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REVIEW OF DISPERSION MODELS AND
POSSIBLE APPLICATIONS IN THE AOSERP STUDY AREA

by

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ALBERTA OIL SANDS ENVIRONMENTAL RESEARCH PROGRAM

Project ME 4.2.1

May 1979

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ABSTRACT

At the request of the Meteorology and Air Quality Technical Research Committee of AOSERP, a literature survey of existing air quality models which may have possible applications in the air quality program of the AOSERP study area was conducted. In addition to reviewing the published literature, several private companies and governmental agencies with available models were contacted as were individuals working in the field. Models which are available for review are described in terms of their applicability, scientific rigor, advantages, and disadvantages. Models which can deal with complex terrain features are recommended in applications of air quality problems in the Alberta Oil Sands.

A user's requirements survey was conducted in order to determine the extent to which existing models can meet the requirements of users. Since no single existing model can meet the requirements of all users, a hierarchy of models is recommended for air quality problems in the oil sands.

ACKNOWLEDGEMENTS

This research project ME 4.2.1 was funded by the Alberta Oil Sands Environmental Research Program, a joint Alberta-Canada research program established to fund, direct, and co-ordinate environmental research in the Athabasca Oil Sands area of northeastern Alberta.

1. INTRODUCTION

The principle objective of this research project is to conduct an extensive search of the literature to identify Air Quality Simulation Models (AQSM) suitable for diagnostic or predictive computations of ground concentration levels of pollutants. The available models are described in terms of selected characteristics that serve to identify practical scenarios for their application. This is not always an easy job since the literature is replete with applications of models to situations for which the models were not meant to apply.

No attempt is made in the present survey either to include all existing models, or to describe each model in a rigorous scientific manner. Such missing information can be obtained from the reference list of articles and reports. Sufficient information, however, is given to aid in the selection of models for the purposes of the Alberta oil sands.

Section 2 of the report describes the essential physical and mathematical principles which govern air quality simulation models. Section 3 outlines some specific details of a selected group of models. Section 4 summarizes the characteristics of some models and in Section 5, the findings of a survey on users' requirements are described. Additional information regarding the agencies that were contacted and verification of models are included in Appendices 9.1 and 9.2.

2. MODELLING APPROACHES

2.1 GENERAL

In selecting a model for the purpose of diagnosing or predicting a meteorological quantity (including pollutants), the resolution in time and space must be specified in advance. This question has not yet been considered in detail in the Alberta Oil Sands Environmental Research Program (AOSERP) study area. So far, emphasis has been put on the requirements for measurements and the need for predictions of air quality quantities. The acquired information is planned to serve as input to decision-making in plant siting, land use planning, control strategies and other important aspects of the environment. There is, therefore, a need to determine the areal extent to which environmental decisions must be applied. Modelling can make a contribution in this aspect of the investigation.

Most models which have been developed to date are solutions to scale approximations of the concentration equation for pollutant mass. The solutions are adjusted to include measured physical quantities such as the widely used dispersion parameters σ_y and σ_z . The basic equation itself, for one species, is based upon the physical principle of mass conservation and can be written as:

$$\frac{\partial C}{\partial t} + \underline{V} \cdot \nabla C = \frac{\partial}{\partial x} \left(K_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial C}{\partial z} \right) + Q + R \quad (1)$$

where C denotes concentration (e.g., SO_2), \underline{V} is the three-dimensional wind velocity, Q is the source of emission rate, and R denotes chemical transformation. In addition, deposition processes (wet and dry) and reflection properties can be parameterized at the horizontal boundaries (surface). Reflection can also occur from an upper inversion lid. To parameterize deposition, data must be accumulated at the ground to estimate removal rates.

Other important processes in equation (1) are the transport ($\underline{V} \cdot \nabla C$) and the diffusion in three-dimensions, described usually

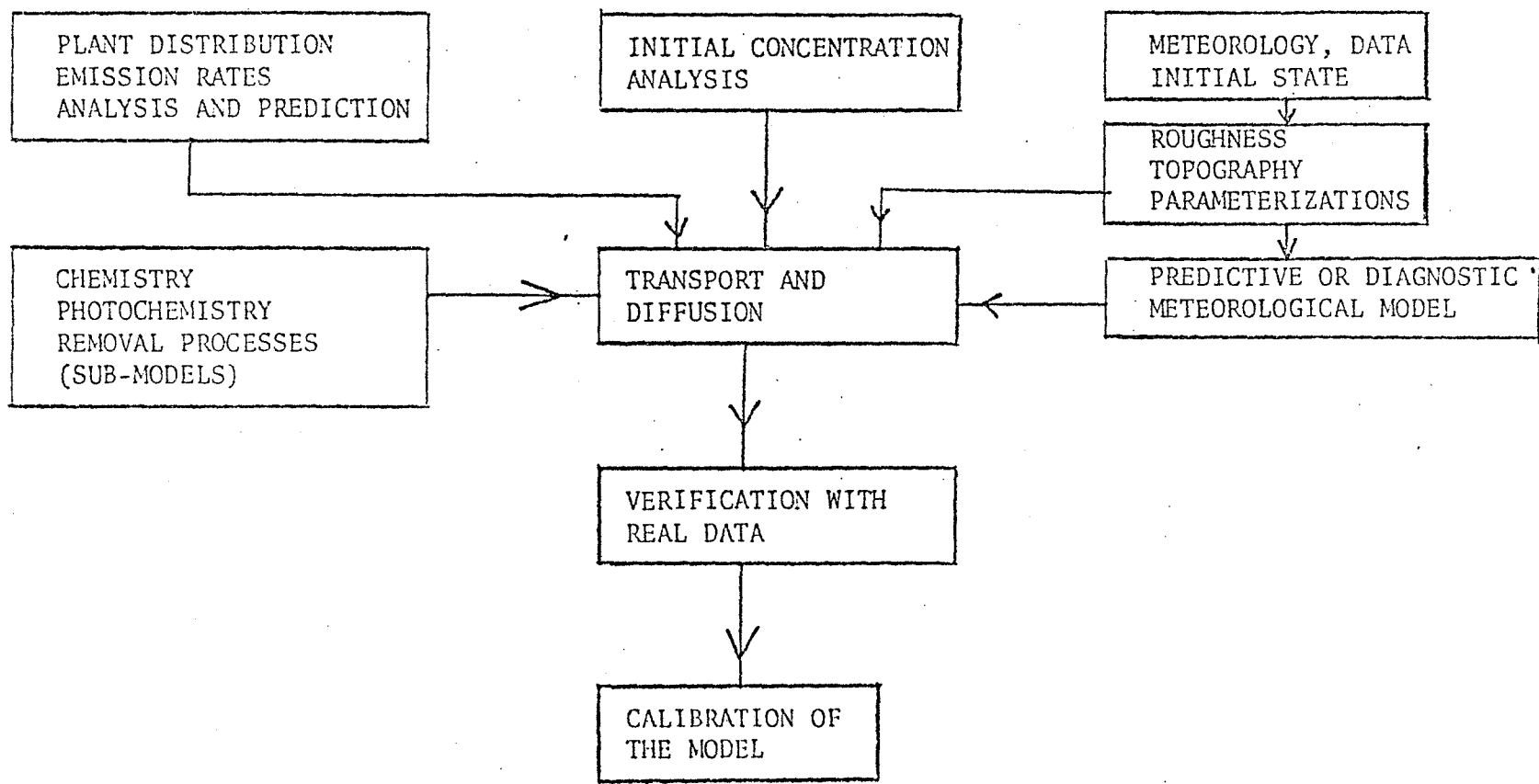


Figure 1. Essential components of an air quality simulation model.

in terms of the K-theory. Figure 1 illustrates a general approach taken in modelling. Each one of the boxes serves as a sub-model to the general model. Data are seldom available in a form required by models; the data must themselves be modelled. Thus, emission rates are frequently interpolated to time intervals required by models and meteorological fields are objectively analyzed to fill in regions of data gaps where measurements are not available. The chemistry can be linear or non-linear and must be modelled with appropriate equations and approximate reaction rates. An example of a sub-model for wet and dry deposition is given below.

2.2 WET OR DRY DEPOSITION

For the purpose of removing SO_2 and sulphates by wet deposition, daily or hourly total precipitation observations must be available. Interpolation to other specified time periods can be done. Deposition rates can then be estimated and applied in a relationship of the form,

$$\frac{C}{C_0} = \text{EXP} [-\Lambda R t] \quad (2)$$

where $C \equiv \text{SO}_2$ concentration at time t

$C_0 \equiv$ initial SO_2 concentration

$\Lambda \equiv$ wet deposition rate (hr^{-1} or $\text{mm}\cdot\text{hr}^{-1}$)

$R \equiv$ precipitation rate ($\text{mm}\cdot\text{hr}^{-1}$ of water)

$t \equiv$ time during which precipitation occurred.

In the case of dry deposition a simpler approximate formula of the form

$$\frac{C}{C_0} = \text{EXP} [-\lambda t] \quad (3)$$

is used. The parameter λ is a dry deposition rate.

The conversion of SO_2 to sulphate aerosol and other compounds and removal from the air by means of cloud droplets (rainout), falling precipitation (washout), and vegetation and soil uptake (dry deposition) is a very complex problem and only simplified forms can be included in models.

2.3 STATISTICAL FORMULATION MODELS

A modelling approach which takes exception to the solution of equation (1) is referred to in the literature as "statistical." It has not received as much attention as other approaches. This method is formulated on the basis of a regression relationship that relates time-average concentrations at a receptor to given statistical parameters. The statistics are primarily valid for the location of the collected data. The predictors can be many in number and the data analysis is usually extremely laborious. Larsen (1974) describes an examples of this type of a model. Calder (1976) encourages modifications of this approach which would lead to reduction in the data analysis.

2.4 GAUSSIAN FORMULATION

The Gaussian approach has been most widely applied to air quality problems and the literature is replete with numerous formulations of the same basic idea. It is based on a Gaussian distribution of pollutants in the stack plume. In two-dimensions, the solution to equation (1) is of the form:

$$C = \frac{Q}{2\pi\sigma_x\sigma_y U} \text{EXP} - \frac{Y^2}{2\sigma_y^2} + \frac{Z^2}{2\sigma_z^2} + \frac{\lambda X}{U} \quad (4)$$

Under the following assumptions:

1. Constant wind speed in time and space,
2. Steady state conditions, i.e., $\frac{\partial C}{\partial t} = 0$,
3. Source strength Q is constant with time,
4. Single point sources in an infinite homogeneous space,

5. No downwind diffusion in the x-direction, and
6. Chemical transformations are linear ($R=\lambda C$).

$$\sigma_y = (2K_y \frac{x}{u})^{\frac{1}{2}} \text{ standard deviation of pollutant concentration in the direction across the plume} \quad (5)$$

(K_y is y-diffusion coefficient).

$$\sigma_z = (2K_z \frac{x}{u})^{\frac{1}{2}} \text{ same as } \sigma_y \text{ but in the z-direction} \quad (6)$$

Co-ordinates (x,y,z) are with respect to the plume center-line and λ is the constant for chemical reaction rate.

The dispersion parameters σ_y , σ_z are obtained from field studies and have been widely used in the manner of Pasquill (1961) and Gifford (1961), in accordance with stability classification. In theory, these models (plume and puff models) are not applicable in regions where the meteorological parameters vary in time and space. Such variations are very important in modelling applications to complex terrain. Similarly, proper forms of σ_y and σ_z must be obtained for regions of complex terrain.

Variations of the Gaussian formula can allow for stack heights, plume rise, reflection from boundaries and overlapping contributions from many single sources. Models in this category have been developed by Turner (1964), Roberts et al. (1970), and many others.

2.5 BOX MODEL

The simplest model based on mass-conservation has been referred to as a box model. It consists of a box on an airshed. Volume flow of clean air into the box is determined by the wind speed U in the direction normal to the face area of the box A . Emission (Q) into the box is assumed to be from below and uniformly distributed. The concentration is

$$C = \frac{Q}{UA} \quad (7)$$

Other variations of the box model idea exist. An example of a box model can be found in the papers of Leahey (1976). Box models lack spatial variability.

2.6 GRID-CELL MODELS

Grid cell models can conveniently include non-uniform wind and temperature fields and complex topography. Grid-models consist of three main classes, under the names of Eulerian (fixed-cell), Lagrangian (moving-cell) and mixed Eulerian-Lagrangian (particle-in-cell or PIC). These models have the following common characteristics:

1. Can treat non-uniform meteorology, chemistry, and topography;
2. Can include time-dependence;
3. Usually utilize K-theory;
4. Can include, in principle, high scale resolution; and
5. Can include more realistic removal formulations.

Eulerian or fixed-cell models have been developed as urban or regional models to relate grid-point concentration values to area distributed emissions. The purpose of Eulerian models is to calculate concentrations of pollutants throughout a region at one time, unlike Gaussian models which do so for source by source or receptor by receptor. In practice, Eulerian models suffer from lack of data, inaccurate numerical schemes for the advection term, and large computer requirements. Their main advantage lies in the flexibility of their predictive ability where the time history of concentration amounts can be stored. Examples of fixed-co-ordinate models are the studies by Reynolds (1973) in which an elaborate effort in source inventory and chemical modelling are made, the work of Pandolfo and Jacobs (1973) where detailed meteorological parameters are predicted as well as concentration levels of carbon monoxide (CO), and the LIRAQ models of MacCracken et al. (1976).

A Lagrangian (moving cell) model considers a moving column of air mass which accepts pollutant emissions as it passes over various sources along a prescribed trajectory. The horizontal

dimensions of the column can vary from 1 m^2 to many square kilometres. The upper boundary of the column is usually the base of an inversion. The position of the column is determined by the local velocity and the time duration of travel. This approach neglects horizontal diffusion. An example of such a model is given by Eschenroeder and Martinez (1973). The main advantages of this approach are that trajectories are followed one at a time and the neglect of vertical wind shear. Lagrangian models are useful for scenarios which are source or receptor oriented. Their main advantage is the simplicity of the mathematics.

Particle-in-cell (PIC) models are a mixture of Eulerian and Lagrangian formulations. The particles within each cell are tracked in a Lagrangian manner but the centre of mass in each cell is defined (based on the number of particles) in a Eulerian manner. This approach has the versatility of Eulerian methods and the simplicity of Lagrangian mathematics.

In selecting a grid-cell model for practical applications, serious consideration must be given to computer requirements. For the purpose of regional modelling, the Eulerian approach is least costly, while for source-oriented siting the PIC approach is least costly.

3. SOME EXISTING MODELS

3.1 LAWRENCE LIVERMORE LABORATORY (LLL) MODELS

During the past few years the LLL group has developed a variety of models which are applicable to regional or source-receptor oriented scenarios. The main objective has been to develop a model which would be flexible enough to deal with the complex terrain of the San Francisco Bay region. The project has been conducted with the co-operation of the Bay Area Air Pollution Control District (BAAPCD) whose main function has been to provide necessary emission quantities.

Two currently used models at LLL are abbreviated as LIRAQ-1 and LIRAQ-2. LIRAQ-1 is utilized to simulate the distribution of inert pollutants over an airshed while LIRAQ-2 is being modified to include sulphur reactions so that it may be applied to the St. Louis (MO) area. Both models are Eulerian in the horizontal and integrated in the vertical. Worthy of mention in the LIRAQ models is the analysis routine used for the initial meteorological fields. The routine, developed by Dickerson (1975) is mass consistent and is abbreviated as MASCON. An earlier model developed by Lange (1975) is a Particle-in-Cell model (ADPIC). It utilizes the mass-consistent wind-field (MATHEW) formulation of Sherman (1975).

LLL supplies a User's Guide and is planning to hold workshops for the benefit of users.

The models which are described are LIRAQ-1, LIRAQ-2 and ADPIC. LIRAQ-2 simulated smog situations while LIRAQ-1 includes only simple chemistry.

The basis equation is:

$$\begin{aligned} \frac{\partial c}{\partial t} + \frac{\partial}{\partial x} (u C_i) + \frac{\partial}{\partial y} (v C_i) + \frac{\partial}{\partial z} (w C_i) &= \frac{\partial}{\partial x} (K_x \frac{\partial C_i}{\partial x}) & (8) \\ + \frac{\partial}{\partial y} (K_y \frac{\partial C_i}{\partial y}) + \frac{\partial}{\partial z} (K_z \frac{\partial C_i}{\partial z}) + \frac{S_i}{\rho H} \\ + R_i (C_1, \dots, C_n) \end{aligned}$$

where C_i represents concentration of species i , and K_x , K_y , and K_z are eddy diffusivity coefficients formulated in the manner of the K-theory approach. S_i represents sources and sinks. R_i denotes chemical reaction and destruction terms for species i , caused by the other species.

Equation (8) is simplified to treat only a single layer below the inversion base when calculating the horizontal layer and chemistry. The layer is bounded by the spatially dependent land surface on the bottom and a time and space varying inversion height at the top. The inversion is treated as a partially leaky lid to allow out-flux of contaminants. The inversion may intersect the topography and prevent flow across the path.

The vertically integrated model takes the form,

$$\begin{aligned}
 & \frac{\partial}{\partial t}(HC_i) - C_i(H) \frac{\partial H}{\partial t} - \frac{\partial}{\partial x}(Hu\bar{C}_i) - u(H)C_i(H) \frac{\partial H}{\partial x} \\
 & + \frac{\partial}{\partial y}(Hv\bar{C}_i) - v(H)C_i(H) \frac{\partial H}{\partial y} + wC_i|_{z_0}^H = \frac{\partial}{\partial x} [K_x \frac{\partial}{\partial y} (HC_i)] \\
 & - \frac{\partial}{\partial x} [KC_i(H) \frac{\partial H}{\partial x}] - [K_x \frac{\partial C_i}{\partial x}]_H \frac{\partial H}{\partial x} + \frac{\partial}{\partial x} [K_x \frac{\partial}{\partial y} HC_i] \\
 & - \frac{\partial}{\partial y} [KC_i(H) \frac{\partial H}{\partial y}] - [K_y \frac{\partial C_i}{\partial y}]_H \frac{\partial H}{\partial y} + [K_z \frac{\partial C_i}{\partial z}]_{z_0}^H + \frac{S_i H}{\rho} \\
 & + HR_i(C_1, \dots, C_n)
 \end{aligned} \tag{9}$$

where $H(x, y, t)$ denotes the top of the mixed layer and $K_x = K_y = K_z = K$ constant. The formulation of the horizontal eddy diffusivity coefficients is based on the principles of the similarity theory (Batchelor 1950):

$$K = A\epsilon^{1/3} \sigma^{4/3} \tag{10}$$

where

$\sigma \equiv$ root-mean square dispersion of the pollutants in a puff

$\epsilon \equiv$ energy dissipation rate

$A \equiv 0.2$ for LIRAQ

$\sigma = \Delta S = \frac{1}{2}$ grid interval, i.e., distance at which a Gaussian has dropped to $1/e$ of its centre point value.

$$\bar{\varepsilon} = 8 \times 10^{-5} \frac{1}{nH} \left(\frac{V_0}{z_0^n} \right)^3 \left[H^{3n} - z_0^{3n} \right] \quad (11)$$

$$\therefore K = 2.7 \times 10^{-2} A \frac{V_0}{z_0^n} \left[\frac{1}{nH} (H^{3n} - z_0^{3n}) \right]^{1/3} \Delta S^{4/3} \quad (12)$$

V_0 is surface velocity and z_0 is roughness length. The vertical diffusivity coefficient is:

$$K_z = \alpha u_x = 0.1 u_1 \text{ where } \alpha = 0.4 \quad (13)$$

Vertical integration requires knowledge of the vertical functional dependence of the concentration and the horizontal wind. The vertical wind profile assumed is:

$$u(x, y, z, t) = u_0(x, y, t) \left(\frac{z}{z_0} \right)^n \quad (14)$$

$$v(x, y, z, t) = v_0(x, y, t) \left(\frac{z}{z_0} \right)^n \quad (15)$$

where n depends upon stability ($n=1/7$). No turning of the wind with height is allowed. This limitation can be relaxed. The vertical concentration is assumed to be logarithmic, i.e.,

$$C_i(x, y, z, t) = a_i(x, y, t) + b_i(x, y, t) \ln \left(\frac{z}{z_0} \right) \quad (16)$$

A procedure exists for determining a_i and b_i .

Pollutant sinks which are not explicitly included in the model's chemistry are of two forms and are incorporated separately. The first is a decay term where a specified fraction of pollutants is removed at each time step. The second mechanism involves interaction with the surface. Some pollutants, such as ozone, have chemical sinks at the surface. Others such as carbon monoxide, have

biological sinks in the surface or vegetation. For these, a deposition velocity is used.

The reaction terms $\bar{R}_i(C_1, \dots, C_n)$ contain linear terms of the form $J_{ij}\bar{C}_j$ and non-linear chemistry of the form $Q_{ijk}\bar{C}_j\bar{C}_k$. The non-linear chemistry requires special mathematical treatment (19 species and 50 reactions are considered).

3.1.1 Source Terms S_i

Source emissions at or below 30 m are assumed to affect the vertical pollutant profile and are included in the surface term. Source emissions above 30 m are treated as elevated sources. Since a solution to regional air quality is sought rather than concentrations in the immediate vicinity of point sources, the elevated source emissions Q_i are assumed to affect only the vertical area concentration. Inversions below stack height are also considered to include pollutants which are trapped above the well-mixed layer.

3.1.2 Scale Considerations

The scales of interest can be as small as 1 km to about 200 km. Grid distances can be 1, 2, or 5 km. A Universal Transverse Mercator system has been used as convenient co-ordinate system. The time scale depends upon the meteorology and the temporal variations of source emissions. A time interval of 1 hour is used.

3.1.3 Data Requirements

Topography, source emission rates, initial and boundary values of pollutants, winds (velocities), inversion heights, cloud amounts, and solar radiation are required data inputs.

Horizontal wind field is specified from data and is objectively analyzed with a variational approach in the computer subroutine MASCON. The surface winds and inversion base heights at time intervals of 3 hours and space scales of 10 km are adjusted, by mass continuity in complex topography, to yield grid point values.

3.1.4 Computer Considerations

The LIRAQ-2 model has been programmed in FORTRAN IV for the CDC-7600 computer. When compiled for 20 by 20 grids, the code essentially fills the large core memory capability of the computer. Approximate running times, with a 5 km grid interval, is 60 minutes for a 24 hour simulation.

The model is programmed with independent subroutines. For example, the chemical kinetics submodel can be revised or removed without affecting significantly the transport submodel or that of meteorology.

In application to the AOSERP study area, LIRAQ-1 would have to include the chemistry of sulphur dioxide. A careful study of the manner in which point sources are included would also have to be conducted. The original intent of LIRAQ-1 was to model area sources. LIRAQ-2 includes detailed photochemistry, a feature which may have to be excluded in the first stages of the model applications.

3.2 ADPIC--ATMOSPHERIC DIFFUSION PARTICLE-IN-CELL

ADPIC is a numerical three-dimensional cartesian coordinate model. It is a time-dependent model, solved for distributions of air pollutants under many conditions. These conditions include strongly distorted advective wind fields, calm conditions, wet and dry deposition, radioactive decay, and space and time diffusion parameters. ADPIC includes short and long time scales with a good accuracy for any specified source term. No chemistry or photochemistry is included. It includes gravitational and precipitation removal effects. The initial data are objectively analyzed with a mass-consistent routine, referred to as MATHEW. The model accepts multiple sources of either a continuous or an instantaneous nature.

Each ADPIC time cycle (Δt) consists of an Eulerian and a Lagrangian part. The diffusivity velocity vector \bar{U}_O and the pseudo-velocity vector \bar{U}_D are calculated in the Eulerian part as functions of the concentration field C , the eddy diffusivity tensor and the mass-consistent regional flow field \bar{U}_A . In the Lagrangian part, the new position vector \bar{R} for each Lagrangian particle is calculated

from its old position vector and from the displacement of the particle in the pseudo-velocity vector-field. The pseudo-velocity is given by,

$$U_D = -\frac{K_x}{C} \frac{\Delta C}{\Delta x} \quad (17)$$

ADPIC was applied to argon plumes at the Savannah River Laboratory for three plume sources modelled by continuous generation of particles. The area coverage was 40 by 40 km² and the vertical dimension was 350 m. The wind field \bar{U}_A was supplied by 15 minute averaged data sets, using interpolation from the three meteorological towers. The meteorological data for wind speed direction and the turbulent intensities (sigmas) were taken at a height of 60 m from two towers and several heights up to 360 m from the third tower.

The horizontal diffusion coefficient K_H was obtained directly from σ_θ as a function of height:

$$K_H = \frac{d}{dt} (\sigma_H^2), \quad \sigma_H = \sigma_\theta |\bar{r}| b \quad (18)$$

where σ_H is the standard deviation of the plume spread, σ_θ is the angular dispersion coefficient, \bar{r} is the distance from the source, b is a constant of stability. The vertical eddy diffusion coefficient K_z is set to increase linear with height:

$$K_z = K_{z0}^+ (K_{zM}/H) Z \quad (19)$$

K_{zM} is the value at the top of the mixed layer height H .

Sensitivity studies with ADPIC indicated great sensitivity of concentrations to wind directions. For modelling plumes on a regional scale, the chief errors in ADPIC, in decreasing order of importance, seemed to depend upon wind directions, topography, diffusion parameters, source strength and wind speed. Typically, 60 percent of the time ADPIC was within a factor of 2 of the observations and 90 percent of the time it agreed to within an order of magnitude (Lange 1975).

Except for excessive computer time, ADPIC seems to be a suitable model for the AOSERP study area. Simple chemistry can be readily added to it. The most attractive feature in the Livermore models is the procedure of objective analysis of meteorological data.

3.3 CEM (PANDOLFO)--CENTRE FOR ENVIRONMENT AND MAN

Pandolfo and Jacobs (1973) have developed a combined three-dimensional meteorological and air quality model for a regional scale on a Eulerian grid. The model is fully time dependent and predicts, in a high vertical resolution boundary layer, the winds, temperature and humidity. This is in contrast to other models (e.g., Sklarew et al. 1971; Eschenroeder and Martinez 1971) which have relied upon incomplete meteorological fields, subjectively and laboriously analyzed.

The model was tested with carbon monoxide (CO) in the complex terrain situation of Los Angeles and compared with the data of 29-30 September, 1969. Forty full test situations were run. The results were favourable and the accuracy on a 10 km grid spacing was equivalent to the model of Sklarew et al. (1971). The model underestimated CO morning peak concentrations.

The simulation of a 24 hour test period takes about 20 minutes of CPU time on the University of Connecticut shared time with IBM 360/65 computer system.

The main drawback of the model is the numerical schemes which are used for the advection terms. Also, a less detailed meteorological model may be more compatible with the accuracy of the mathematics and physics and yield predictions which are not significantly different. The total model is a combined meteorological and air quality model.

The basic predictive equation of the model is:

$$\frac{\partial x_i}{\partial t} + \bar{v} \cdot \nabla x_i = \frac{\partial}{\partial z} \left\{ \left[K_i(R_i, Z) \right] \frac{\partial x_i}{\partial z} \right\} + A_i \quad (20)$$

where x_j denotes any one of the variables (u,v), T, q (humidity), and pollutant concentration and A_j represents sources and sinks. The dependence of K upon the Richardson number leads to longer computations than are traditional in K-theory models. The external parameters which drive the small scale motions (dimensions of a city) are the geostrophic wind and surface temperature which is obtained from a solution of the heat balance equation. The radiation part of the heat balance equation requires knowledge of the cloud amount. Initially, winds and temperatures must be objectively analyzed from available observations.

The upstream numerical differencing scheme was used for the advective term. The scheme suffers from numerical diffusion. For a grid network of 25x25x15 grid points and a grid distance of 2 miles, a 24 hour simulation on an IBM 360-65 requires about 5 hours at a cost of about \$1,000.

The model was applied to carbon monoxide (CO) in Los Angeles. The station network for CO was much less dense than the meteorological network. The surface meteorological network consisted of more stations than the radiosonde network. The model is designed to deal with such inadequacies in input data.

It is possible to reduce the complexity of the model without too much loss of accuracy for practical situations. Such a simplification is available in Padro (1974).

The model requires the following physical parameters: albedo, soil heat conductivity, soil specific heat, soil density, moisture parameter, and an artificial heat source (urban).

3.4 ERT (EGAN)--ENVIRONMENTAL RESEARCH AND TECHNOLOGY INC.

The model is a three-dimensional adaptation of the advection-diffusion model of Egan and Mahoney (1972a). The model is Eulerian and includes the processes of advection, diffusion, emission, chemical transformation, and deposition.

The model has been developed for the Sulfate Regional Experiment in Eastern United States (SURE) program to study the long range sulphate transport and transformation. It is presently

formulated on a grid distance of 80 km and covers a region of 2,080 km by 1,360 km in the eastern U.S. and southern Canada. It has been reported that a good correlation was obtained between model predictions and observations. For assessing alternate control strategies further developments seem to be needed in the analysis of emission inventories, meteorological fields, and reactive chemistry transformation rates. ERT has paid special attention to the formulation of a proper numerical scheme for advection.

The model deals with two types of pollutants, SO_2 and SO_4 (C_1, C_2):

$$\frac{\partial C_1}{\partial t} = -u \frac{\partial C_1}{\partial x} - v \frac{\partial C_1}{\partial y} + \frac{\partial}{\partial z} \left(K \frac{\partial C_1}{\partial z} \right) + \frac{Q}{h} - k_t C_1 \quad (21)$$

$$\frac{\partial C_2}{\partial t} = -u \frac{\partial C_2}{\partial x} - v \frac{\partial C_2}{\partial y} + \frac{\partial}{\partial z} \left(K \frac{\partial C_2}{\partial z} \right) + \frac{3}{2} k_t C_2 \quad (22)$$

Deposition is described by the boundary condition:

$$\left[K \frac{\partial C}{\partial z} \right]_{z=0} = (1-r) \bar{K} \frac{C_0}{h} \quad (23)$$

k_t - 1 to 2% per hour, transformation rate

where $r = 1 - V_d \bar{h} / \bar{K}$, a reflection coefficient

Q = emission rate

\bar{h} = mean depth of the lowest two layers

\bar{k} = mean eddy diffusivity of lowest two layers

V_d = deposition velocity

The top boundary was assumed perfectly reflecting. V_d depends upon the pollutant type, surface conditions and meteorological conditions. Lateral diffusion is neglected in the model. The model is famous for its treatment of the advective part in a non-diffusive numerical fashion. In each grid cell, the pollutant mass is conserved, as are the first and second moments of the distribution.

Emissions were classified by effective height, season and species. Emissions were allocated to the three layers depending upon the effective effluent release height. Briggs' (1969) plume rise formula was used. All ground-level point and area source emissions occur at the lowest layer to the ground.

The levels are displaced vertically parallel to the local topography. The mixing depth is allowed to vary temporally and spatially. The model specifies vertical profiles of K according to the conditions of stability.

A region of 2,080 km by 1,360 km is used with 80 km grid distance. In the vertical, three levels are used up to 1,500 km. Standard meteorological input is required every 12 hours.

In applications to the oil sands, the model would have to be modified to include complex topography, horizontal diffusion, and a smaller grid distance.

3.5 INTERA ENVIRONMENTAL CONSULTANTS LTD. (EMS)

The model is Eulerian, based upon a solution of the pseudo velocity potential in complex terrain. It is reported to apply over short length scales of the order of a few kilometres for concentration predictions for 24 hours. It is meant to replace Gaussian models which are not applicable in complex terrain.

The model was applied to a number of real situations, such as the power plants in Arizona and the EPA-sponsored tracer study in Huntington Canyon, Utah. The results of verification in the Huntington Canyon do not seem to be conclusive as they are reported from different points of view by two groups. Intera concluded, in a comparison study with the "Valley" (EPA model) model and the Southwest Energy Study group model (SWES), that the Intera model does well in estimating average concentrations and patterns, and the "Valley" model underestimates and the SWES overpredicts by an order of magnitude. On the other hand, the EPA group concluded that the Huntington data were representative for short term periods (up to one hour) and inappropriate for comparison with the 24 hour average "Valley" model predictions, and the Intera model underpredicts peak concentrations

by about an order of magnitude. The author has not been able to analyze these viewpoints in more detail. However, it may be that a potential flow in complex terrain is not sufficient to describe the wind field. The contribution due to vorticity may have to be included.

Input parameters to the Intera model are:

1. Emission rates,
2. Total flow rate,
3. Exit temperature and velocity,
4. Meteorology of vertical temperature and wind gradients,
5. Topography, and
6. Source distribution.

Intera has a wide experience in measuring and analyzing diffusion coefficients, suitable for modelling.

The model was run on a CDC 6600 and required computing time of a few seconds for a steady state case and a few minutes for a case of transient meteorological conditions.

Some of Intera's results are reproduced in Table 1.

The model is Eulerian, solved by finite difference methods and it includes chemical reactions (in a simplified form) and adsorption. The following quotation is from the comparison cited above:

Intera's Environmental Modelling System (EMS) gives numerical solutions to the three-dimensional material balances describing wind flow and pollutant diffusion. Wind flow over and around terrain is calculated using a modified form of the velocity potential equation. The modification includes inviscid potential flow above the boundary layer and height-dependent coefficients recognizing surface friction effects in the boundary layer. It is this calculation which distinguishes the model from Gaussian models and provides for the realistic treatment of terrain influences. Moreover, the calculations have been kept somewhat simple to minimize computer time, and to consider far field applications which are most common for elevated releases.

Table 1. Model comparisons for test cases of tracer releases at Garfield, Utah.

Test	Model	Ratio Calc/Obs	Logarithmic Mean Ratio
2	Numerical (INTERA)	0.90	0.82
	NOAA	0.26	0.20
	EPA	0.36	0.36
3	Numerical	0.45	0.44
	NOAA	0.35	0.26
	EPA	0.34	0.36
7	Numerical	1.5	1.25
	NOAA	1.5	0.78
	EPA	2.69	2.23

Instead of assuming normal concentration distributions in the cross wind and vertical directions, the model approximates turbulent fluctuations by a Fickian-type eddy diffusivity. These eddy properties are height dependent, as is the wind. This differs from the wind and dispersion coefficients averaged over height used in a Gaussian model or those used in a constant diffusivity model.

Winds are computed (including topography) from:

$$\nabla \cdot \bar{V} = q \quad (\text{form of } q \text{ is not given})$$

$\bar{V} \equiv$ time averaged velocity vector

$q \equiv$ source and sink volume rate per unit volume which generates winds

In terms of the velocity potential ϕ , this becomes:

$$\nabla^2 \phi = q \quad (24)$$

The modified form with viscosity is:

$$\nabla \cdot K \nabla \phi = q \quad (25)$$

Neglected in this approach is the change in wind direction with elevation which occurs in the Ekman spiral.

3.6 DIFFUSION MODEL

The basis of Intera's concentration model is the following equation:

$$\nabla \cdot K \nabla C - \bar{U} \cdot \nabla C + r = \frac{\partial C}{\partial t} + q_s + q_a \quad (26)$$

- C \equiv pollutant concentration
- K \equiv eddy diffusivity coefficient
- r \equiv chemical reaction sink
- q_s \equiv pollutant source rate
- q_α \equiv pollutant ground adsorption rate
- ∇ \equiv three dimensional del operator

Input:

1. (a) Emission strengths,
 (b) Total flow rate,
 (c) Temperature of emission, and
 (d) Exit velocity.
2. (a) Ambient air temperature,
 (b) Temperature sounding,
 (c) Wind velocity and height measurement,
 (d) Wind profile, and
 (e) Wind direction.

3.7 SHIR AND SHIEH MODEL

This is a three-dimensional Eulerian model which applies to homogeneous terrain. It accepts objectively analyzed (in space and time) dependent meteorological data. Other input parameters include the stack height, plume rise and surface roughness. Emission rates are averaged for 2 hour periods for each source according to the formulas of Turner and Edmisten (1968).

Twenty-four hour predictions of the model were verified with SO_2 data in the St. Louis area during 25 consecutive days in February 1965. The results agreed favourably with measurements for both strong and light wind conditions. The model was also applied to Venice, Italy by the Donegani Research Institute. Although the results were favourable, it was reported that they were critically dependent upon input of good wind field data.

The computer time for a 24 hour simulation on IBM 360-195 is about 5 minutes.

3.7.1 Input Data

Emission rates over a 2 hour period (obtained from 24 hour and 2 hour averages) are required. For each area source and point source the emission rates are computed from equations developed by Turner and Edmisten (1968). The following are required:

1. Stack heights of point sources, and plume rises,
2. Hourly averaged meteorological data,
3. Surface wind speeds and directions,
4. Sky cover and surface temperature, and
5. Hourly values of three meteorological stations on the periphery of the domain of integration.

Information from one tower provided wind and temperature for three height levels and two daily mixing heights (morning minimum and afternoon maximum).

The basic equation is:

$$\frac{\partial C}{\partial t} + \nabla \cdot VC = K_H \nabla_H^2 C + \frac{\partial}{\partial z} K_Z \frac{\partial C}{\partial z} + Q + R \quad (27)$$

and

$$K_Z \frac{\partial C}{\partial z} = 0 \text{ at } z = 0, H \quad (28)$$

Absorption of SO_2 by the ground is neglected (no deposition). The vertical wind profiles assumed are of the form:

$$|\bar{V}| = |V_s| (z/z_m)^P \quad (29)$$

and P is selected in accordance with Pasquill's (1974) stability classification.

In the surface layer K_Z is obtained from the similarity theory. At higher levels, the mixing length concept is used. The horizontal eddy diffusivity coefficient K_H is taken as a constant and the chemical reaction rate is linear.

The model's grid distance is 1,524 m with 30 by 40 by 14 grid points.

The modellers recommend that the monitoring sites be selected such that they are free from local influences and are representative of the ambient air quality.

3.8 ENVIRONMENTAL PROTECTION AGENCY MODEL (CRSTER)

EPA has in its possession a number of models. The one selected for discussion here is CRSTER, which is a Gaussian plume model which calculates hourly and daily SO_2 concentrations for an array of 180 receptor locations and also computes maximum daily SO_2 concentrations for a year.

The model has been extensively used by EPA to estimate air quality impact of fossil fueled steam-electric power plants. Primary emphasis has been placed on the maximum 24 hour concentration of SO_2 . The model is still undergoing further development.

CRSTER uses the following input parameters:

1. Source Related Parameters:
 - (a) Stack height,
 - (b) Stack gas temperature and exit velocity,
 - (c) Stack diameter,
 - (d) Emission rate,
 - (e) Terrain adjustments for plume height, and
 - (f) Monthly variation factors.
2. Meteorological Parameters:
 - (a) Mixing height,
 - (b) Wind speed,
 - (c) Ambient temperature and stability class, and
 - (d) Flow vector.

The model estimates SO_2 concentrations, downwind from large power plants for 1 hour and 24 hour averages, caused by emissions from single sources. The computations can be carried out for a period of a year during which identification is made of meteorological conditions associated with maxima of hourly and daily concentrations for an array of 180 receptors. Selection is made for 36 azimuths at 5 distances away from the source.

The model is Gaussian and hence requires the usual input of data. The wind speed increase with height is assumed to be:

$$u = u_0 (h/h_0)^p \quad (30)$$

where h is stack height and h_0 is the instrument level. Briggs' (1969) plume rise formula is utilized in the model.

3.9 CLIMATOLOGICAL DISPERSION MODEL (CDM)

The Climatological Dispersion Model (CDM) determines long term (seasonal or annual) pollutant concentrations at any ground-level receptor using average emission rates from point and area sources and a joint frequency distribution of wind direction, wind speed and stability for the same period.

The average concentration \bar{C}_A due to area sources at a particular receptor is given by:

$$\bar{C}_A = \frac{16}{2\pi} \int_0^{\infty} \left[\sum_{k=1}^{16} q_k(\rho) \sum_{e=1}^6 \sum_{m=1}^6 \phi(k,e,m) S(\rho,z;U_e,P_m) \right] d\rho \quad (31)$$

$k \equiv$ index for wind direction sector

$$q_k(\rho) \equiv \int Q(\rho,\theta) d\theta \quad \text{for the } k \text{ sector}$$

$Q(\rho,\theta) \equiv$ emission rate of the area source per unit area and unit time

$\rho \equiv$ distance from the receptor to an infinitesimal area source

$\theta \equiv$ angle relative to polar coordinates centered on the receptor

$e \equiv$ index for wind speed class

$m \equiv$ index for Pasquill stability category

$\phi(k,e,m) \equiv$ joint frequency function

$S(\rho,z;U_e,P_m) \equiv$ dispersion function (Gaussian)

For $\sigma_z(\rho) < 0.8L$,

$$S(\rho, 0; U_e, P_m) = \frac{2}{\sqrt{2\pi} U_e \sigma_z(\rho)} * \exp \left[-\frac{1}{2} \left(\frac{h}{\sigma_z(\rho)} \right)^2 \right] * \exp \left(-\frac{0.692\rho}{U_e T} \right) \quad (32)$$

For $\sigma_z(\rho) > 0.8L$

$$S(\rho, 0; U_e, P_m) \equiv \frac{1}{U_e L} \exp \left(-\frac{0.692\rho}{U_e T} \right) \quad (33)$$

z \equiv height of receptor above ground level

U_e \equiv representative wind speed

P_m \equiv Pasquill stability category

σ_z \equiv vertical dispersion function

h \equiv effective stack height of source distribution

L \equiv afternoon mixing height

T \equiv half life of pollutant

The term $\exp \left(-\frac{0.692\rho}{U_e T} \right)$ represents removal by physical or chemical processes.

For point sources the average concentration \bar{C}_ρ due to n point sources is given by

$$\bar{C}_\rho \equiv \frac{16}{2\pi} \sum_{n=1}^n \sum_{e=1}^6 \sum_{m=1}^6 \frac{\phi(k_m, e, m) G_n S(e_n, z, U_e, P_m)}{\rho_n} \quad (34)$$

\equiv wind sector appropriate to the n^{th} point source

G_n \equiv emission rate of the n^{th} point source

ρ_n \equiv distance from the receptor to the n^{th} point source

The total concentration for the averaging period is the sum of concentrations of the point and area sources for that averaging period.

The computer program is dimensioned to accept 250 area sources and 200 point sources. Computations can be performed for any number of receptor points. There are 576 entries in the joint frequency function with 16 wind sectors, 6 wind speed classes, and 6 stability classes. Hourly meteorological data are processed and the Pasquill-Gifford stability classes are used in the following form:

$$\sigma_z(\rho) = a\rho^b \quad (35)$$

The wind profile used is of the form:

$$U(z) = U_e \left(\frac{z}{z_o} \right)^p \quad (36)$$

where p depends upon stability. For point sources z_o has been made a function of height of the stack above the ground.

Briggs' (1969) plume rise formula is used:

$$\Delta h = 1.6 F^{1/3} U^{-1} \rho^{2/3} \quad \rho \leq 3.5X^* \quad (37)$$

$$\Delta h = 1.6 F^{1/3} U^{-1} (3.5X^*)^{2/3} \quad \rho > 3.5X^* \quad (38)$$

$$X^* = 14F^{5/8} \quad \text{if} \quad F \leq 55 \quad (39)$$

$$F = gV_s R_s^2 \left[\frac{(T_s - T_a)}{T_s} \right], \text{ buoyancy flux parameter} \quad (40)$$

$$X^* = 34F^{2/5} \quad \text{if} \quad F > 55 \quad (41)$$

V_s = exit velocity

R_s = radius of stack

U = wind speed at the stack height

Afternoon and nocturnal mixing heights are needed. The hourly atmospheric stability category P_m is based on ground-level meteorological observations only (surface wind speed, cloud amount and height), supplemented by solar elevation data.

3.10 ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL) MODELS (GIFFORD AND HANNA)

The Atmospheric Turbulence and Diffusion Laboratory (ATDL) had developed a number of different models in the past few years. It is now embarking on developing Eulerian models suitable for complex pollution scenarios.

Among the simpler models at ATDL is the one developed by Gifford and Hanna, which mathematically can be written as:

$$C = M \frac{Q}{U}$$

The concentration C is directly related to source Q . The proportionality factor M depends on stability and the wind U is computed from a distribution function of wind speed classes.

In this model, transport from other sources are neglected. The source is assumed to cover an area of 1 km^2 .

There exists another ATDL model, of a Gaussian nature, which has been widely used for climatological purposes (not necessary for the present report). It uses large point sources, modified to account for the frequency of time that the wind blows toward a specified sector. Input parameters are based on annual means.

3.11 WESTERN RESEARCH AND DEVELOPMENT (LEAHEY 1976)

This is a box model, applied to smooth terrain. Input parameters include velocity, stability, ambient temperature, and source characteristics.

The model was applied to New York City, Calgary, and Edmonton. All three cases verified very well with correlation

coefficient of about 0.8.

The model is simple and inexpensive to run. It is meant to apply to small scale lengths of a few kilometres and short time intervals.

3.12 ACRES CONSULTING SERVICES LTD. (1975)

This model is referred to as Atmospheric Transport and Loading Model. It is a box model, developed to estimate the atmospheric loading on the Upper Great Lakes which result from major industrial centers, hundreds of kilometres away.

The model is reported to have been verified against precipitation chemistry field data. It is presently run on a GE415 computer and requires about 30 minutes per year of data.

3.13 RICHARD ANTHES AND RICHARD KEYSER

The authors' model (Anthes and Keyser 1976) is a two-dimensional PIC model for a passive contaminant. The model has the attractive feature of providing predictions of meteorological fields from a planetary boundary layer model over complex terrain. The concentration patterns in the resulting plume appear reasonable and lend credibility to the model's potential for predicting the distribution of a passive contaminant on a regional scale. No chemistry has yet been introduced into the model. The model indicates sensitivity to the meteorological fields which vary in space and time in applications to regional modelling. Since the model is two-dimensional (x-z), it does not include diffusion in the y-direction (i.e., the cross-wind flow). The model includes dry deposition. Typical errors in the total concentration for a 12 hour prediction was estimated at 10%. This error does not include errors in input meteorological data.

4. SUMMARY OF MODELS

The primary objective of the present report is to survey the existing AQSM which may have a possible application for short range (about 24 hours) predictions of pollutant concentrations in the AOSERP study area. It is hoped that, after a decision is made on the space and time scales of the pollution problems in the AOSERP study area, the survey will provide the necessary information for selecting pertinent models.

A variety of Grid-cell and Gaussian air quality simulation models have been described in this report. The models are categorized in terms of their mathematical and physical characteristics. This classification provides a framework for associating the models with various environmental scenarios. For example, in an environmental impact study for a region with geometrical dimensions of 100 km by 100 km, a suitable Eulerian or PIC model with appropriate input information may be an adequate choice. On the other hand, a study which is oriented towards a source-receptor situation along specified paths, may benefit from a trajectory or Gaussian model. Gaussian models are considered adequate for homogeneous terrain and for short distances downwind from a source.

Since the AOSERP study area is characterized by complex terrain, models which include that property are recommended. A map of the AOSERP study area is given in Figure 2. Among the outstanding features of the terrain are the Athabasca River Valley, the Birch Mountains, Stoney Mountain and Muskeg Mountain to the east of Fort MacKay.

4.1 COMPUTER COSTS

Eulerian and PIC models have the largest computer requirements. Gaussian and box models impose least demands on computers. The analysis of computer costs, as given by Nappo (1975) in Table 2 of Appendix B and the discussions of computer requirements of the individual models indicate that the cost for a 24 hour prediction could be as high as \$300 per run on a large modern computer. For

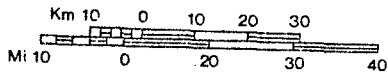
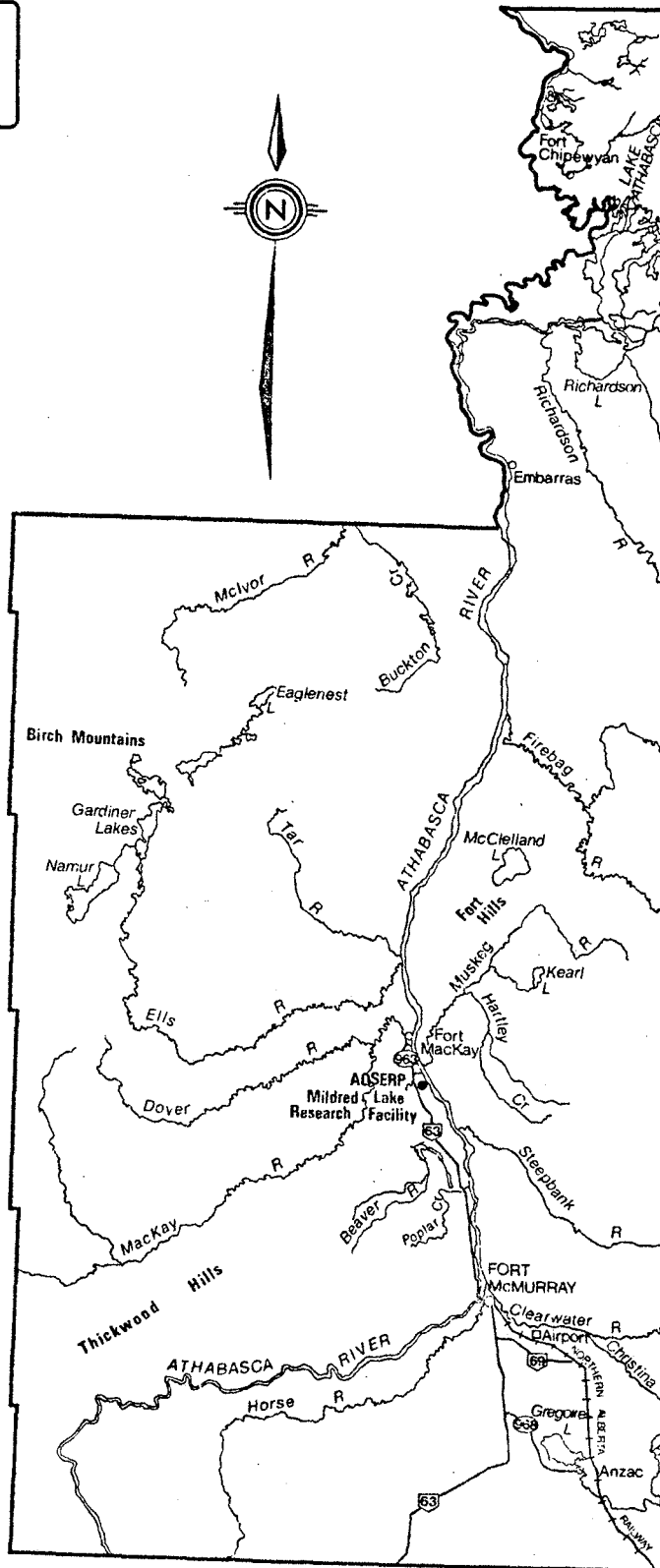
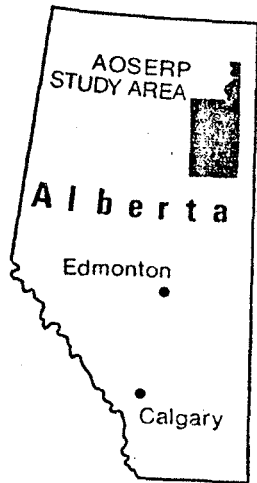


Figure 2. The Alberta Oil Sands Environmental Research Program study area.

forecast models, the annual cost of running a sophisticated Eulerian model can be estimated at \$250,000. However, for research purposes which require 30 to 40 runs per year for planning purposes, a yearly cost of \$10,000 is estimated. Gaussian models cost much less and box models may have no need for computers at all.

Models which have the flexibility of varying as many of the input parameters as possible are recommended for sensitivity studies. Sensitivity studies, although model dependent, are often used to prepare air quality impact statements. Model sensitivity can be defined as the response of model computed concentration levels to changes in input parameters. Results from such tests can be very useful for decision making processes.

4.2 METEOROLOGICAL CONSIDERATIONS

In Figure 1, the various important sub-models required in an AQSM were outlined. For real-time predictive models, the meteorological input must come from a real-time predictive meteorological model. In the case of Eulerian AQSM, the coupling must be with a planetary boundary layer model (PBL). Both models must be consistent with respect to a number of properties such as space and time resolutions. For Gaussian and box models the requirements for meteorological predictions are less demanding since local forecasts can be made available from weather offices. There are situations for which weather office forecasts may not be adequate.

If the input meteorological data come from history files, an appropriate objective analysis procedure would have to be coupled to the AQSM. Such procedures do exist in the literature. The availability of either the objective analysis routines or predictive PBL models is scarce. Pandolfo and Jacobs' (1973) model is among the few which have a coupled PBL-AQSM system of models. Other potential models are those of Pielke (1974) and Padro (1974). The latter two have not been coupled to an AQSM and require further testing for small areas.

Table 2 provides a summary of the principle characteristics of models which have been selected for discussion.

Table 2. Air quality models--summary of characteristics.

Model Agency Author	Type	General Characteristics	Scale and Resolution		Input		Advantages	Disadvantages
			Space	Time	Emission	Met		
EPA, Climatological Dispersion Model CDM	Gaussian	long term, seasonal, annual ground level concentration	regional, 1 km ²	annual seasonal	major point or area sources annual average	annual freq. dist. of wind, stability mixing ht.	simple, minimal computing time; can be expanded.	assumes steady state cannot be applied to light variable winds rough terrain
EPA, CRSTER	Gaussian	predict 1-24 hr average GLC SO ₂ , Briggs plume rise, monthly	regional and local	24 hr., monthly	point source stack data	mixing ht wind speed, T stability	predicts for 180 receptors SO ₂ included	limitations of Gaussian models
Lawrence Livermore LIRAQ 1	Eulerian	handles complex terrain	regional 200 km to 1 km ²	variable down to 1 hr.	topography source rates	wind, inversion hts	consider complex topography; can be extended to include chemistry, deposition, variable wind etc.	require space dependent data 60 min. computer time for 24 hr. simulation.
LIRAQ 2	Eulerian	similar to LIRAQ1, incorporates chemistry, photochemistry	"	"	"	"		

Table 2. Continued.

Model, Agency Author	Type	General Characteristics	Scale and Resolution		Input		Advantages	Disadvantages
			Space	Time	Emission	Met		
ADPIC	PIC	numerical 3-D mod. deposition but no chem; chem could be added	regional	short and long term	multi-source	wind - 60 m and 360 m	flexible, complete	high computer, time
Centre for Environment and man - CEM Pandolfo and Jacobs	Eulerian	urban scale Los Angeles	short range 2 miles	short term 24 hr.		albedo, Soil T, heat source	complete, can be simplified	cost to run 24 hr on IBM 360.50 \$1000
Environmental Research and Technology (ERT) Egan	Eulerian	deals with SO ₂ , SO ₄ ; good deposition Briggs plume rise	2080 x 1360 km large scale		mixing ht., season, species	13 hr.	good correlation between prediction and measured	would have to be modified to accept computer topography large scale
Intera (EMS)	Eulerian	includes chemistry can handle terrain	few km	24 hr.	flow rate temp.	T. mini-sonde wind	variable wind profile simplified equations reduce comp time	critically dependent upon good wind data short range

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continued ...

Table 2. Concluded

Model, Agency Author	Type	General Characteris- tics	Scale and Resolution		Input		Advantages	Disadvantages
			Space	Time	Emission	Met		
Shir and Shieh	Eulerian 3-D	homogeneous terrain St. Louis	small	24 hr.	stack ht plume rise roughness	2 hr data tower temp., wind	includes SO ₂	critically dependent upon good wind data
Western Research and Develop- ment	Box	smooth terrain New York, Calgary Edmonton	small - urban area average	short	source character- istics	T, wind, stability	simple, inexpensive	area average
Acres Consulting Services	Box	great lakes application	large scale regional	24 hr.	source charact- eristics	geostro- phic wind	30 min of computer time for 1 yr	
ATDC (a) Hanna-Gifford (b)	Box Gaussian	regional regional scale	regional regional	hourly	long term average	mean wind stability	simple inexpensive	cannot handle chem, terrain
Richard Anthes Richard Keyser	PIC- 2 0 X, Z axes	can handle complex terrain, chemistry dry deposition	regional			wind, stability mixing height	small error 10% in predicted values	2 - dimension model

5. USERS' REQUIREMENT SURVEY OF AIR QUALITY SIMULATION MODELS

5.1 INTRODUCTION

As part of an investigation to identify Air Quality Simulation Models (AQSM) which may be suitable for the AOSERP study area, a survey of users' requirements was conducted. The users who were interviewed are members of Alberta Environment, the Technical Research Committees of AOSERP, and Syncrude:

- J. Padro and A. Mann, conducted the interviews
- F. Burbidge, Atmospheric Environment Service
- S. Dobko, Alberta Environment
- R. Angle, Alberta Environment
- R. Hursey, AOSERP Research Manager, Vegetation Sector
- S. Brown, AOSERP Vegetation Sector
- D. Lindsay, University of Alberta, soils
- S. Malhotra, Canadian Forestry Service
- S. Sakar, Canadian Forestry Service
- P. Addison, Canadian Forestry Service
- R. Weatherill, AOSERP Research Manager, Terrestrial Fauna
- S. Djurfors, Syncrude Canada Ltd.
- D. Barton, AOSERP Aquatic Fauna Sector
- M. Lock, AOSERP Aquatic Fauna Sector
- R.K. Deeprise, Alberta Environment, Hydrology Sector
- C.R. Froelich, AOSERP Research Manager, Hydrology Sector
- B.R. Croft, Stanley Associates Engineering Ltd.

The following basic questions were discussed:

1. Types of pollutants which may be important for the model users;
2. Resolution in space and time of computations of pollutant concentrations;
3. Areal extent of the specific scientific investigations;
4. The need for real time operational predictions of pollutant concentrations; and
5. Other comments.

Discussions of the above questions were conducted in an interactive manner among the scientists who participated. It was recognized that insufficient information exists, at the present time, to assess the various factors affecting the environment of the AOSERP study area. Most of the Technical Research Committees have a clear idea of the general effects of pollutants upon the environment but would need guidance from AQSM in order to determine the extent of these effects in the area. For example, the areal extent of the influence of the various pollutants depends critically upon the local atmospheric characteristics of transport, diffusion, removal, and more generally upon chemical transformation. These can be effectively studied through the application of a suitable AQSM with appropriate data. Some of the Committees expressed the need for AQSM results to aid in the design of their experiments. Immediate needs may be satisfied with results from data and models which can be implemented reasonably quickly. These results would be considered tentative until a more comprehensive model becomes available for application.

5.2 ALBERTA ENVIRONMENT

The discussion revolved around the requirements of air quality standards and control. Alberta Environment has the responsibility to control emissions and maximum permissible concentrations of air contaminants in the ambient air.

5.2.1 Types of Pollutants

At the present time provincial regulations exist for the following pollutants: sulphur dioxide, hydrogen sulphide, nitrogen dioxide, carbon monoxide, oxidants, suspended particulates, and dustfall. It is expected that this list will increase as more is learned about the local environment. For example, it is recognized that some of the precursors of photochemical smog do exist in the oil sands. If photochemical reactions are significant, then the product species may be of concern.

5.2.2 Time and Space Scales

Values of ambient air concentrations must be known for averaging times of 0.5 hour, 1 hour, and 24 hours to protect against violations of the provincial regulations of maximum permissible concentration amount in the ambient air. However, the licence-to-operate issued to an industrial facility may stipulate maximum ambient concentrations for pollutants other than those for which a regulation exists and/or a lower level than that set out in the regulations. As more is learned about the local environment the terms and conditions of the Licence can be amended to incorporate the findings. The discussion did not clarify the exact role that a model would play in assessing ambient air concentrations in Alberta as opposed to actual measurements. It is known, however, that in locations where no stations exist, a model can be used to estimate concentrations. Also, air quality models are used to determine the stack height (and possibly the need for additional source control) required to ensure that the ambient air quality standards are met for the worst case situation.

No requirement was expressed to include horizontal and vertical resolutions of concentration amounts in models. Such details may be included in the future.

For long time scales, the requirement was expressed for frequency distributions of events. This can be studied with climatological models and may yield more information about critical seasons.

5.2.3 Areal Extent

When additional plants begin to operate in the Athabasca Oil Sands area, it may be necessary, through sensitivity studies, to trace the sources of various pollutants. This may require that the selected model have the capability of covering a linear distance of 100 km.

5.2.4 Real Time Predictions

There is at the present time no requirement for real time operational predictions of air quality parameters. This would require an elaborate station network and communication system.

5.2.5 Other Comments

Additional discussions dealt with the following requirements:

1. Chemical transformations may be important to meet the requirements of Alberta Environment. SO_2 conversion to sulphates may be most important at the present time. Concerns about acid rain are probably minimal in the AOSERP study area at this time.
2. Model guidelines are needed to design optimum station networks for various meteorological conditions; and
3. Evaluate impact of additional plants.

5.3 VEGETATION COMMITTEE

5.3.1 Types of Pollutants

Heavy metals (including vanadium, cadmium), NO_x , SO_2 , sulphuric acid, and sulphates are types of pollutants of main interest. They would like to have estimates of concentration amounts.

5.3.2 Time and Space Scales

Very little guidance exists at this time for vegetation scientists in the AOSERP study area to aid in determining high priority locations for field studies.

The time scale of greatest concern is the long term accumulation of pollutants (chronic effects, seasonal time scale), which can be estimated with a climatological model.

For shorter time scales, large dosages of pollutants in localized areas can be harmful to vegetation. The question that must be answered is the extent and frequency of such damage in the AOSERP study area.

It is suspected that, if at all important, H_2SO_4 and

and sulphates would be of concern at large distances from the sources.

5.4 TERRESTRIAL FAUNA

5.4.1 Types of Pollutants

Heavy metals, and toxic substances are pollutants of main interest.

5.4.2 Areal Extent

Snow depths determine movement of wildlife. Areal estimates of depth would be important.

In general, wildlife is not affected directly by the quality of the air. The effects depend upon the quality of the vegetation which is available for food.

The above comments indicate necessity of an areal extent of about 100 by 100 km².

5.5 SYNCRUDE CANADA LTD.

5.5.1 Types of Pollutants

NO_x, SO₂, and heavy metals (vanadium, mercury, and arsenic) are pollutants of main interest. No problem is envisaged with other particulates in view of the effective filtering mechanisms which will be in operation. No thought has yet been given to photochemistry.

5.5.2 Time and Space Scales and Areal Extent

A requirement exists for short range forecasts of episodes and fumigation events. Short range, hourly forecasts are important in planning against possible violations of provincial regulations. For longer range predictions, an areal extent of 100 km by 100 km would be adequate.

Syncrude sees the need to conduct sensitivity studies for short and long time scales in attempts to isolate various contributing effects of pollution.

5.5.3 Real Time Predictions

Syncrude intends to set up a meteorological station network which will provide adequate information for real time (short term) predictions of ground level concentrations. Such a network would also provide details of wind velocity and temperature profiles.

Additional requirements indicated the need for AQSM guidance in testing chemical and deposition rate formulations.

5.6 AQUATIC FAUNA

5.6.1 Types of Pollutants

SO₂, acid rain, sulphates, particulates (including heavy metals) and dust (wind erosion) are pollutants of main interest.

5.6.2 Time and Space Scales and Areal Extent

Short term predictions require a 24 hour maximum concentration prediction. For long term computations, snow pack accumulations of pollutants are very important.

Areal extent is estimated to cover 100 km by 100 km, depending on results from tests with models.

5.6.3 Other Comments

Isopleths of pollutant concentrations available to water bodies would aid the experiments of aquatic fauna.

5.7 HYDROLOGY

5.7.1 Types of Pollutants

Sulphates, and particulates (heavy metals, and fly ash) are pollutants of main interest.

5.7.2 Time and Space Scales and Areal Extent

For long term computations, there exists a requirement for estimates of annual buildup of pollutants, particularly of heavy

metals. The northeastern lakes in the AOSERP study area have been identified as needing special attention.

5.8 STANLEY ASSOCIATES ENGINEERING LTD.

5.8.1 Types of Pollutants

SO₂, particulates, and water vapour are pollutants of main interest.

5.8.2 Time and Space Scales and Area! Extent

Short and long range, generally long term, effects for environmental impact studies, were cited as being of major interest.

5.8.3 Real Time Prediction

No specific requirement was stated.

Table 3 summarizes the results of the survey.

Table 3. Air quality--statement of interest by sector.

Agency or Sector	Albert Environment	Vegetation Committee	Terrestrial Fauna	Aquatic Fauna	Hydrology	Syncrude	Stanley Associates
Type of Pollutant	SO ₂ , H ₂ S, NO ₂ , CO, particulates, oxidants, dust-fall	SO ₂ , NO _x , SO ₄ , H ₂ SO ₄ , heavy metals (incl. V, Cd)	heavy metals toxic compounds	SO ₂ , acid rain SO ₄ particulates (incl heavy metals)dust from wind erosion	SO ₄ particulates (incl. heavy metals, fly ash)	SO ₂ , NO _x , heavy metals (incl. V, Hg, As)	SO ₂ , particulates water vapor
Nature of Impact	ambient air, surface conc. to ensure levels described in regulations are not exceeded	evaluate effect on vegetation of high conc. events, evaluate effects of buildup of sulphur and heavy metals in soil	pollutants may affect vegetation which in turn may effect habitat. Snow depth is important to animal migration patterns	changes in pH in lakes and rivers may affect plant and invertebrate species distribution. Primary production and fish may be affected	document changes in water quality of lakes and rivers, evaluate buffering capability, absorbitive capability for heavy metals	short range forecasts of fumigation events	environmental impact studies
Space Scale and resolution	100 x 100 km is satisfactory	100 x 100 km OK 4 x 4 km resolution	100 x 100 km	100 x 100 km initial interest on river basin scale	100 x 100 km	short range, also long range environmental effects	short and long range

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Continued

Table 3. Concluded

Agency or Sector	Alberta Environment	Vegetation Committee	Terrestrial Fauna	Aquatic Fauna	Hydrology	Syncrude	Stanley Associates
Time Scale and Resolution	½ hr., 1 hr., 24 hr.	short period high concentration events long term buildup	short period high concentration events seasonal averages	seasonal total sulphur deposition heavy metals	seasonal deposition over area	short term hourly forecast	generally long term
Real Time Prediction	No	No	No	No	No	Yes	No
Type of Model	CDM CRSTER LIRAQ	CDM CRSTER LIRAQ	CDM CRSTER LIRAQ	CDM CRSTER	CDM CRSTER	CRSTER LIRAQ	CRSTER

6. CONCLUSIONS

Although the intent of the present survey is to provide information from users which will aid in selecting a suitable Air Quality Simulation Model (AQSM), the results of the survey indicate that an AQSM is itself a necessary tool for providing some of the answers. The environmental problem is interactive. The results from the survey can, however, be used as a first step in selecting a model. Model users are so varied in their requirements that no one existing model can supply all the necessary information. For example, models for short term predictions are not suitable for long term predictions. It is also quite clear that to provide answers to some questions in the content of the AOSERP study area will require modifications to existing models. No existing AQSM provide answers to all air quality questions.

The survey indicates that a number of projects have a pressing need for some approximate isopleths of SO_2 concentration in the Athabasca Oil Sands area. In order to respond to this immediate need, as quickly as possible, steps must be taken to implement a simple model, while at the same time preparing the stage for a more versatile model. The latter model requires more time for adaptation to the AOSERP study area and should be capable of testing the relevance of the various pollutants, their chemical transformation, and removal rates.

7. RECOMMENDATIONS

It is recommended that the model which is selected should be sufficiently flexible to accept realistic formulations of physical processes as they become available in the AOSERP study area. To do otherwise would be a very laborious and costly approach. The property of complex terrains should be in the model at the start of the numerical simulations in order to treat properly the time and space dependent meteorological variables.

It is also recommended that two models should be considered as early as possible. One model is Gaussian, which can be implemented relatively quickly, and the other is Eulerian, which is relatively flexible. The Eulerian model can be applied to answer fundamental questions about the environment of the AOSERP study area. The Gaussian type model which will respond to some immediate requirements is the CRSTER which was developed by EPA. For more complex considerations the Eulerian type LIRAQ or ADPIC models are recommended. The following summary presents the main features of these models.

7.1 GAUSSIAN MODEL

The CRSTER model:

1. Can provide hourly and daily SO_2 concentrations, and maximum daily SO_2 concentrations;
2. Has been extensively used by EPA;
3. Includes terrain adjustments for plume height;
4. Incorporates emissions from single sources;
5. Carries out computations for a period of one year to identify meteorological conditions associated with maxima of hourly and daily concentrations for an array of 180 receptors;
6. Uses average wind from the vertical profile $U = U_0 (h/h_0)^P$;
7. Uses Briggs' (1969) plume rise formula;
8. Assumes the wind is constant in space (no deflection or dilution due to windshear);

9. Assumes stability is constant in space;
10. Defines dispersion parameters only for the plumes, and gives consideration to turbulence in the rest of the boundary layer;
11. Lacks influence of complex terrain on meteorological variables;
12. Cannot deal with smog situations;
13. Can incorporate linear chemistry only;
14. Uses simple deposition formulations only;
15. Cannot deal with multiple inversions;
16. Is suitable for channeling situations where wind may be assumed constant; and
17. Cannot deal with "sloshing" of pollutants up and down the valley as temperature gradient between mountain and valley changes sign during day and night.

7.2

EULERIAN MODELS

The LIRAQ I and II model:

1. Can provide hourly and daily concentration values;
2. Has been used by San Francisco pollution control;
3. Is most suitable for area sources, but can deal with single sources and daily computations;
4. Assumes vertical profile of wind except when computing horizontal transport;
5. Incorporates variable wind in horizontal and integrated value in the vertical for transport processes (not for diffusion);
6. Incorporates turbulence for the whole boundary layer;
7. Is especially suitable for complex terrain since it includes terrain as a constraint in objective analysis of data (LIRAQ II is designed specifically to deal carefully with smogs [photochemistry] and can incorporate complex chemical formulations);
8. Can accept any physical formulation of depositions (when they become available);

9. Can be conveniently modified to deal with multiple inversions and can deal with channeling effects; and
10. Can include anabatic and katabatic winds to include effects of day and night situations.

The ADPIC model:

1. Is the same as LIRAQ I (no photochemistry but is flexible enough to include it);
2. Incorporates many single sources;
3. Incorporates multiple inversions;
4. Incorporates variable winds in horizontal and vertical;
5. Has good objective analysis, including complex terrain as a constraint; and
6. Is an ideal model, except that the computer time required may be large; this factor must still be discussed carefully with the appropriate agency (Livermore).

8. REFERENCES

- Acres Consulting Services Ltd. 1975. Atmospheric loadings of the Upper Great Lakes, Phase II. Acres Consulting Services, Earth Science Consultants. Ontario.
- Anthes, R., and R. Keyser. 1976. A mesoscale air quality model. Internal Report, Dep. of Meteorology, Penn. State University.
- Batchelor, G.K. 1950. The application of the similarity theory of turbulence to atmospheric diffusion. Q. J. Meteorol. Soc. 76:133.
- Bornstein, R.D. 1975. The two-dimensional URBMET urban boundary layer model. J. Appl. Meteorol. 8:1459-1477.
- Briggs, G.A. 1969. Plume rise. Atomic Energy Commission Critical Review Series TID-25075, National Technical Information Service. 81 pp.
- Calder, K.L. 1976. Empirical techniques for analyzing air quality and meteorological data. Part II, feasibility study of a source-oriented empirical air quality simulation model. Environmental Monitoring Series, EPA-600/4-76-029b. Environmental Sciences Research Laboratory, Environmental Protection Agency, Research Triangle Park, N.C. 27711.
- Dickerson, M.H. 1975. MASCON-A mass-consistent atmospheric flux model for regions with complex topography. Lawrence Livermore Laboratory. Report UCRL-76157. Rev. 1.
- Duewer, W.H., M.C. MacCracken, and J.J. Walton. 1976. The Livermore regional air quality model: II, verification and sample application in the San Francisco Bay area.
- Egan, B.A., and J.R. Mahoney. 1972a. Numerical modelling of advection and diffusion of urban area source pollution. J. Appl. Meteorol. 2:312-322.
- Egan, B.A., and J.R. Mahoney. 1972b. Applications of a numerical air pollution transport model to dispersion in the atmospheric boundary layer. J. Appl. Meteorol. 7:1023-1039.
- Eschenroeder, A.Q., and J.R. Martinez. 1973. Concepts and applications of photochemical smog models. Advan. Chem. Ser. No. 113.
- Gifford, F.A. 1961. Uses of routine meteorological observations for estimating atmospheric dispersions. Nuclear Safety 34:47-51.
- Gifford, F.A. 1974. Sensitivity of the Gaussian plume model. Atmos. Environ. 8(8):870-871.

- Heinbach, J.A., and Y. Sasaki. 1975. A variational technique for mesoscale objective analysis of air pollution. *J. Appl. Meteorol.* 2:197-203.
- Hengenson, P.L., and A.L. Morris. 1974. Forecasting the behaviour of the St. Louis, Missouri, pollutant plume. *J. Appl. Meteorol.* 8:901-909.
- Knox, B.J. 1976. Recent advances in the simulation of regional air quality. August, 1976. Lawrence Livermore Laboratory. Univ. of California.
- Lange, R. 1975. ADPIC-A three-dimensional transport diffusion model for the dispersal of atmospheric pollutants and its validation against regional tracer studies, Livermore, California.
- Larsen, R.J. 1974. An air quality data analysis system for inter-relating effects, standards and needed source reduction. *Air Pollut. Cont. Assoc.* 25(6):551-558.
- Leahey, D.M. 1976. Application of an urban air pollution model to the City of Edmonton. Western Research Development Ltd., Calgary, Alberta.
- Lebedeff, S.A., and S. Harneed. 1976. Laws of effluent dispersion in the steady-state atmospheric surface layer in stable and unstable conditions. *J. Appl. Meteorol.* 4:326-336.
- Leonard, R.E., and C.A. Federer. 1973. Estimated and measured roughness parameters for a pine forest. *J. Appl. Meteorol.* 2:302-307.
- Liu, C.Y., and W.R. Goddin. 1976. A two-dimensional model. *Atmos. Environ.* 10:513-526.
- Luna, R.E., and H.W. Church. 1974. Estimation of long-term concentrations using a "universal" wind speed distribution. *J. Appl. Meteorol.* 8:910-916.
- MacCracken, M.C., D.J. Whebbles, J.J. Walton, W.H. Duewer, and K.E. Grant. 1976. The Livermore regional air quality model: I, concept and development. October 1976.
- Marziano, G.I., A. Sutera, L. Gianolio, and M. Cipriano. 1976. Further developments in the application of Shir's model to the Venice area. G. Donegani Research Institute, Montedison S.P.A., Novara, Italy.
- McElroy, J.L. 1969. A comparative study of urban and rural dispersion. *J. Appl. Meteorol.* 1:19-31.

- Nappo, C.J. 1975. Time dependent mesoscale wind fields over complex terrain. Presented at the First Conference on Regional Mesoscale Modelling, Analysis, and Prediction. Amer. Meteorol. Soc., Las Vegas, Nevada, 6-9 May, 1975.
- Nappo, C.J. 1976. A method for evaluating the accuracy of air pollution prediction models. Proceedings of Symp. on Atmos. Diff. and Air Pollut., Santa Barbara, California.
- Neale, R.J. 1975. A comparative study of atmospheric dispersion models. Report No. 444-1, Committee on Air Quality Pollution Abatement Research, Canadian Forestry Service, Ottawa, Ontario.
- Padro, J. 1974. Forecasting in the planetary boundary layer. Proceedings of Second Annual Symp. on Forecast Research, 1974, Atmospheric Environment Service, Toronto, Ontario. 16 pp.
- Pandolfo, J.P., and C.A. Jacobs. 1973. Tests of an urban meteorological pollutant model using CO validation data in the Los Angeles metropolitan area. Vol. 1, Centre for Environment and Man, Hartford, Connecticut, 06120.
- Pasquill, F. 1961. The estimation of the dispersion of windborne material. Meteorology Magazine. 90(1063):33-49.
- Pasquill, F. 1971. Atmospheric dispersion of pollution. Q. J. R. Meteorol. Soc. 97:414.
- Pasquill, F. 1974. Atmospheric diffusion. Ellis Horwood, Chichester, U.K. 429 p.
- Peterson, E.W. 1971. Predications of the momentum exchange coefficient for flow over heterogeneous terrain. J. Appl. Meteorol. 5:958-961.
- Pielke, R.A. 1974. A three-dimensional numerical model of the sea breeze over south Florida. Monthly Weather Review. 102:115-139.
- Prahm, L.P. 1974. Comments on the background level of the summer tropospheric aerosol over Greenland and the north Atlantic Ocean. J. Appl. Meteorol. 6:730-732.
- Reynolds, S. 1973. Urban air shed photochemical simulation model study, Vol. II. User's guide and description of computer programs. Systems Applications, Inc., U.S. Environmental Protection Agency Pub. No. EPA-R4-73-030f.
- Roberts, J., E. Croke, A. Kennedy, J. Narco, and L. Conley. 1970. Chicago air pollution analysis program. Argonne National Laboratory, ANL/ES-CC-007.

- Rosen, C.L. 1977. A review of air quality modelling techniques. Lawrence Livermore Laboratory, UCID-17382.
- Rote, D.M. 1976. Current uses and requirements for air quality models. Energy and Environmental Systems Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois, 60439, U.S.A.
- Sherman, C.A. 1975. A mass-consistent model for wind fields over complex terrain. Lawrence Livermore Laboratory, Univ. of California.
- Shieh, C.M. 1972. A theoretical study of the diurnal wind variation in the planetary boundary layer. J. Atmos. Sci. 5:995-998.
- Shir, C.C. and L.J. Shieh. 1974. A generalized urban air pollution model and its application to the study of SO₂ distribution in the St. Louis Metropolitan area. J. Appl. Meteorol. 2:185-204.
- 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 application to air pollution problems. Final Report 35R-844, Systems, Science, and Software, La Jolla, California.
- Takle, E.W., R.H. Shaw, and H.C. Vaughan. 1976. Low-level stability and pollutant trapping potential for a rural area. J. Appl. Meteorol. 1:36-42.
- Turner, D.B. 1964. A diffusion model for an urban area. J. Appl. Meteorol. 3:81-83.
- Turner, D.B. 1970. Workbook of atmospheric dispersion estimates. U.S. Environmental Protection Agency, Research Triangle Park, N.C.
- Turner, D.B., and N.G. Edmisten. 1968. St. Louis SO₂ dispersion model study--description of basic data. Unpublished Report, Air Pollution office, Environmental Protection Agency, Durham, N.C.

9. APPENDICES

9.1 INPUT TO AIR QUALITY MODEL AND PROCEDURE OF THE LITERATURE SURVEY

9.1.1 Ideal Input

1. Wind field $\bar{V}(x, y, z)$,
2. Stability (clouds, time of day, and season),
3. Surface and upper air temperature T,
4. Mixing heights (at least twice daily),
5. Topography,
6. Emission rates,
7. Diffusion coefficients, and
8. Plume stack parameters (plume rise).

Included in Appendix 9.1 is a description of the approach which was taken to survey the literature of AQSM.

9.1.2 Method of Analysis

Air quality simulation models (AQSM) are being developed at a very rapid rate. This is indicated in the numerous published papers and literature survey reports which have appeared in the past few years. Such surveys are regularly updated to include new models and computational techniques. The following reports comprise a useful sample of literature surveys:

Environmental Research Laboratories, Atmospheric Turbulence and Diffusion Laboratory. 1975. 1974 Annual Report. Oak Ridge, Tennessee.

Hoffert, M.I. 1972. Atmospheric transport, dispersion and chemical reactions in air pollution. AIAA Journal, Vol. 10, No. 4.

IEC International Environmental Consultants Ltd. 1975. Comparative study of atmospheric dispersion models. Final Report to 31 October, 1975. CPAR Project Report 444-1.

- Lamb, D.V., F.I. Badgley, and A.T. Rossano. 1973. A critical review of mathematical diffusion modelling techniques for predicting air quality with relation to motor vehicle transportation. Washington State Dept. of Highways. Distributed by NTIS, U.S. Dept. of Commerce.
- Randerson, D. 1976. An overview of regional-scale numerical models. Bulletin of the Amer. Meteorol. Soc., Vol. 57, No. 7.
- Rote, D.M. N.D. A preliminary report prepared for the NATO/CCMS expert panel on air quality simulation modelling. Available from Energy and Environmental Systems Div., Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois, 60439.
- Stern, A.C., ed. 1976. Air pollution, volume 1. Environmental Sciences. An Interdisciplinary Monograph Series, Academic Press Inc., New York, San Francisco, London.

In addition to literature surveys and published reports, specific details regarding selected models were requested from companies, organizations, or individuals that appeared to have made some contribution or refinements in AQSM.

Table 4 presents a list of names and addresses of companies and individuals who were contacted and some responses from these contacts. Other papers which were included, were found in proceedings of various symposia.

Models described in the present investigation have played an important part in the following major U.S. air quality programs:

1. SURE--Sulfate Regional Experiment in eastern U.S.;
2. ETTEX--Eastern Tennessee Trajectory Experiment;
3. Los Angeles data base--mainly for photochemical smog;
4. San Francisco Bay Area--test site for complex terrain;
5. St. Louis--METROMEX;
6. NTS--Nevada test site; and
7. MAP³S--Multistate Atmospheric Power Production Pollution Study.

Table 4. Agencies under study.

NAME & ADDRESS	CONTACTED	RESPONSE	REASON FOR CONTACT	EXPERIENCE
Environmental Research & Technology (ERT) Inc., 696 Virginia Road, Concord, Mass. 01742, U.S.A.	Met at a Conference Bruch Egan	Several papers	Model deals with SO ₂ and sulfates. Good numerical schemes	was applied to SURE
Intera Environmental Consultants Ltd., 603-7th Ave. S.W., Calgary, Alberta, Canada T2P 2T5	A visit with C.C. Fortems	Letter and several papers	Wind applied to complex terrain	Huntington Canyon terrain Uta and other sites. (EPA study).
Lawrence Livermore, Radiation Laboratory, P.O. Box 808, Livermore, California 94550, U.S.A.	Letter and telephone with M.H. Dickerson	several reports	sophisticated application to complex terrain, Good wind procedure	applied to San Francisco Bay area
Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711, U.S.A.	Met at a Conference Letter to W.P. Freas	several papers User's Guide to the Models	A good organization for Gaussian models. Compute SO ₂ for 180 receptor locations	applied to many sites in the U.S. Applied to the Canal Plant of Cape Cod.
International Environmental Consultants (IEC), 333 Cavendish Boulevard, Suite 400, Montreal, P.Q. A4B 2M5				

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Continued ...

Table 4. Continued.

NAME & ADDRESS	CONTACTED	RESPONSE	REASON FOR CONTACT	EXPERIENCE
Western Research & Development, #3, 1313 - 44th Ave. N.E., Calgary, Alberta, Canada T2E GL5	Visit with and telephone D.M. Leahey	several reports	simple, low-cost box model	Applied to Calgary, Edmonton
G. Donegani, Research Institute, Montedison S.P.A. Novara, Italy	letter	two papers	another applica- tion of Shir Model	Applied to Venice, Shir applied it to St. Louis
IBM Scientific Centre, Venice, Italy	letter	a paper	example of the numerical scheme of fractional steps	
A.Q. Eschenroeder General Research Corporation, P.O. Box 3587, Santa Barbara, California 93104, U.S.A.	Indirectly	a paper	not available in the open litera- ture. Detailed photochemical model. Lagrangian	
R.C. Shlarew, Systems, Science and Software La Jolla, California, U.S.A.	Indirectly	a report	One of the original Particle- in-cell Method	SO ₂ particulates & photochem- istry
R.J. Neale, Committee on Pollution Abatement Research, Canadian Forestry Service, Ottawa, Ontario, K1A 0H3	letter	a survey report by IEC	a good survey report	

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Continued ...

Table 4. Continued.

NAME & ADDRESS	CONTACTED	RESPONSE	REASON FOR CONTACT	EXPERIENCE
Environmental Research Lab., Air Resources, Atmospheric Turbulence & Diffusion Laboratory, Oak Ridge, Tennessee, U.S.A.	letter	annual report	a variety of models and model comparisons	ETTEX
Pacific Environmental Services, Inc. 1930 14th Street Santa Monica ,CA 90404				Validation against Los Angeles data
(TRC) Research Corporation of New England, 125 Silas Dean Highway, Weathersfield, CT 06109				
R.A. Anthes, Penn. State Univ., Dept. of Meteorology, College of Earth & Mineral Sciences, 503 Deike Bldg., University Park, Penn. 16802	A visit to the university	interview and a report	Meteorologist Input and numerical scheme	sensitivity studies
H.A. Panofsky, Penn. State University	discussion at Penn. State	State of the Art of parameteriz- ation and similarity theory		

Continued ...

Table 4. Concluded.

NAME & ADDRESS	CONTACTED	RESPONSE	REASON FOR CONTACT	EXPERIENCE
J.P. Pandolfo & M.A. Atwater The Center for the Environment and Man, Inc., 275 Windsor Street, Hartford, Connecticut 06103	met at Conference	report	unique model in its prediction of the meteorolog- ical fields	applied to Los Angeles for CO.
IBM Scientific Center, Palo Alt, California 94304	letter	a paper	a model for SO ₂	applied to St. Louis SO ₂ in 1965

9.2 APPLICATION OF AIR QUALITY SIMULATION MODEL AND VERIFICATION PROCEDURES

A detailed list of possible applications of AQSM is reproduced in this Appendix from Rote (1976). This gives an idea of the types of activities in which various air quality groups are involved.

Also included is a brief analysis of model verification procedures as discussed by Nappo (1975).

9.2.1 Summary of Air Quality Model Applications

9.2.1.1 Characterization of existing air quality in multi-source area.

1. Determination of spatial and temporal air quality patterns;
2. Worst case identification;
3. Source Culpability determination:
 - a) by range of source and effect of background,
 - b) by source class or stack height, and
 - c) by geographic location (e.g., windsector);
4. Separation of anthropogenic and natural causes; and
5. Selection of clean air sites for hospitals, schools, etc.

9.2.1.2 Air quality impact analysis (sensitivity studies).

1. Existing sources;
2. Plans involving changes in existing emission patterns:
 - a) modification of existing sources,
 - b) addition of new sources,
 - c) urban expansion and development,
 - d) commercial/industrial development and expansion,
 - e) transportation system changes,
 - f) centralization of space heating facilities, and
 - g) fuel use pattern changes;
3. Government policies affecting emission patterns directly or indirectly; and

4. Review of impact statements by government officials.

9.2.1.3 The integration of air quality impact analysis and the planning process.

1. Alternative site selection--minimization of adverse impacts; and
2. Analysis of tradeoffs with other types of development.

9.2.2 Air Quality Model Verification Procedures--Nappo (1975)

In his report, Nappo (1975) provides an interesting commentary on model verification techniques. He presents a table (reproduced here as Table 5) of evaluations of the temporal characteristics of a number of models. He points out the weakness of temporal correlation coefficients which depend on time-varying parameters at individual stations. If the same verification between predictions and observations is done spatially, a different picture of a model's accuracy emerges. In fact, for the models in Table 5, a spatial verification indicated that models which verified poorly on a temporal analysis, verified quite well in a spatial analysis.

All the models, with the exception of MacCracken et al. (1971), were verified with CO data in the Los Angeles basin. MacCracken's model was applied to the San Francisco Bay area.

Table 5 also includes estimates of computer time and cost necessary to run the models on IBM 360/65.

Table 5. Model evaluation based on temporal characteristics.

Model	Average Temporal Correlation Coefficient	Computer Time for 24 Hour Prediction (min.)	Computer Cost for 24 Hour Prediction (dollars)
MacCracken et al. (1971) multi-box	0.37	106	350
24 Hour Persistence	0.47	None	None
Roth et al. (1971) primitive equation	0.52	60	200
Hanna (1973) ATDL simple model	0.60	None	None
Sklarew et al. (1972) particle-in-cell	0.65	49	160
Pandolfo and Jacobs (1973) primitive equation	0.66	20	70
Reynolds et al. (1973) primitive equation	0.73	30	100
Eschenroeder et al. (1972) trajectory	0.73	15	50
Lamb and Neiburger (1971) trajectory	0.90	35	115

10. AOSERP RESEARCH REPORTS

1. AOSERP First Annual Report, 1975
2. AF 4.1.1 Walleye and Goldeye Fisheries Investigations in the Peace-Athabasca Delta--1975
3. HE 1.1.1 Structure of a Traditional Baseline Data System
4. VE 2.2 A Preliminary Vegetation Survey of the Alberta Oil Sands Environmental Research Program Study Area
5. HY 3.1 The Evaluation of Wastewaters from an Oil Sand Extraction Plant
6. Housing for the North--The Stackwall System
7. AF 3.1.1 A Synopsis of the Physical and Biological Limnology and Fisheries Programs within the Alberta Oil Sands Area
8. AF 1.2.1 The Impact of Saline Waters upon Freshwater Biota (A Literature Review and Bibliography)
9. ME 3.3 Preliminary Investigations into the Magnitude of Fog Occurrence and Associated Problems in the Oil Sands Area
10. HE 2.1 Development of a Research Design Related to Archaeological Studies in the Athabasca Oil Sands Area
11. AF 2.2.1 Life Cycles of Some Common Aquatic Insects of the Athabasca River, Alberta
12. ME 1.7 Very High Resolution Meteorological Satellite Study of Oil Sands Weather: "a Feasibility Study"
13. ME 2.3.1 Plume Dispersion Measurements from an Oil Sands Extraction Plant, March 1976
15. ME 3.4 A Climatology of Low Level Air Trajectories in the Alberta Oil Sands Area
16. ME 1.6 The Feasibility of a Weather Radar near Fort McMurray, Alberta
17. AF 2.1.1 A Survey of Baseline Levels of Contaminants in Aquatic Biota of the AOSERP Study Area
18. HY 1.1 Interim Compilation of Stream Gauging Data to December 1976 for the Alberta Oil Sands Environmental Research Program
19. ME 4.1 Calculations of Annual Averaged Sulphur Dioxide Concentrations at Ground Level in the AOSERP Study Area
20. HY 3.1.1 Characterization of Organic Constituents in Waters and Wastewaters of the Athabasca Oil Sands Mining Area

21. AOSERP Second Annual Report, 1976-77
22. HE 2.3 Maximization of Technical Training and Involvement of Area Manpower
23. AF 1.1.2 Acute Lethality of Mine Depressurization Water on Trout Perch and Rainbow Trout
24. ME 4.2.1 Air System Winter Field Study in the AOSERP Study Area, February 1977.
25. ME 3.5.1 Review of Pollutant Transformation Processes Relevant to the Alberta Oil Sands Area
26. AF 4.5.1 Interim Report on an Intensive Study of the Fish Fauna of the Muskeg River Watershed of Northeastern Alberta
27. ME 1.5.1 Meteorology and Air Quality Winter Field Study in the AOSERP Study Area, March 1976
28. VE 2.1 Interim Report on a Soils Inventory in the Athabasca Oil Sands Area
29. ME 2.2 An Inventory System for Atmospheric Emissions in the AOSERP Study Area
30. ME 2.1 Ambient Air Quality in the AOSERP Study Area, 1977
31. VE 2.3 Ecological Habitat Mapping of the AOSERP Study Area: Phase I
32. AOSERP Third Annual Report, 1977-78
33. TF 1.2 Relationships Between Habitats, Forages, and Carrying Capacity of Moose Range in northern Alberta. Part I: Moose Preferences for Habitat Strata and Forages.
34. HY 2.4 Heavy Metals in Bottom Sediments of the Mainstem Athabasca River System in the AOSERP Study Area
35. AF 4.9.1 The Effects of Sedimentation on the Aquatic Biota
36. AF 4.8.1 Fall Fisheries Investigations in the Athabasca and Clearwater Rivers Upstream of Fort McMurray: Volume I
37. HE 2.2.2 Community Studies: Fort McMurray, Anzac, Fort MacKay
38. VE 7.1.1 Techniques for the Control of Small Mammals: A Review
39. ME 1.0 The Climatology of the Alberta Oil Sands Environmental Research Program Study Area
40. VE 7.1 Interim Report on Reclamation for Afforestation by Suitable Native and Introduced Tree and Shrub Species
41. AF 3.5.1 Acute and Chronic Toxicity of Vanadium to Fish
42. TF 1.1.4 Analysis of Fish Production Records for Registered Traplines in the AOSERP Study Area, 1970-75
43. TF 6.1 A Socioeconomic Evaluation of the Recreational Fish and Wildlife Resources in Alberta, with Particular Reference to the AOSERP Study Area. Volume I: Summary and Conclusions
44. VE 3.1 Interim Report on Symptomology and Threshold Levels of Air Pollutant Injury to Vegetation, 1975 to 1978
45. VE 3.3 Interim Report on Physiology and Mechanisms of Air-Borne Pollutant Injury to Vegetation, 1975 to 1978

46. VE 3.4 Interim Report on Ecological Benchmarking and Biomonitoring for Detection of Air-Borne Pollutant
47. TF 1.1.1 A Visibility Bias Model for Aerial Surveys of Moose on the AOSERP Study Area
48. HG 1.1 Interim Report on a Hydrogeological Investigation of the Muskeg River Basin, Alberta
49. WS 1.3.3 The Ecology of Macrobenthic Invertebrate Communities in Hartley Creek, Northeastern Alberta
50. ME 3.6 Literature Review on Pollution Deposition Processes
51. HY 1.3 Interim Compilation of 1976 Suspended Sediment Data in the AOSERP Study Area
52. ME 2.3.2 Plume Dispersion Measurements from an Oil Sands Extraction Plant, June 1977
53. HY 3.1.2 Baseline States of Organic Constituents in the Athabasca River System Upstream of Fort McMurray
54. WS 2.3 A Preliminary Study of Chemical and Microbial Characteristics of the Athabasca River in the Athabasca Oil Sands Area of Northeastern Alberta.
55. HY 2.6 Microbial Populations in the Athabasca River
56. AF 3.2.1 The Acute Toxicity of Saline Groundwater and of Vanadium to Fish and Aquatic Invertebrates
57. LS 2.3.1 Ecological Habitat Mapping of the AOSERP Study Area (Supplement): Phase I

These reports are not available upon request. For further information about availability and location of depositories, please contact:

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