Atmospheric Transport Models for Complex Terrain

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(Manuscript received 6 April 1983, in final form 26 September 1983)

ABSTRACT

Two codes, ATOMS1 and ATOMS2, have been developed to model respectively, wind fields and pollutant transport in three dimensions with particular application to complex terrain. ATOMS1 models wind fields with the use of a mass conservation error minimization principle employing available observations. ATOMS2 employs these wind fields to model transport by advection and diffusion using a Crowley second-order flux estimation. Both codes employ terrain-following vertical coordinates which provide critical resolution of the boundary layer and simplify boundary conditions at the surface. A companion paper provides three examples of models produced by the codes with comparison to observation.

1. Introduction

The modeling of pollutant transport over complex terrain is a matter of practical importance for environmental concerns of various regions of the country. We describe here several codes which have been developed and tested to model such transport. For the case studies considered, a reasonably large meteorological database is available. The codes use these data to develop self-consistent wind fields which are, in turn, used as inputs for the pollutant transport calculations. Of course, the codes can be used also for applications where complex terrain is not a factor.

Our approach has been to separate the calculations into two computer codes: the first develops a three-dimensional wind field and the second uses this wind field to compute the transport. By using terrain-following coordinates and an expanded vertical grid system in the wind field and transport codes, we insure resolution near the surface where the drainage flow occurs and where pollutants are normally concentrated. Conformal coordinates with an expanded grid system in the vertical direction not only allow improved resolution near the surface but make the application of boundary conditions more direct. On the other hand, the usual Cartesian coordinate system has to deal with a mesh that protrudes through the surface and has difficulty in increasing the resolution near the surface.

Only a brief description of the codes will be given here since a more extensive description appears in Dickerson (1980) and in Traci et al. (1978). A statistical analysis of these codes appears in a Savannah River Laboratory report (Buckner, 1981).

We solve the concentration equation utilizing eddy diffusion coefficients that are developed from observations. The advection is accomplished using a second-order explicit differencing scheme by Crowley (1968). Implicit finite-difference equations are used in the vertical direction in order to maintain a reasonable time step. Modifications of the governing equations in the terrain-following coordinates are discussed in Section 2. The wind field code (ATOMS1) is discussed in Section 3 and the advection diffusion code (ATOMS2) in Section 4. An application of these techniques in modeling pollutant transport is given in a companion paper (King and Bunker, 1984) where the details of comparisons to observations are discussed.

2. Terrain-following coordinates

The use of conformal or terrain-following coordinates, such as used in some primitive equation models (e.g., Anthes and Warner, 1978), increases the complexity of the differential equations but allows for better resolution near the surface if combined with an expanded grid system in the vertical direction. Treatment of the surface boundary conditions becomes much easier than with Cartesian coordinates. It is possible that finite element methods that assume functional fits to variables may have advantages in handling complex boundaries, but the applicability of this approach in a three-dimensional condition has not yet been substantiated (Gresho et al., 1980; Pepper and Baker, 1979).

The functional form of the transformation used in ATOMS1 is

$$\sigma = \frac{Z_{\text{top}} - Z}{Z_{\text{top}} - Z_S} = \frac{Z_{\text{top}} - Z}{\pi},$$

(1)

where $Z_S$ is the ground elevation, $Z_{\text{top}}$ the top of the computational domain, $Z$ the original vertical coordinate and $\sigma$ the transformed vertical coordinate (Fig. 1). The hydrostatic approximation ($dP/dZ = -\rho g$) gives the relationship between height $Z$ and pressure $P$. The upper boundary $Z_{\text{top}}$ is held constant.
The modification of the governing equations in the sigma-coordinate system are obtained from the rule of chain-differentiation:

\[
\begin{align*}
\left( \frac{\partial f}{\partial x} \right)_{y,z} &= \left( \frac{\partial f}{\partial x} \right)_{y,\sigma} + \frac{\sigma}{\pi} (Z_s)_x \left( \frac{\partial f}{\partial \sigma} \right)_{x,y} \\
\left( \frac{\partial f}{\partial y} \right)_{x,z} &= \left( \frac{\partial f}{\partial y} \right)_{x,\sigma} + \frac{\sigma}{\pi} (Z_s)_y \left( \frac{\partial f}{\partial \sigma} \right)_{x,y} \\
\left( \frac{\partial f}{\partial Z} \right)_{x,y} &= -\frac{1}{\pi} \left( \frac{\partial f}{\partial \sigma} \right)_{x,y}
\end{align*}
\]

where

\[(Z_s)_x = \left( \frac{\partial Z_s}{\partial x} \right)_{y,z}, \quad (Z_s)_y = \left( \frac{\partial Z_s}{\partial y} \right)_{y,z}.
\]

When these transformations are introduced into the continuity equation,

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial Z} = 0,
\]

various other partial derivatives occur, such as \(\partial^2 f/\partial x \partial y\), \(\partial^2 f/\partial x^2\), etc., that must be evaluated in order to insure that the terrain effects of channeling, blocking and the diverting of flows is correctly modeled. Discussions on the use of other conformal coordinates in meteorological codes are given by Phillips (1957), Kasahara (1974), Bleck (1978) and others.

3. Diagnostic wind fields (ATMOS1)

It is essential that mass consistency be maintained in the wind fields as developed, in order to insure that no artificial mass transport occurs in the advection-diffusion part of the calculation (ATMOS2). The technique used to solve the variational equation for the Lagrange multiplier \(\lambda\) is based on minimization of the integral,

\[
I = \int_V \left\{ \alpha_1^2[(\pi u - \pi u_0)^2 + (\pi v - \pi v_0)^2] + \alpha_2^2(\pi \tilde{w} - \pi \tilde{w}_0)^2 + \pi \tilde{w}_0 \frac{\partial \pi u}{\partial x} + \frac{\partial \pi v}{\partial y} + \frac{\partial \pi \tilde{w}}{\partial \sigma} \right\} dx, dy, d\sigma,
\]

where

\[
\tilde{w} = \frac{\sigma}{\pi} \left[ (Z_s)_x u + (Z_s)_y v \right] - w. \tag{5}
\]

A discussion of Eq. (4) is given by Sherman (1978).

The squared variation of the wind field is minimized under the constraint of nondivergence. The alphas in Eq. (4) are the Gauss precision moduli, and \(u_0\) and \(v_0\) are the components of the initial wind field. The effective velocity in the sigma-coordinate direction is \(w\) and \(w_0\), the initial vertical velocity component, is usually assumed to be zero. The method of solution uses the successive overrelaxation (SOR) technique, and convergence occurs in a reasonable number of iterations.

The procedure we use at present for developing the initial wind profiles relies on interpolation and extrapolation of the data. We normally develop the vertical profile from surrounding wind soundings. Calculated drainage-flow profiles are also used if they seem appropriate. Synoptic data may be used in the event that there are no local data available. After obtaining a vertical profile at the location of each wind station, we interpolate wind fields in the horizontal directions. The procedure is to fill the computational mesh with winds using 1/R^2 interpolations, possibly with weighting, from the vertical wind structures. Presumably, this initial wind field \((u_0, v_0\) etc.) is close to the actual wind field in the region and adjustments will be small.

As discussed by Sherman (1978) and Dickerson (1978), the \(\alpha\) in Eq. (4) are related to observational errors \(\epsilon\) through \(\alpha = \frac{\epsilon}{\pi}\). These \(\epsilon\) can be considered as deviations of the observed field from the adjusted field. In a stable atmosphere, \((\alpha_1/\alpha_2)^2\) would be small, O(10^-4), while under unstable conditions it would tend toward infinity.

4. The advection diffusion code (ATMOS2)

To resolve the distribution of concentration near the surface we have resorted to sigma coordinates with an expanded grid system only in the vertical direction. The basic equation to be solved is the concentration equation, assuming Fickian diffusion,

\[
\frac{\partial c}{\partial t} = - \frac{\partial (\pi uc)}{\partial x} - \frac{\partial (\pi vc)}{\partial y} - \frac{\partial (\pi \tilde{w} c)}{\partial \sigma} + \left[ \frac{\partial}{\partial x} \left( K_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial \sigma} \left( K_\sigma \frac{\partial c}{\partial \sigma} \right) + S \right], \tag{6}
\]
where $K_r = K_Z/\pi^2$, $\pi = Z_{top} - Z_s$ and $S$ is the source. Here, the $K$'s are the eddy diffusivities, $c$ the concentration, and $u$, $v$ and $w$ the velocity vectors as obtained from ATMOS1. In order to retain a reasonable time step, we use an implicit scheme for diffusion and advection in the sigma direction. The method of finite differencing of the flux $F$ is based on Crowley's (1968) second-order form or

$$F_{j+1/2} = \frac{\Delta t}{\Delta x} \left( \frac{\beta_{j+1/2}}{2} (c_{j+1} + c_j) - \frac{\beta_{j+1/2}^2}{2} (c_{j+1} - c_j) \right),$$  

where $\beta_{j+1/2} = u_{j+1/2} \Delta t / \Delta x$. This method is much better than standard upwind or donor cell differencing and can be improved on by the use of flux corrector techniques (Boris and Book, 1973). The uncertainty of the physical diffusion is of such a magnitude that the artificial diffusion only increases the error in known concentration by a small amount. We are conducting more studies on this question, using analytic solutions and intercomparisons with existing codes. As we improve the accuracy in the wind field determination, we may need to improve the accuracy in our advection diffusion calculation. With our present scheme, however, we have found good correlations with various observations. We have provisions for introducing time-dependent sources in selected (generally near-surface) zones. The source is centered in the computational cell while the velocities are centered in the cell surface along with the eddy diffusivities.

For the vertical diffusivities in the plume transport equation we rely on the work of Smith and Howard (1972). In this method, empirical relationships for the variance in vane direction ($\sigma_E$) and the turbulence length $L$ are used in a manner formulated by Hanna (1968). The basic equation is

$$K_Z = k u \sigma_E L,$$

where $k$ is the Von Karman constant with a value near 0.45. This formulation depends on stability class as defined by Pasquill (1974) and varies with height up to 100 m. Tables for $\sigma_E$ and $L$ are included for interpolation in the code. The relationship of the horizontal diffusivities to the vertical diffusivities is given by

$$K_h = \gamma K_Z,$$

where $\gamma$ is in a table that was derived from observations.

The code at present is quite simple. It treats advection in second order to reduce the artificial diffusion that is common in the usual "donor" cell schemes. The use of higher order schemes or the modified advection velocity scheme (depending on cell size), as devised by Lange (1978), does not seem to be needed in our complex terrain models. The estimated diffusivities we use are local, depending on the Pasquill–Gifford stability profiles and therefore, are limited to short range dispersion. They may be sufficient for a mesoscale area since transport dominates. One of our major problems for pollutant transport over complex terrain is the correct estimation of the vertical winds. The mass-consistent code develops its own vertical winds, but critically depends on the vertical profiles assumed. Measurements of the vertical winds are being analyzed at the Geyseres should help to test the assumptions used.

5. Conclusions

In general, wind fields and their subsequent use in the advection diffusion calculation result in concentration distributions which agree reasonably well with data. These results are discussed in the companion paper. We used a simple mass consistent model to obtain wind fields, since sufficient amounts of data exist. The advection diffusion calculations are performed in three dimensions. The finite difference approximation for the advection term inadvertently develops artificial diffusion (Eulerian flow). Accurate estimates of the magnitude of the artificial diffusion are hard to make. Estimates by Freeman (1976) indicate that the off-diagonal terms of the tensor diffusivity matrix can in some cases be as large as the physical diffusion coefficients used in our present simulations. Inclusion of second-order closure methods to determine diffusivities may be the next step in improving this part of our calculation. Results so far are encouraging (see the companion paper) but improvements will be necessary in order to make this procedure applicable to regional-scale pollutant transport.

Acknowledgments. The codes described rely heavily on the work by Freeman (a Los Alamos consultant), Patnaik and Philips at SAI (Science Applications, Incorporated). This work was carried out under the auspices of the U.S. Department of Energy.

REFERENCES


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