OPERATION:

CORE REQUIREMENTS? 150k bytes.
ON LINE STORAGE REQUIREMENTS? None.
COMPUTATIONAL TIME REQUIREMENTS? 30 mins./data year (IBM 370) dependent on puff resolution used.
INPUT DATA PREPARATION TIME REQUIREMENTS? 1 hour
OTHER HARD WARE REQUIREMENTS? 2 tape drives/met station

REFERENCES FOR MESODIF MODEL:

G. E. Start and L. L. Wendell,1974: "Regional Effluent Dispersion Calculations Considering Spatial and Temporal Meteorological Variations", NOAA Technical Memorandum ERL ARL-44

Wendell, L. L.,1972:"Mesoscale Wind Field and Transport Estimates Determined From a Network of Wind Towers",Mon. Wea. Rev. Vol 100 No.7 pp 565-578

Wendell, L. L.,1970:"A preliminary examination of mesoscale wind fields and transport determined from a network of towers", NOAA Tech. Memo. ERLTM-ARL 25, U.S.Dept. of Commerce,Air Resources Lab.,Silver Spring, Md.,25 p + appendices.

Start, G. E., and E. H. Markee, Jr.,1967:"Relative dose factors from long-period point source emissions of atmospheric pollutants", Proc. of the USAEC Meteorological Information Meeting, Chalk River Nuclear Labs.,Chalk River, Ontario, Sept 11-14, 1967, C.A. Manson (ed.) AECL-2787, pp 59-67

Dickson, C. R., G. E. Start, E. H. Markee, Jr, A. P. Richter, and J. Kearns, 1967:"Meteorology for the Loss-of-Fluid Test Reactor", 2d. Progress Report, Jan 1966 - Jan. 1967, IDO-12059, ESSA, Air Resources Field Research Office, Idaho Falls, Idaho

10. ELIASSEN-SALTBONES ONE-LAYER MODEL

This model is a simple Lagrangian dispersion model which incorporates deposition and a linear transformation of sulfur dioxide to sulfates. The pollutants are modeled as marked particles with the concentrations attached to each particle modified at each time step as indicated by the removal, deposition, and transformation equations. The particles are advected by a method described by Petterssen [1956].

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? None.
SINGLE STATION? No.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? No.
SPATIAL EXTRAPOLATION TECHNIQUE? Analyzed.
INPUT TIME INTERVAL? 6 hour.
TEMPORAL INTERPOLATION TECHNIQUE? Linear.
SMOOTHING? Analyzed.
ADJUSTED FOR MIXING LID? No.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

TURBULENCE DATA: None.

OTHER METEOROLOGICAL DATA? None.

EMISSIONS:

SOURCE INVENTORY: Gridded source inventory.

ELEVATED SOURCES? No.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN? Not considered.

TRANSPORT:

ADVECTIVE METHOD?

Every hour particles are advected by an iterative 2-point Runge-Kutta technique described by Petterssen [1956]. Every 12 hours, the particles are condensed to one particle per grid cell.

DIFFUSIVE METHOD? None.
HORIZONTAL DIFFUSION? None.
VERTICAL DIFFUSION? None.
PSEUDO-DIFFUSION? No.
SPATIAL RESOLUTION AND EXTENT OF MESH? 32 by 32 grid with a spacing of 270 km.

RESOLUTION AND EXTENT OF TIME INCREMENT?
Time step of 1 hour, 6 month duration.

BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? None.
BACKGROUND DATA? None.

SPECIES:

MULTIPLE SPECIES? Yes.
WHICH REACTIVE SPECIES? SO2, SO4
WHICH NON-REACTIVE SPECIES? None.
DEPOSITION? Yes.
WET? No.
DRY? Yes, using the deposition velocity concept.

DECAY? Removal rate for sulfates.
CHEMISTRY? Yes.
LINEAR? Yes.
NON-LINEAR? No.
WHAT CHEMICAL SYSTEM? SO2 to SO4

COMPUTED DATA:

AVERAGES? Yes.
LONG TERM(ANNUAL)? Yes.
SHORT TERM? Yes.
1 HOUR? No.
3 HOUR? No.
24 HOUR? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? No.

VALIDATION HISTORY?

"Sulfur Transport and Dry Depostion Over Europe Described by a Simple Lagrangian Dispersion Model", A. Eliassen and J. Saltbones, Norwegian Institute for Air Research (1976)

APPLICABLE TO FOUR CORNERS REGION?
Given its limitations, it is applicable to the Four Corners Region if modified to include terrain.
INCORPORATION OF OBSERVED DATA? Yes.
CALIBRATION POTENTIAL? Unknown at this time.

USAGE CRITERIA:

USER'S MANUAL? Unknown at this time.
AVAILABILITY OF THE MODEL? Developmental
EASE OF MODIFYING MODEL? Unknown at this time.
EASE OF USING MODEL? Unknown at this time.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Unknown at this time.
ERROR DIAGNOSTICS? Unknown at this time.
EASE OF MODEL INSTALLATION ON UNIVAC? Unknown at this time.
EASE OF MODEL MAINTENANCE? Unknown at this time.
OUTPUT INTERPRETATION REQUIREMENTS? Unknown at this time.

OPERATION:

CORE REQUIREMENTS? Unknown at this time.
ON LINE STORAGE REQUIREMENTS? Unknown at this time.
COMPUTATIONAL TIME REQUIREMENTS? Unknown at this time.
INPUT DATA PREPARATION TIME REQUIREMENTS? Unknown at this time.

REFERENCES FOR ELIASSEN-SALTBONES ONE-LAYER MODEL:

Eliassen, A. and J. Saltbones, 1976: "Sulphur Transport and Dry Deposition Over Europe Described by a Simple Lagrangian Dispersion Model.", Norwegian Institute for Air Research

Petterssen, S.,1956: Weather Analysis and Forecasting, McGraw Hill p 27

Elisen A. and J. Saltbones, 1975: "Decay and Transformation Rates of SO2 as Estimated from Emission Data,Trajectories,and Measured Air Concentrations" Atmos.Env. Vol 9 pp 425-429

Bolin B. and Persson C.,1975: "Regional Dispersion and Deposition of Atmospheric Pollutants with Particular Application to Sulfur Pollution over Western Europe." Tellus Vol 27 pp 281-310

11. ELIASSEN-SALTBONES TWO-LAYER MODEL

This model is an extension of the one-layer model to two layers (to account for low and high sources) with different wind fields for horizontal advection in each layer, and with a simple turbulent exchange mechanism between the layers.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Two layers.
SINGLE STATION? No.
GRIDDED INPUT? Yes.
ARBITRARY STATION INPUT? No.
SPATIAL EXTRAPOLATION TECHNIQUE? Analyzed.
INPUT TIME INTERVAL? 6 hour.
TEMPORAL INTERPOLATION TECHNIQUE? Linear.
SMOOTHING? Analyzed.
ADJUSTED FOR MIXING LID? No.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

TURBULENCE DATA: Turbulent exchange velocity field.

OTHER METEOROLOGICAL DATA? None.

EMISSIONS:

SOURCE INVENTORY: Gridded source inventory.

ELEVATED SOURCES? Yes.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.

ARBITRARY LOCATIONS? No.

TERRAIN? Not considered.

TRANSPORT:

ADVECTIVE METHOD?

Every hour particles are advected by an iterative 2-point Runge-Kutta technique described by Petterssen [1956]. Every 12 hours, the particles are condensed to one particle per grid cell.

DIFFUSIVE METHOD?

The vertical flux of q from the top to the bottom layer is approximated by

$$F = 2 K (q1-q0)/(h1+h0)$$

where q1,q0,h1,h0 are the SO_2 concentrations and depths of the top and bottom layers, and K is the vertical eddy-diffusivity between the layers.

HORIZONTAL DIFFUSION? None.
VERTICAL DIFFUSION? Yes.

PSEUDO-DIFFUSION? No.

SPATIAL RESOLUTION AND EXTENT OF MESH? 32 by 32 by 2 grid with a spacing of 270 km. in the horizontal, 200m and 800m in the vertical.

RESOLUTION AND EXTENT OF TIME INCREMENT?
Time step of 1 hour, 6 month duration.

BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? Two.
BACKGROUND DATA? None.

SPECIES:

MULTIPLE SPECIES? Yes.
WHICH REACTIVE SPECIES? SO_2, SO_4
WHICH NON-REACTIVE SPECIES? None.

DEPOSITION? Yes.
WET? No.
DRY? Yes, using the deposition velocity concept.

DECAY? Removal rate for sulfates.

CHEMISTRY? Yes.
LINEAR? Yes.
NON-LINEAR? No.
WHAT CHEMICAL SYSTEM? SO_2 to SO_4

COMPUTED DATA:

AVERAGES? Yes.
LONG TERM(ANNUAL)? Yes.
SHORT TERM? Yes.
1 HOUR? No.
3 HOUR? No.
24 HOUR? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? No.

VALIDATION HISTORY? Limited.

APPLICABLE TO FOUR CORNERS REGION?
Given its limitations, it is applicable to the Four Corners Region if modified for terrain.
INCORPORATION OF OBSERVED DATA? Yes.
CALIBRATION POTENTIAL? Unknown at this time.

USAGE CRITERIA:

USER'S MANUAL? Unknown at this time.
AVAILABILITY OF THE MODEL? Developmental.
EASE OF MODIFYING MODEL? Unknown at this time.
EASE OF USING MODEL? Unknown at this time.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Unknown at this time.
ERROR DIAGNOSTICS? Unknown at this time.
EASE OF MODEL INSTALLATION ON UNIVAC? Unknown at this time.
EASE OF MODEL MAINTENANCE? Unknown at this time.
OUTPUT INTERPRETATION REQUIREMENTS? Unknown at this time.

OPERATION:

CORE REQUIREMENTS? Unknown at this time.
ON LINE STORAGE REQUIREMENTS? Unknown at this time.
COMPUTATIONAL TIME REQUIREMENTS? Unknown at this time.
INPUT DATA PREPARATION TIME REQUIREMENTS? Unknown at this time.

REFERENCES FOR ELIASSEN-SALTBONES TWO-LAYER MODEL:

Eliassen, A. and J. Saltbones,1976: "Sulphur Transport and Dry Deposition Over Europe Described by a Simple Lagrangian Dispersion Model.", Norwegian Institute for Air Research

Petterssen, S.,1956: Weather Analysis and Forecasting, McGraw Hill , p27

Elaissen, A. and Saltbones, J.,1975: "Decay and transformation rates of SO2 as Estimated From Emission Data,Trajectories and

Measured Air Concen- trations.",Atmos.Env. Vol 9 pp 425-429

Bolin B. and Persson C.,1975: "Regional Dispersion and Deposition of Atmospheric Polutants with Particular Application To Sulfur Pollution over Western Europe",Tellus Vol 27 pp 281-310

Eliassen, A. and Saltbones, J. 1975: "A Two Layer Dispersion Model: Description and a Few Results", Norwegian Institute for Air Research,

12. WENDELL-POWELL-DRAKE MODEL

This model is a trajectory model intended primarily for calculating the transport, diffusion, and deposition of effluents on regional and continental scales. A month, season, or year of trajectories at 6-hourly time intervals may be calculated forward or backward in time from any origin in the Northern Hemisphere for durations up to 10 days.

Th[illegible] plume is modeled as a series of plume segments which are diff[illegible] the Gaussian formula in the vertical and in the directi[illegible] normal to the wind flow. The downwind length of each segment i[illegible] U dt where U is the mean wind speed and dt is the time increment.

The model incorporates wet and dry deposition as well as linear transformation of SO_2 to SO_4.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Vertically averaged winds.
SINGLE STATION? Yes.
GRIDDED INPUT? Yes (analyzed).
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE?

This model computes grid point winds from station winds by weighting the observations of all stations within a radius R by distance and alignment. While the user may select various parameter values, the model is set up for a radius R=300 nautical miles and for a distance weighting factor of 1/r**2 and an alignment weighting factor of 1-.5 abs(sin(a)) if r is the distance to the station and a its angle relative to the wind at a.

The model uses a bilinear interpolation from corner grid points to the interior of a cell.

INPUT TIME INTERVAL? 12 hours or 6 hours.
TEMPORAL INTERPOLATION TECHNIQUE?
The model assumes persistence of the winds reported closest to the calculation time. (No trajectory is calculated if the wind data is missing for the 2 or 3 closest time periods.)

DIVERGENCE FREE? No.
SMOOTHING? If analyzed.
ADJUSTED FOR MIXING LID? Vertically averaged.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Stability.
INPUT SPATIAL REQUIREMENT? Constant.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? Yes.

AMBIENT TEMPERATURE? No.
AMBIENT PRESSURE? No.
PRECIPITATION RATE? Yes.
SOLAR RADIATION? No.
SURFACE HEAT FLUXES? No.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? No.
MULTIPLE SOURCE SITES? No.
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.

ARBITRARY LOCATIONS? No.

TERRAIN? No.

TRANSPORT:

This model computes trajectories for up to 10 days using U dt increments where dt=1 hours and U is the computed wind at the current point in space and time. Trajectories are started every six hours.

DIFFUSIVE METHOD?

The plume is modeled as a series of plume segments which diffuse vertically and crosswind according to the ground level Gaussian formula for a continuous point source. The vertical and crosswind standard deviations are approximated by a function of downwind distance and stability class. Each segment has a downwind length equal to U dt where U is the mean wind speed and dt is the time increment.

HORIZONTAL DIFFUSION? Yes (on option).
VERTICAL DIFFUSION? Yes.

PSEUDO-DIFFUSION? No.

SPATIAL RESOLUTION AND EXTENT OF MESH?

The model is organized to compute on a large scale grid which is about 34 km square.

RESOLUTION AND EXTENT OF TIME INCREMENT?

Intended for monthly, seasonal applications with a time increment of 3 hours.

BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? None.
BACKGROUND DATA? None.

SPECIES:

MULTIPLE SPECIES? Yes.

WHICH REACTIVE SPECIES? SO2,SO4.
WHICH NON-REACTIVE SPECIES? SO2,TSP,etc.

DEPOSITION? Yes.

WET?

Precipitation scavenging is based on an empirically derived average scavenging ratio (Engelmann,1970).

DRY?

The concept of deposition velocity is used to calculate dry deposition amounts along a trajectory.

DECAY? No.
CHEMISTRY? No.

COMPUTED DATA:

AVERAGES? Yes.
LONG TERM(ANNUAL)? Yes.
SHORT TERM? No.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? Yes.

VALIDATION HISTORY? Limited.
APPLICABLE TO FOUR CORNERS REGION?
Yes, with suitable modifications.
CALIBRATION POTENTIAL? Good, given adequate observed data.

USAGE CRITERIA:

USER'S MANUAL? No.
AVAILABILITY OF THE MODEL? In the public domain.
EASE OF MODIFYING MODEL? Some difficulty due to lack of documentation.
EASE OF USING MODEL? Some difficulty due to lack of documentation.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Moderate.
ERROR DIAGNOSTICS? Unable to assess.
EASE OF MODEL INSTALLATION ON UNIVAC? Moderate.
EASE OF MODEL MAINTENANCE? Moderate.
OUTPUT INTERPRETATION REQUIREMENTS? Minor.

OPERATION:

CORE REQUIREMENTS? Moderate.
ON LINE STORAGE REQUIREMENTS? Moderate.
COMPUTATIONAL TIME REQUIREMENTS?
15 minutes/data month for 30 sources on CDC 6600
INPUT DATA PREPARATION TIME REQUIREMENTS? ???

REFERENCES FOR WENDELL-POWELL-DRAKE MODEL:

Wendell, L., L. Powell, D. C., Drake R. L.,1976:"A Regional Scale Model For Computing Deposition and Ground Level Air of SO2 and Sulfates From Elevated and Ground Sources", Proc. Third Symposium on Atmos. Turbulence, Diffusion and Air Quality, AMS, Raleigh, NC ,pp 318-324

13. HEFFTER-TAYLOR-FERBER LONG-TERM MODEL

This model is a trajectory model intended primarily for calculating the transport, diffusion, and deposition of effluents on regional and continental scales. A month, season, or year of trajectories at 6-hourly time intervals may be calculated forward or backward in time from any origin in the Northern Hemisphere for arbitrary durations. A Gaussian plume model is combined with the trajectory model to calculate long-term mean average surface air con- centrations and deposition amounts. Both wet and dry deposition are incorporated into the model.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Vertically averaged winds.
SINGLE STATION? Multiple Station.
GRIDDED INPUT? Yes (analyzed).
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE?

For station input, this models computes three hour trajectory segments from station winds by weighting the observations of all stations within a radius R by distance and alignment. While the user may select various parameter values, the model is set up for a radius R=300 nautical miles and for a distance weighting factor of 1/r**2 and an alignment weighting factor of 1-.5 abs(sin(a)) if r is the distance to the station and a its angle relative to the wind at a station.

The model uses a bilinear interpolation from corner grid points to the traject segment in the cell for gridded input.

INPUT TIME INTERVAL? 12 hours or 6 hours.
TEMPORAL INTERPOLATION TECHNIQUE?

All winds are linearly interpolated to the periods 00Z,06Z,12Z, and 18Z.

DIVERGENCE FREE? No.
SMOOTHING? If analyzed.
ADJUSTED FOR MIXING LID? Vertically averaged.

MIXING LID: Temperature profile at stations.

INPUT SPATIAL REQUIREMENT? At each station.
SPATIAL EXTRAPOLATION? Yes.

INPUT TEMPORAL REQUIREMENT? Same as winds.
TEMPORAL INTERPOLATION? Yes.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? Constant.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? Yes.

AMBIENT TEMPERATURE? Yes.
AMBIENT PRESSURE? No.
PRECIPITATION RATE? Yes.
SOLAR RADIATION? No.
SURFACE HEAT FLUXES? No.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? No.
AREA SOURCES? No.
MULTIPLE SOURCE SITES? No.
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? Yes.
ARBITRARY LOCATIONS? Yes.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD?

This model computes trajectories for up to 10 days using U dt increments where dt=3 hours and U is the computed wind at the current point in space and time. Trajectories are started every six hours.

DIFFUSIVE METHOD?

Ground-level air concentration calculations along a trajectory are based on the Gaussian plume equation for a instantaneous point source assumed to be at ground level. Here sigma z is the square root of 2 Kt where K is the vertical diffusivity and sigma y is assumed to be .5 t.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? No.
SPATIAL RESOLUTION AND EXTENT OF MESH?
The model is organized to compute on a large scale grid of about 80 by 80 in extent with a spacing of .5 degrees in latitude or longitude.

RESOLUTION AND EXTENT OF TIME INCREMENT?
Intended for monthly, seasonal applications with a time increment of 3 hours.

BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? None.
BACKGROUND DATA? None.

SPECIES:

MULTIPLE SPECIES? No.
WHICH REACTIVE SPECIES? None.
WHICH NON-REACTIVE SPECIES? SO2,TSP,etc.
DEPOSITION? Yes.
WET?
Precipitation scavenging is based on an empirically derived average scavenging ratio (Engelmann,1970).

DRY?
The concept of deposition velocity is used to calculate dry deposition amounts along a trajectory.

DECAY? No.
CHEMISTRY? No.

COMPUTED DATA:

AVERAGES? Yes.
LONG TERM(ANNUAL)? Yes.
SHORT TERM? No.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? Yes.

VALIDATION HISTORY? Limited: Heffter et al.,1975.
There are current plans for extensive testing during the coming year.

APPLICABLE TO FOUR CORNERS REGION?
Yes if suitably modified to take terrain into account.
INCORPORATION OF OBSERVED DATA? In principle, yes.
CALIBRATION POTENTIAL? Not ascertained.

USAGE CRITERIA:

USER'S MANUAL? Model not externally documented.
AVAILABILITY OF THE MODEL? In the public domain.
EASE OF MODIFYING MODEL? Dependent on documentation.
EASE OF USING MODEL? Relatively easy.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Moderate.
ERROR DIAGNOSTICS? Minimal.
EASE OF MODEL INSTALLATION ON UNIVAC? Already on UNIVAC.
EASE OF MODEL MAINTENANCE? Good.
OUTPUT INTERPRETATION REQUIREMENTS? Minor.

OPERATION:

CORE REQUIREMENTS? Less than 256K on IBM 360/195
ON LINE STORAGE REQUIREMENTS? Moderate.
COMPUTATIONAL TIME REQUIREMENTS? On IBM 360/195, one data month takes 1 minute (4 trajectories per day,5 day trajectories).
INPUT DATA PREPARATION TIME REQUIREMENTS? Not ascertained.

REFERENCES FOR HEFFTER-TAYLOR-FERBER LONG-TERM MODEL

Heffter J.L., Taylor, A.D., Ferber, G.J.,1975:"A Regional-Continental Scale Transport, Diffusion, and Deposition Model", NOAA Technical Memorandum ERL ARL-50

Englemann R.J.,1970:"Scavenging Prediction Using Ratios of Concentrations in Air and Precipitation",Proc. Symposium on Precipitation Scavenging, AEC Symposium Series 22, pp 475-485

Heffter, J.L.,1965:"The Variation of Horizontal Diffusion Parameters with Time for Travel Periods of one Hour or Longer", JAM Vol 4 , pp 153-156

Machta, L., Ferber, G. J., and Heffter, J.L.,1974:"Regional and Global Scale Dispersion of Krypton-85 for Population-Dose Calculations",Proc. Symposium on the Physical Behavior of Radioactive Contaminants in the Atmosphere,IAEA,Vienna,pp 411-425

14. HEFFTER, TAYLOR AND FERBER: SHORT-TERM MODEL

This model is a trajectory model intended primarily for calculating the transport, diffusion, and deposition of effluents on regional and continental scales. A month, season, or year of trajectories at 6-hourly time intervals may be calculated forward or backward in time from any origin in the Northern Herimsphere for durations up to 10 days. The continuous emission source is modeled as a series of instantaneous "puffs" which are advected along the trajectory and diffused according to the Gaussian formula for an instantaneous release. The diffusion is assumed to be horizontally isotropic.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Vertically averaged winds.
SINGLE STATION? Yes.
GRIDDED INPUT? Yes (analyzed).
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE?

This models computes grid point winds from station winds by weighting the observations of all stations within a radius R by distance and alignment. While the user may select various parameter values, the model is set up for a radius R=300 nautical miles and for a distance weighting factor of 1/r**2 and an alignment weighting factor of 1-.5 abs(sin(a)) if r is the distance to the station and a its angle relative to the wind at a.

The model uses a bilinear interpolation from corner grid points to the interior of a cell.

INPUT TIME INTERVAL? 12 hours or 6 hours.
TEMPORAL INTERPOLATION TECHNIQUE?

The model assumes persistence of the winds reported closest to the calculation time. (No trajectory is calculated if the wind data is missing for the 2 or 3 closest time periods.)

DIVERGENCE FREE? No.
SMOOTHING? If analyzed.
ADJUSTED FOR MIXING LID? Vertically averaged.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform.
SPATIAL EXTRAPOLATION? None.

INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? Constant.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? No.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? No.
AREA SOURCES? No.
MULTIPLE SOURCE SITES? No.
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? Yes.
ARBITRARY LOCATIONS? Yes.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD?

This model computes trajectories for up to 10 days using U dt increments where dt=3 hours and U is the computed wind at the current point in space and time. Trajectories are started every six hours.

DIFFUSIVE METHOD?

The continuous emission source is modeled as a series of instantaneous "puffs". Each puff is advected along the trajectory and sampled a few times daily. The concentrations at the receptors are calculated by the Gaussian equation for an instantaneous source. Here the vertical standard deviation is the square root of 2 K t, where K is the vertical diffusivity, and the horizontal standard deviation is assumed to be .5 t where t is the travel time in seconds.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? No.
SPATIAL RESOLUTION AND EXTENT OF MESH?
The model is organized to compute concentrations at receptors within one or two days travel time of the the source.

RESOLUTION AND EXTENT OF TIME INCREMENT?
The recommended time increment is 3 hours with the extent of a run limited only by the availability of input data and computation time.

BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? None.
BACKGROUND DATA? None.

SPECIES:

MULTIPLE SPECIES? No.
WHICH REACTIVE SPECIES? None.
WHICH NON-REACTIVE SPECIES? SO2,TSP,etc.
DEPOSITION? No.

DECAY? No.
CHEMISTRY? No.

COMPUTED DATA:

AVERAGES? Yes.
LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.
1 HOUR? Yes.
3 HOUR? Yes.
24 HOUR? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? Yes.

VALIDATION HISTORY? Limited: Heffter et al.,1975.
There are current plans for extensive study during the coming year.
APPLICABLE TO FOUR CORNERS REGION?
A higher resolution, numerical model would be more appropriate for short-term events in the Four Corners region.
INCORPORATION OF OBSERVED DATA? In principle,yes.
CALIBRATION POTENTIAL? Not ascertained.

USAGE CRITERIA:

USER'S MANUAL? No external documentation.
AVAILABILITY OF THE MODEL? In the public domain.
EASE OF MODIFYING MODEL? Dependent on documentation.
EASE OF USING MODEL? Relatively easy.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Moderate.
ERROR DIAGNOSTICS? Minimal.
EASE OF MODEL INSTALLATION ON UNIVAC? ???
EASE OF MODEL MAINTENANCE? Dependent on documentation.
OUTPUT INTERPRETATION REQUIREMENTS? Minor.

OPERATION:

CORE REQUIREMENTS? Not ascertained.
ON LINE STORAGE REQUIREMENTS? Not ascertained.
COMPUTATIONAL TIME REQUIREMENTS? Not ascertained.
INPUT DATA PREPARATION TIME REQUIREMENTS? Not ascertained.

REFERENCES FOR HEFFTER-TAYLOR-FERBER SHORT-TERM MODEL:

Heffter J.L., Taylor A.D., Ferber G.J.,1975:"A Regional-Continental Scale Transport, Diffusion, and Deposition Model", NOAA Technical Memorandum ERL ARL-50

Heffter J.L.,1965:"The Variation of Horizontal Diffusion Parameters with Time for Travel Periods of One Hour or Longer", J.A.M. Vol 4 , pp 153-156

Machta L,Ferber G. J., and Heffter J.L.,1974:"Regional and Global Scale Dispersion of Krypton-85 for Population-Dose Calculations",Proc. Symposium on the Physical Behavior of Radioactive Contaminants in the Atmosphere,IAEA,Vienna,pp 411-425

15. SHEIH-MOROZ MODEL

This is a Lagrangian puff model that takes into account temporal and spatial inhomogeneity, notably wind shear; integrates plume-rise calculation into the puff model; and can optimally tailor its Lagrangian coordinates to the need of the multi-scale sources of urban modeling. It can be used to provide treatment of sub-grid scale phenomena in regional scale grid models.

The plume from a point, line, or area source is treated as a series of puffs emitted successively from the specific source. Each of the puffs is characterized by the amount of pollutant emitted and by the coordinates of three axes and, for the case where buoyant plume rise is important, the temperature and vertical velocity of the puff. At each time step, the position of the three axes are computed from local variables taking into account advection, eddy diffusion, wind shear, and plume-rise entrainment.

The concentration distribution within each puff is determined by fitting an ellipsoid around the axes and assuming a Gaussian distribution with the length of the principal axes of the ellipsoid as standard deviations. The final concentration at a point of interest is obtained by summing the contributions from nearby puffs.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Yes.
SINGLE STATION? Yes.
GRIDDED INPUT? In principle, yes.
ARBITRARY STATION INPUT? In principle, yes.
SPATIAL EXTRAPOLATION TECHNIQUE? Not ascertained
INPUT TIME INTERVAL? Not ascertained

MIXING LID:

INPUT SPATIAL REQUIREMENT? Not ascertained.
SPATIAL EXTRAPOLATION? Not ascertained.
INPUT TEMPORAL REQUIREMENT? Not ascertained.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? Constant.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? Yes.

AMBIENT TEMPERATURE? Yes.
AMBIENT PRESSURE? Yes.
PRECIPITATION RATE? No.
SOLAR RADIATION? No.
SURFACE HEAT FLUXES? No.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? ???
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? Yes.

BUOYANT ENTRAINMENT? Yes.

Buoyancy entrainment is incorporated into the puff motion by an iterative solution to the conservation laws of volume, momentum, and heat of an instantaneous source (eg, Morton et al.) for the puff radius.

VERTICAL WIND SHEAR? Yes.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? In principle, yes.
POLAR GRID? In principle, yes.
ARBITRARY LOCATIONS? In principle, yes.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD?

The plumes are modeled as a series of puffs represented by 8 Lagrangian particles. The first six particles are for translation and the last two for wind shear rotation.

At each time step the first six particles are displaced an amount u dt where dt is the time step and u is the three dimensional wind vector. In addition, during the first time interval of release, the particle advection takes account of the stretching of the puff due to the difference in exposure time of the various parts of the puff to the advection wind.

Wind shear rotation about the vertical axis is neglected. Rotation about the horizontal axes is incorporated by a displacement proportial to the variation of the wind field over the puff.

DIFFUSIVE METHOD?

The Lagrangian particles are also displaced by a diffusive velocity estimated from the Gaussian puff diffusion equation given by Sutton. This velocity is the square root of 2 K/2 t, where K is the diffusivity is the relevant direction and t is the time from release.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? No.
SPATIAL RESOLUTION AND EXTENT OF MESH? Not ascertained.
RESOLUTION AND EXTENT OF TIME INCREMENT? Not ascertained.
BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? None.

SPECIES:

MULTIPLE SPECIES? No.
WHICH REACTIVE SPECIES? None.
WHICH NON-REACTIVE SPECIES? SO_2
DEPOSITION? No.
DECAY? No.
CHEMISTRY? No.

COMPUTED DATA:

AVERAGES? Yes.
LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.
1 HOUR? Yes.
3 HOUR? Yes.
24 HOUR? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? No.

VALIDATION HISTORY?
Comparison of plume with TVA observation, Sheih and Moroz, "A Lagrangian Puff Diffusion Model for the Prediction of Pollutant Concentrations over Urban Areas", (1973)

APPLICABLE TO FOUR CORNERS REGION? Not in isolation; see Section 16.
INCORPORATION OF OBSERVED DATA? Not ascertained.
CALIBRATION POTENTIAL? Not ascertained.

USAGE CRITERIA:

USER'S MANUAL? No external documentation.
AVAILABILITY OF THE MODEL? Developmental
EASE OF MODIFYING MODEL? Unknown.
EASE OF USING MODEL? Unknown.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Unknown.
ERROR DIAGNOSTICS? Unknown.
EASE OF MODEL INSTALLATION ON UNIVAC? Unknown.

EASE OF MODEL MAINTENANCE? Unknown.
OUTPUT INTERPRETATION REQUIREMENTS? Unknown.

OPERATION:

CORE REQUIREMENTS? Not presently known.
ON LINE STORAGE REQUIREMENTS? Not presently known.
COMPUTATIONAL TIME REQUIREMENTS? Not presently known.
INPUT DATA PREPARATION TIME REQUIREMENTS? Not presently known.

REFERENCES:

Morton B. R., Taylor G.I., Turner J. S.,1953:"Turbulent gravitational convectin from maintained and instantaneous sources", Proc. of the Roy. Soc. 234 pp 1-23

Sutton, O. G. ,1953: Micrometerology, p 134, Mc Graw -Hill,NY

Sheih,C.M. Moroz, W.J.,1973:"A Lagrangian Puff Diffusion Model for the Prediction of Pollutant Concentrations over Urban Areas.", Proc. Third Inter. Clean Air Congress, Dusseldorf, FDR,VDI-Verlag, B43-B52

16. SHEIH PUFF-GRID MODEL

This is a mesoscale model combining a Lagrangian puff model (see Section 15) with a particle-in-cell grid model. The puff model is used to handle sub-grid scale phenomena. The pollutant in each puff is passed to the grid system and henceforth is treated with the grid model after the puff has grown to a size comparable with the grid volume. Area sources comparable with or larger than the grid dimension are treated with the grid model. The final concentration at a point of interest is obtained by summing the contributions from the grid model and nearby puffs.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Yes.
SINGLE STATION? Yes.
GRIDDED INPUT? No.
ARBITRARY STATION INPUT? No.
SPATIAL EXTRAPOLATION TECHNIQUE? None.

INPUT TIME INTERVAL? Hourly.
DIVERGENCE FREE? Yes.
SMOOTHING? No.
ADJUSTED FOR MIXING LID? No.

MIXING LID: None.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? Constant.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? Yes.

AMBIENT TEMPERATURE? Yes.
AMBIENT PRESSURE? Yes.
PRECIPITATION RATE? No.
SOLAR RADIATION? No.
SURFACE HEAT FLUXES? No.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? Yes.

BUOYANT ENTRAINMENT? Yes.

Buoyancy entrainment is modeled by an iterative numerical solution to the equations of conservation of volume, momentum, and heat.

VERTICAL WIND SHEAR? Yes.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD?
DIFFUSIVE METHOD?

The plume from a source small in comparison to the grid dimension is modeled as a series of puffs, with the shape of each puff determined by 6 Lagrangian particles. At each time step the particles are advected by the local wind field, with displacements due to wind shear and buoyancy entrainment and due to a diffusive velocity. When the puff and grid dimension are comparable, the puff is merged with the grid particles.

The grid scale advection solves the conservation of mass equation by the particle-in-cell method. Briefly, this method assumes that the total pollutant in each grid cell is concentrated in a single particle at the grid center. In each time step the particle is displaced to a new location by the sum of advective and diffusive velocities multiplied by the time increment. Upon reaching another location, the pollutant in the particle is then redistributed to the surrounding grid points, inversely weighting the mass distribution according to distance.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? Yes.
SPATIAL RESOLUTION AND EXTENT OF MESH?

The model covers a 5 km by 5 km area with an 11 by 11 horizontal grid and 11 levels from the surface up to a height of 1 km.

RESOLUTION AND EXTENT OF TIME INCREMENT? 30 Sec. for 24 hr.
BOUNDARY CONDITIONS?

No pollutant deposited on the ground, all grid and puff pollutants are removed from the field after they are transported out of the region of interest.

INITIAL CONDITIONS? Initial SO_2 field is 0.
NUMBER OF VERTICAL LAYERS? 11
BACKGROUND DATA? No.

SPECIES:

MULTIPLE SPECIES? No.
WHICH REACTIVE SPECIES? None.
WHICH NON-REACTIVE SPECIES? SO_2
DEPOSITION? No.
DECAY? No.
CHEMISTRY? No.

COMPUTED DATA:

AVERAGES? Yes.

LONG TERM(ANNUAL)? No.
SHORT TERM? Yes.
1 HOUR? Yes.
3 HOUR? Yes.
24 HOUR? Yes.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? No.

VALIDATION HISTORY?
Comparison of observed and prediction over State College, Pa: "A Puff-Grid Model for Predicting Pollutant Transport Over an Urban Area", C.M. Sheih (1976)
APPLICABLE TO FOUR CORNERS REGION?
If suitably modified, yes.
INCORPORATION OF OBSERVED DATA? Not ascertained.
CALIBRATION POTENTIAL? Not ascertained.

USAGE CRITERIA:

USER'S MANUAL? Lacks basic documentation.
AVAILABILITY OF THE MODEL? Developmental.
EASE OF MODIFYING MODEL? Depends on documentation.
EASE OF USING MODEL? Depends on documentation.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Unknown.
ERROR DIAGNOSTICS? Unknown.
EASE OF MODEL INSTALLATION ON UNIVAC? Depends on documentation.
EASE OF MODEL MAINTENANCE? Depends on documentation.
OUTPUT INTERPRETATION REQUIREMENTS? Unknown.

OPERATION:

CORE REQUIREMENTS? Unknown.
ON LINE STORAGE REQUIREMENTS? Unknown.
COMPUTATIONAL TIME REQUIREMENTS? 500 sec. for 24 hours, IBM 370
INPUT DATA PREPARATION TIME REQUIREMENTS? Unknown.

REFERENCES:

Sheih C. M. and Moroz W. J.,1973:"A Lagrangian Puff Diffusion Model for the Prediction of Pollutant Concentrations over Urban Areas", Proc. The Third International Clean Air Congress, B43-B52

Sklarew, R. C.,1970:"Preliminary Report of the SSS Urban Air Pollution Model Simulation of Carbon Monoxide in Los Angeles", System,Science, and Software, Inc. La Jolla, California

Sklarew, R.C. , "A New Approach: The Grid Model of Urban Air Pollution", JAPCA, 20, p 79 (1970)

17. BNL TRAJECTORY MODEL

This model is the Heffter, Taylor and Ferber model modified by the BNL Meteorology Group to include chemical transformations and deposition. The model was furthur modified to consider multiple sources by combining their individual sulfur dioxide and sulfate patterns for the time period modeled.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? Vertically averaged winds.
SINGLE STATION? Yes.
GRIDDED INPUT? Yes (analyzed).
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE?

This models computes grid point winds from station winds by weighting the observations of all stations within a radius R by distance and alignment. While the user may select various parameter values, the model is set up for a radius R=300 nautical miles and for a distance weighting factor of 1/r**2 and an alignment weighting factor of 1-.5 abs(sin(a)) if r is the distance to the station and a its angle relative to the wind at a.

The model uses a bilinear interpolation from corner grid points to the interior of a cell.

INPUT TIME INTERVAL? 12 hours or 6 hours.
TEMPORAL INTERPOLATION TECHNIQUE?

The model assumes persistence of the winds reported closest to the calculation time. (No trajectory is calculated if the wind data is missing for the 2 or 3 closest time periods.).

DIVERGENCE FREE? No.
SMOOTHING? If analyzed.
ADJUSTED FOR MIXING LID? Vertically averaged.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

TURBULENCE DATA:

DIFFUSIVITY OR STABILITY? Diffusivity.
INPUT SPATIAL REQUIREMENT? Constant.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Constant.
TEMPORAL INTERPOLATION? None.

OTHER METEOROLOGICAL DATA? Yes.

AMBIENT TEMPERATURE? No.
AMBIENT PRESSURE? No.
PRECIPITATION RATE? Yes.
SOLAR RADIATION? No.
SURFACE HEAT FLUXES? No.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? No.
AREA SOURCES? No.
MULTIPLE STACKS AT ONE SITE? Yes.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? No.
INSTANTANEOUS SOURCE EMISSIONS? No.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? No.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD?

This model computes trajectories for up to 10 days using U dt increments where dt=3 hours and U is the computed wind at the current point in space and time. Trajectories are started every six hours.

DIFFUSIVE METHOD?

Ground-level air concentration calculations along a trajectory are based on the Gaussian plume equation for a continuous point source assumed to be at ground level. The plume is modeled as a series of plume segments (or "puff-slices") each with a downwind length of U dt, where U is the mean wind speed and dt is the time increment.

The standard deviation of the plume's mass normal to the wind direction is assumed to be proportional to the travel time, t, and the vertical standard deviation is equal to the square root of 2 K t, where K is the diffusivity.

HORIZONTAL DIFFUSION? Yes.
VERTICAL DIFFUSION? Yes.
PSEUDO-DIFFUSION? No.
SPATIAL RESOLUTION AND EXTENT OF MESH?
The model is organized to compute on a large scale grid of about 80 by 80 in extent with a spacing of .5 degrees in latitude or longitude.

RESOLUTION AND EXTENT OF TIME INCREMENT?
Intended for monthly, seasonal applications with a time increment of 3 hours.

BOUNDARY CONDITIONS? None.
INITIAL CONDITIONS? None.
NUMBER OF VERTICAL LAYERS? None.
BACKGROUND DATA? None.

SPECIES:

MULTIPLE SPECIES? Yes.
WHICH REACTIVE SPECIES? SO2,SO4
WHICH NON-REACTIVE SPECIES? SO2,TSP,etc.
DEPOSITION? Yes.
WET?
Precipitation scavenging is based on an empirically derived average scavenging ratio (Engelmann,1970).

DRY?
The concept of deposition velocity is used to calculate dry deposition amounts along a trajectory for both SO2 and SO4.

DECAY? No.
CHEMISTRY?
Linear chemistry is used to convert SO2 to SO4 along a trajectory. The conversion rate is a parameter. In addition 2% of the initial SO2 is immediately converted to SO4 to simulate in-stack production of SO4.

COMPUTED DATA:

AVERAGES? Yes.

LONG TERM(ANNUAL)? Yes.
SHORT TERM? No.
MAXIMUM CONCENTRATIONS? No.
PLUME TRAJECTORY? Yes.

VALIDATION HISTORY? Limited: Heffter et al.,1975
APPLICABLE TO FOUR CORNERS REGION?
Yes, if suitably modified.
INCORPORATION OF OBSERVED DATA? Not ascertained.
CALIBRATION POTENTIAL? Not ascertained.

USAGE CRITERIA:

USER'S MANUAL? None.
AVAILABILITY OF THE MODEL? Not presently available.
EASE OF MODIFYING MODEL? Not now ascertained.
EASE OF USING MODEL? Not now ascertained.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Unknown.
ERROR DIAGNOSTICS? Not now ascertained.
EASE OF MODEL INSTALLATION ON UNIVAC? Not now ascertained.
EASE OF MODEL MAINTENANCE? Not now ascertained.
OUTPUT INTERPRETATION REQUIREMENTS? Minor.

OPERATION:

CORE REQUIREMENTS? Not now ascertained.
ON LINE STORAGE REQUIREMENTS? Not now ascertained.
COMPUTATIONAL TIME REQUIREMENTS? Not now ascertained.
INPUT DATA PREPARATION TIME REQUIREMENTS? Not now ascertained.

REFERENCES:

Heffter J.L., Taylor A.D., Ferber G.J.,1975:"A Regional-Continental Scale Transport, Diffusion, and Deposition Model", NOAA Technical Memorandum ERL ARL-50

Englemann R.J.,1970:"Scavenging Prediction Using Ratios of Concentrations in Air and Precipitation",Proc. Symposium on Precipitation Scavenging, AEC Symposium Series 22, pp 475-485

Heffter, J.L.,1965:"The Variation of Horizontal Diffusion Parameters with Time for Travel Periods of one Hour or Longer", J.A.M. Vol 4 , pp 153-156

Machta, L,Ferber, G. J., and Heffter J.L.,,1974:"Regional and Global Scale Dispersion of Krypton-85 for Population-Dose Calculations",Proc. Symposium on the Physical Behavior of Radioactive Contaminants in the Atmosphere,IAEA,Vienna,pp 411-425

Meyers, R. and R. Cederwall, 1975: BNL RESP Annual Report, BNL 50478

18. STRAM MODEL

STRAM (Source-Transport-Receptor Analysis Model) is basically a version of the Gaussian Plume Model modified to account for temporal variations in point source emission rates and both spatial and temporal variations in wind speed, wind direction and plume dispersion parameters. The model formulation also allows for dry deposition, washout and chemical transformation. Although the model is described as being able to treat non-linear chemistry, there is the implicit assumption that each chemical species involved in the reaction is emitted from a single source so that the chemical kinetics associated with interacting plumes is ignored. In fact, for the example test case presented in the User's Manual, only the first order transformation of SO2 to sulfate is analyzed.

The basic driving force in the model is the advection of plume increments (points) in response to a wind field updated at specified intervals. A plume segment is defined to be a portion of the plume between successive plume increments. The wind field is derived from pibal and rawinsonde data reduced from ETAC upper air data tapes. These data are then processed by the program RNGRD (Random-to-Grid) to obtain gridded wind directions and wind speeds at 12-hour intervals. The gridded wind field is generated from measured wind speeds and wind directions by use of a inverse distance squared weighting procedure. The wind field is adjusted for the mixing height but not smoothed or divergence free. The wind speed and wind direction for a particular plume increment is obtained through a bi-linear interpolation of the gridded wind field in space and time. Since ETAC upper air data is used for the wind field generation, both the advection and sampling grid systems must be subsets of the NMC 47 by 47 octagonal grid system. Present dimensions of the code allow for an advection grid with not more than 17 intersections in the horizontal direction of the NMC grid and not more than 13 intersections in the vertical direction. The sampling grid is currently limited to 13 by 13 equally spaced intersections. The program also allows for concentrations to be computed for up to 10 special receptor locations.

After each advection step for a plume increment, a numerical calculation is performed to determine the amount of a chemical constituent lost or gained during the advection time due to chemical transformation, dry deposition and washout. To carry out this calculation of a new effective source strength, the advection distance is subdivided according to program input specifications. Since chemical transformations generally occur at a higher rate for shorter downwind distances the model provides for successively larger integration step sizes for those plume segments located at larger downwind distances from the source. For each downwind integration step, the calculation of the gain or loss of a substance due to chemical transformation requires an integration over the y and z coordinates perpendicular to the plume axis.

In addition to updating the wind speed and effective source strength at each plume increment, the vertical and horizontal dispersion parameters are increased by an amount depending upon the advection distance and the stability class in force at the appropriate simulation time. Concentrations are then calculated at each of the plume increment points and at three equally spaced points at either side of the plume increment points along lines perpendicular to the plume segment axis. The calculation points are spaced so that the distance between the extreme points (plume "width") is six times the horizontal dispersion parameter. For each plume segment each of the sampling grid points and special sampling locations are examined to determine whether they lie within a trapezoid defined by the plume widths at adjacent plume increments and the straight lines connecting the end points of these widths. If the sampling point is found to lie within this region, then the concentration for this location is obtained through an interpolation of the appropriate crosswind concentrations for the plume increment points at the opposite ends of the plume segment.

FUNCTIONAL CRITERIA:

METEOROLOGY:

WIND FIELD:

VERTICAL RESOLUTION? None.
GRIDDED INPUT? Yes, after running the meteorological preprocessor program RNGRD (Random-to-Grid).
ARBITRARY STATION INPUT? Yes.
SPATIAL EXTRAPOLATION TECHNIQUE? 1/r**2 extrapolation to grid points, linear interpolation from grid points to plume increments.
INPUT TIME INTERVAL? Variable.
TEMPORAL INTERPOLATION TECHNIQUE? Linear.
DIVERGENCE FREE? No.
SMOOTHING? No.
ADJUSTED FOR MIXING LID? Yes, if the limited mixing height for of the Gaussian plume model is

specified.

MIXING LID:

INPUT SPATIAL REQUIREMENT? Uniform in space.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly or at each advection step.
TEMPORAL INTERPOLATION? Persistence.

TURBULENCE DATA: Stability Class

DIFFUSIVITY OR STABILITY? Stability.
INPUT SPATIAL REQUIREMENT? Uniform.
SPATIAL EXTRAPOLATION? None.
INPUT TEMPORAL REQUIREMENT? Hourly or at each advection step.
TEMPORAL INTERPOLATION? Persistence.

OTHER METEOROLOGICAL DATA? None.

EMISSIONS:

SOURCE INVENTORY:

ELEVATED SOURCES? Yes.
AREA SOURCES? No.
MULTIPLE SOURCE SITES? Yes.
TIME DEPENDENT SOURCE STRENGTHS? Yes.
INSTANTANEOUS SOURCE EMISSIONS? Yes.

PLUME RISE? No.

RECEPTOR GEOMETRY:

RECTANGULAR GRID? Yes.
POLAR GRID? No.
ARBITRARY LOCATIONS? Yes, up to ten.

TERRAIN? No.

TRANSPORT:

ADVECTIVE METHOD? Simple Euler integration.
DIFFUSIVE METHOD? The vertical and horizontal plume standard deviations at each plume increment point are based upon the total distance traveled and the current stability class, as well as the accumulated sigmas acquired thus far.

HORIZONTAL DIFFUSION? Yes.

VERTICAL DIFFUSION? Yes.

PSEUDO-DIFFUSION? None.

SPATIAL RESOLUTION AND EXTENT OF MESH? STRAM has an advection grid with 17 intersections in the horizontal direction and 13 intersections in the vertical. The advection grid must be a subset of the NMC grid.

RESOLUTION AND EXTENT OF TIME INCREMENT? The number of hours for each basic advection step is a user input variable.

BOUNDARY CONDITIONS? None.

INITIAL CONDITIONS? None.

NUMBER OF VERTICAL LAYERS? None.

BACKGROUND DATA? Yes.

SPECIES:

MULTIPLE SPECIES? Yes.

WHICH REACTIVE SPECIES? Any for which the reaction rates can be specified.

WHICH NON-REACTIVE SPECIES? Any.

DEPOSITION? Yes.

WET?

DRY?

DECAY? Yes.

CHEMISTRY? No problem with linear chemistry, but if non-linear chemistry is invoked, the effects of interacting plumes may not be included.

COMPUTED DATA:

AVERAGES? Yes. (Non-overlapping)

LONG TERM(ANNUAL)? Yes.

SHORT TERM? Yes.

1 HOUR?

3 HOUR?

24 HOUR?

MAXIMUM CONCENTRATIONS? Yes.

PLUME TRAJECTORY? Currently not printed out but an easy modification.

VALIDATION HISTORY? None.

APPLICABLE TO FOUR CORNERS REGION? The model is, with the necessary modifications, applicable to the Four Corners region.

INCORPORATION OF OBSERVED DATA? No.

CALIBRATION POTENTIAL? Good, given adequate observed data.

USEAGE CRITERIA:

USER'S MANUAL? Very detailed and user oriented (well flow charted).
AVAILABILITY OF THE MODEL? In the public domain.
EASE OF MODIFYING MODEL? The code is broken down into a number of subroutines which deal with separate model functions, so that modifications to the model can be made with little disruption to the structures of the entire code. Changes in deposition and chemical kinetics parameters must be made within the code itself.
EASE OF USING MODEL? Relatively easy, given meteorological data.
VOLUME OF DATA REQUIRING MANUAL PREPARATION? Moderate.
ERROR DIAGNOSTICS? Good.
QUALITY ASSURANCE?
EASE OF MODEL INSTALLATION ON UNIVAC? Presently in process of being setup to run on the UNIVAC 110.
EASE OF MODEL MAINTANANCE? Relatively easy.
OUTPUT INTERPRETATION REQUIREMENTS? Average.

OPERATION:

CORE REQUIREMENTS? 176K bytes (for 6 chemical constituents).
ON LINE STORAGE REQUIREMENTS? None.
COMPUTATIONAL TIME REQUIREMENTS? No timing information available. Would depend upon number of chemical species, sources and plume increments.
INPUT DATA PREPARATION TIME REQUIREMENTS? 4 hours.
OTHER HARD WARE REQUIREMENTS? 2 tape drives.

REFERENCES FOR STRAM MODEL:

Hales, J. M., Powell, D.C., and T.D. Fox, 1977, "STRAM - An Air Pollution Model Incorporating Non-linear Chemistry, Variable Trajectories and Plume Segment Diffusion", EPA-450/3-77-012.

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
4. TITLE AND SUBTITLE A REVIEW OF REGIONAL-SCALE AIR QUALITY MODELS FOR LONG DISTANCE DISPERSION MODELING IN THE FOUR CORNERS REGION		5. REPORT DATE October 1977 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) John A. Nuber, Arthur Bass, Michael T. Mills, and Charles S. Morris		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Environmental Research & Technology, Inc. 696 Virginia Road Concord, MA 01742		10. PROGRAM ELEMENT NO. EHE 625 C 11. CONTRACT/GRANT NO. 03-6-02-35254/NOAA Contract
12. SPONSORING AGENCY NAME AND ADDRESS Environmental Protection Agency Office of Research and Development Washington, DC 20460		13. TYPE OF REPORT AND PERIOD COVERED Contract Report 14. SPONSORING AGENCY CODE EPA-600/7

15. SUPPLEMENTARY NOTES

Performed under contract to the National Oceanic and Atmospheric Administration

16. ABSTRACT

A review of available long-range air quality transport and diffusion models has been prepared to select, modify, and apply such a model for the simulation of air quality impact associated with emissions from new energy resource development in the Four Corners area of the Western United States. Primary emphasis has been placed upon the review of models that are presently operational and currently available for use and adaptation.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
*Air Pollution *Reviews *Atmospheric Diffusion *Transport properties		13B 05B 07D 14B

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 82
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE

EPA Form 2220-1 (9-73)

☆U.S. GOVERNMENT PRINTING OFFICE: 1978-0-777-167/1259

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Research and Development
Environmental Research Information Center
Cincinnati, Ohio 45268

If your address is incorrect, please change on the above label tear off; and return to the above address.
If you do not desire to continue receiving these technical reports, CHECK HERE ☐, tear off label, and return it to the above address,

EPA-600/7-78-066