MESOSCALE NUMERICAL MODELING OF POLLUTANT TRANSPORT IN COMPLEX TERRAIN

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ABSTRACT. This paper discusses the dispersion of atmospheric pollution by synoptic-, meso- and micro-scale motions. It is shown that synoptic baroclinicity, mesoscale thermal circulations, and boundary-layer turbulence can separately, or together, act to enhance dispersion as well as substantially influence transport time of the center of mass of the polluted air. Both a mathematical description and examples of numerical model simulations are used to illustrate expected dispersion characteristics in the atmosphere. An example of an analysis for worst-case impacts of power plant plumes on U.S. National Park lands in south Florida is presented based on calculations of a regional atmospheric meteorology-dispersion modeling system.

1. INTRODUCTION

A continuous or short-term release of air pollution can be represented by the introduction to the atmosphere of a large number of infinitesimally small parcels whose motion through the air can be approximated by

$$
\begin{aligned}
x(t + \delta t) &= x(t) + u(x,y,z,t)\ \delta t \\
y(t + \delta t) &= y(t) + v(x,y,z,t)\ \delta t \qquad (1) \\
z(t + \delta t) &+ z(t) + w(x,y,z,t)\ \delta t
\end{aligned}
$$

The position of each parcel at time t is given by x(t), y(t), z(t), where δt is a time interval. The horizontal advecting velocity, $\mathbf{V} = u\mathbf{i}$

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+ vj can be expressed as $\mathbf{V}_H = \mathbf{V}_R + \mathbf{V}_D$ (Haltiner, 1971, pg. 51) where $\mathbf{V}_R$ is the rotational component of the wind ($\mathbf{V}_R = k \times \nabla\psi$) and $\mathbf{V}_D$ is the divergent component ($\mathbf{V}_D = \nabla\chi$). The total advecting velocity, (u, v, w), can also be decomposed into three components, i.e.,

$$
\begin{aligned}
u(x,y,z,t) &= u_o(x,y,z,t) + u'(x,y,z,t) + u''(x,y,z,t) \\
v(x,y,z,t) &= v_o(x,y,z,t) + v'(x,y,z,t) + v''(x,y,z,t) \\
w(x,y,z,t) &= w_o(x,y,z,t) + w'(x,y,z,t) + w''(x,y,z,t),
\end{aligned} \tag{2}
$$

which have the following definitions:

i) u_o, v_o, and w_o denote <u>synoptic-scale motion</u>. Above the planetary boundary layer u_o and v_o are close to gradient wind balance ($u_o i + v_o j \cong \mathbf{V}_R$) while within the planetary boundary layer, u_o and v_o turn towards low pressure as a result of turbulent friction decelerating the flow. The synoptic vertical velocity w_o occurs due to the frictional convergence within the planetary boundary layer, and as an atmospheric response to maintain the gradient wind balance in the absence of friction. The rotational component of the wind is usually much larger in magnitude at this scale than the divergent component ($|\mathbf{V}_R| \gg |\mathbf{V}_D|$). The "omega-equation" (Haltiner, 1971) is a mathematical representation of the vertical motion that develops in an atmosphere which is close to gradient wind balance. Motion on this scale is hydrostatic.

ii) u', v', and w' denote <u>mesoscale motion</u>. These velocities represent the residual atmospheric motions which are still in hydrostatic balance, but are not accounted for in u_o, v_o and w_o. The divergent component of the wind is significant as compared with the rotational component at this scale ($|\mathbf{V}_D| \sim |\mathbf{V}_R|$).

iii) u'', v'', and w'' denote <u>microscale motion</u>. This scale represents the nonhydrostatic motions. Pielke (1982, 1984) discusses this dynamic definition of scale separation in more detail.

In this paper, these definitions can be used to illustrate the influence of atmospheric flow on the transport and dispersion of pollution.

Dispersion is caused by diffusion (represented by u'', v'', w'' in mesoscale meteorological models) plus differential advection (resulting from values of u_o, u', v_o, v', w_o and w' which vary spatially and temporally). Thus we use the term "diffusion" to refer to the spread of pollutants due to the unresolvable part of the flow field. Note that in synoptic-scale models, diffusion would be due to both the mesoscale and microscale motions, while in large-eddy simulation models, the resolved microscale eddies would contribute to dispersion through differential advection. On the synoptic scale, to the extent that the winds are in geostrophic balance, the change of u_o and v_o with height can be estimated from (Stevens and Crum, 1986)

$$\Delta u_o = -\frac{R}{f} \ln \frac{p_1}{p_2} \frac{\partial T}{\partial y} = -\frac{g}{f} \frac{\partial(\Delta z)}{\partial y}$$

$$\Delta v_o = \frac{R}{f} \ln \frac{p_1}{p_2} \frac{\partial T}{\partial x} = \frac{g}{f} \frac{\partial(\Delta z)}{\partial x}$$

where Δz is the thickness between the two pressure surfaces, p_1 and p_2, R is the gas constant for air, f is the Coriolis parameter, and g is the gravitational constant. When $\Delta u_o \neq 0$ and/or $\Delta v_o \neq 0$, the flow is baroclinic.

As an example, if between 1000 mb and 850 mb, $\frac{\partial T}{\partial x} = \frac{\partial T}{\partial y} = -10^oC/200$ km, then in the Northern Hemisphere at about 43° of latitude (where $f \cong 10^{-4}$ sec^{-1}), $\Delta u_o \cong 23$ ms^{-1} and $\Delta v_o \cong -23$ ms^{-1}. If at 1000 mb, $u_o = v_o = 0$, then at 850 mb there would be a northwest wind of 32.5 ms^{-1}. A pollutant plume distributed initially uniformly in the vertical between 1000 mb and 850 mb would be sheared out towards the southeast. After twelve hours of such flow, the pollutants at 850 mb would have traveled 1404 km from their source point while those at 1000 mb would not have moved at all. Obviously, the concept of transport is difficult to define when a layer of pollution is smeared by baroclinically-driven wind shear.

Superimposed on this horizontal synoptic baroclinic dispersion are the diurnally varying values of u_o and v_o within the boundary layer (i.e., u_o and v_o turn less towards low pressure during the night when there is reduced turbulent coupling between the boundary layer and the free atmosphere above), and the vertical motion, w_o, which occurs in order to maintain approximate gradient wind balance.

Dispersion by mesoscale flow is somewhat more difficult to illustrate, since it does not have a quasi-balanced state as occurs on the synoptic scale. Figure 1 presents a schematic of a vertical cross section associated with one type of thermally-forced mesoscale flow - sea and land breezes. Although an idealization, several major influences of this mesoscale wind circulation on dispersion can be interpreted from this figure. If a vertically uniform column of pollution was inserted at the coastline during the mid afternoon, those parcels aloft in the return circulation would be advected seaward, whereas those in the onshore sea breeze flow would move inland. Ascent (i.e., mesoscale venting), associated with the low-level sea breeze convergence zone inland and the subsidence offshore, would result in a recirculation of the pollution back towards its source region. The influence of the Coriolis effect (not shown in the figure) would produce a turning of the winds with time, resulting in a helical path of the pollution (to the right in the northern hemisphere) as the air parcels repeatedly move onshore, upwards, offshore, and then subside to begin the circulation pattern again (as observationally verified by Lyons and Cole, 1976, and Lyons and Olsson, 1973). When a prevailing synoptic flow is superimposed on this mesoscale system, recirculation may not occur, but an ascent/descent couplet will still result.

When mesoscale organized regions of deep cumulus convection occur (e.g., mesoscale convective complexes, squall lines), a similar pattern occurs with low-level convergence of pollution, its venting aloft (in this case to high in the troposphere), and its sinking in a region removed from the region of ascent.

Microscale motion has been investigated deterministically using cumulus cloud and cloud field models (e.g., Cotton, 1987), and by applying large eddy simulation (LES) models (e.g., Deardorff, 1974, and Wyngaard and Brost, 1984). Applications to pollution dispersal, however, have often treated microscale motions statistically where u", v", and w" are selected randomly from probability density functions whose functional forms are determined from the intensity and structure of turbulence (which should include, for example, cumulus cloud motions, and internal gravity wave influences). If the probability density functions are normally distributed, assuming zero mean values, the standard deviations of the microscale velocities, i.e., $\sigma_{u''}$, $\sigma_{v''}$, $\sigma_{w''}$, are used to characterize the statistical character of the small-scale flow.

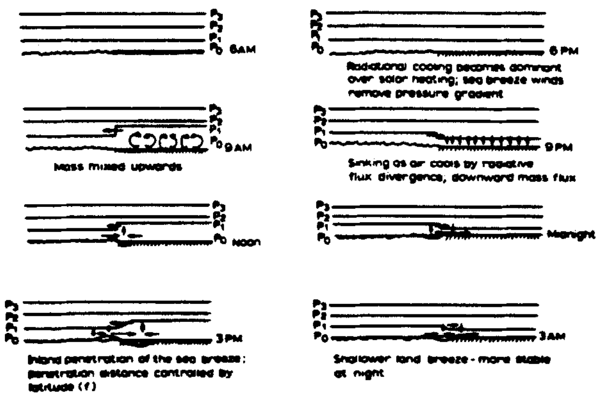

Figure 1. Schematic of the diurnal evolution of the sea and land breeze in the absence of synoptic flow (from Pielke, 1981).

The microscale flow influences synoptic and mesoscale motions directly. This can most easily be shown by writing a one-dimensional diffusion equation for velocity, i.e.,

$$\frac{\partial(V_o + V')}{\partial t} = \frac{\partial}{\partial z} K \frac{\partial(V_o + V')}{\partial z} \tag{3}$$

where K is an exchange coefficient. The term $K \frac{\partial(V_o + V')}{\partial z}$ is a representation of the influence of microscale motions on the larger scale motion. Equation (3) can be decomposed into two components (e.g., Pielke, 1974),

$$\frac{\partial V_o}{\partial t} = \frac{\partial}{\partial z} K_o \frac{\partial V_o}{\partial z}, \tag{4a}$$

$$\frac{\partial V'}{\partial t} = \frac{\partial}{\partial z} K_o \frac{\partial V'}{\partial z} + \frac{\partial}{\partial z} K' \frac{\partial V_o}{\partial z} + \frac{\partial}{\partial z} K' \frac{\partial V'}{\partial z} \tag{4b}$$

where $K_o \frac{\partial V_o}{\partial z}$ represents a large-scale (i.e., averaged) value of turbulence intensity. The remainder of the influence of microscale turbulence on larger scale motions is expressed by the right-hand side of 4b. The term $K_o \frac{\partial V_o}{\partial z}$ represents the turbulent frictional retardation on the synoptic scale mentioned earlier in this section, which causes flow within the boundary layer to turn towards low pressure. K_o represents the turbulent microscale motions generated by V_o, while K' is associated with the microscale motions caused by V'.

Further discussion of the separation of the atmospheric flow field into synoptic, mesoscale and microscale motions is presented in Pielke (1984, Chapters 4 and 7) and Pielke et al. (1986). The remainder of this paper will illustrate the influences of these scales of motion in the dispersion of pollution with results of simulations from two coupled numerical models.

2. THE METEOROLOGICAL MODEL AND THE POLLUTION DISPERSION MODEL

A mesoscale meteorological model described, for instance, in Pielke and Mahrer (1978) and McNider and Pielke (1981) can be used to obtain estimates of u_o, u', v_o, v', w_o, and w', and of the microscale (i.e., turbulence) statistical characteristics of u'', v'', and w'' for the simulated flow. This information can then be applied to represent the spread of a field of particles whose movement is described using equation (1). Values of u_o, u', v_o, v', w_o, and w' are then specified directly in the pollution dispersion (i.e., Lagrangian particle) model from the meteorological model, while u'', v'', and w'' are evaluated statistically using a Markov chain approach. This technique permits treatment of subgrid-scale diffusion on shorter time scales and smaller space scales than the K-theory advection-diffusion approach is capable of. Figure 2 illustrates schematically how this meteorology-dispersion modeling system works. A detailed description of the particle model is presented in McNider (1981), Arritt (1985) and Segal et al. (1986a).

The particle positions simulated by this modeling system represent the most likely distribution of particles (i.e., an ensemble average), since the turbulence parameterization from which they are obtained is an ensemble representation. The microscale turbulent velocity of each individual particle is not cross-correlated with any other particle; consequently this model is not applicable for relative diffusion simulations.

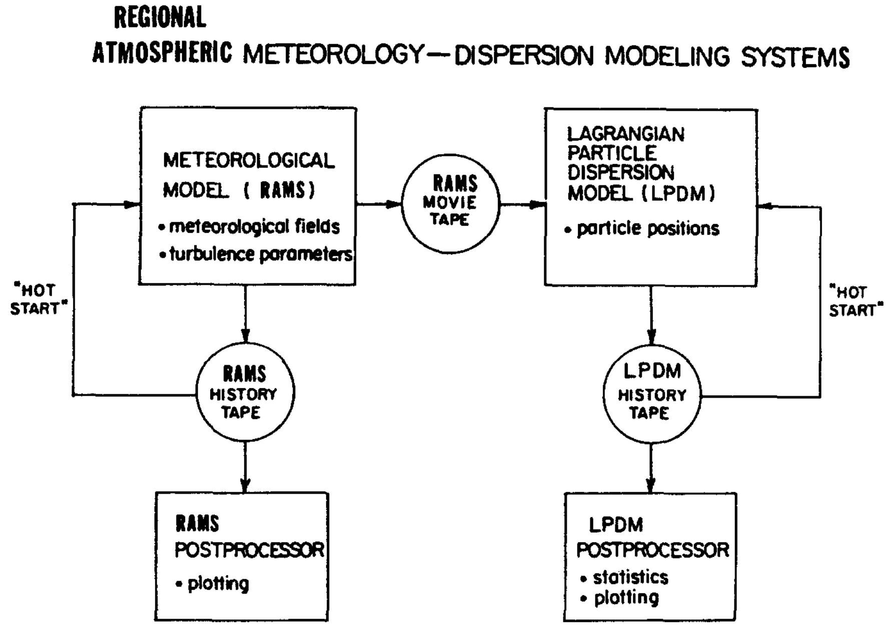

Figure 2. Two numerical models are used in combination to examine meteorological influences on pollutant transport and dispersion. This flowchart shows the logical relationships between the two numerical models and their attendant postprocessors. (From Moran et al., 1986b).

3. EXAMPLES OF MODEL SIMULATIONS

3.1 Influence of the Diurnal Heating/Cooling Cycle and Synoptic Baroclinic Effects On Dispersion

Results from a wintertime case study of the Mt. Isa smelter plume in the Northern Territory, Australia (approx. 20^{o}S latitude) are used to show the relative contributions to the dispersion of an elevated plume by the synoptic component of the wind field. Details of this study are reported in McNider et al. (1987). In the simulations shown here, the synoptic wind field was taken to be horizontally homogeneous but still possessed a complete diurnal cycle. A 7.5 ms^{-1} easterly synoptic wind was assumed. In Figure 3, the plume at 0600 LST, 42 hours after the initiation of the plume at 1200 LST two days previously, is shown for 5 separate experiments. Particles were emitted every 600 seconds in panels (a), (b) and (e), and every 100 seconds in panels (c) and (d), from a height of 300 meters.

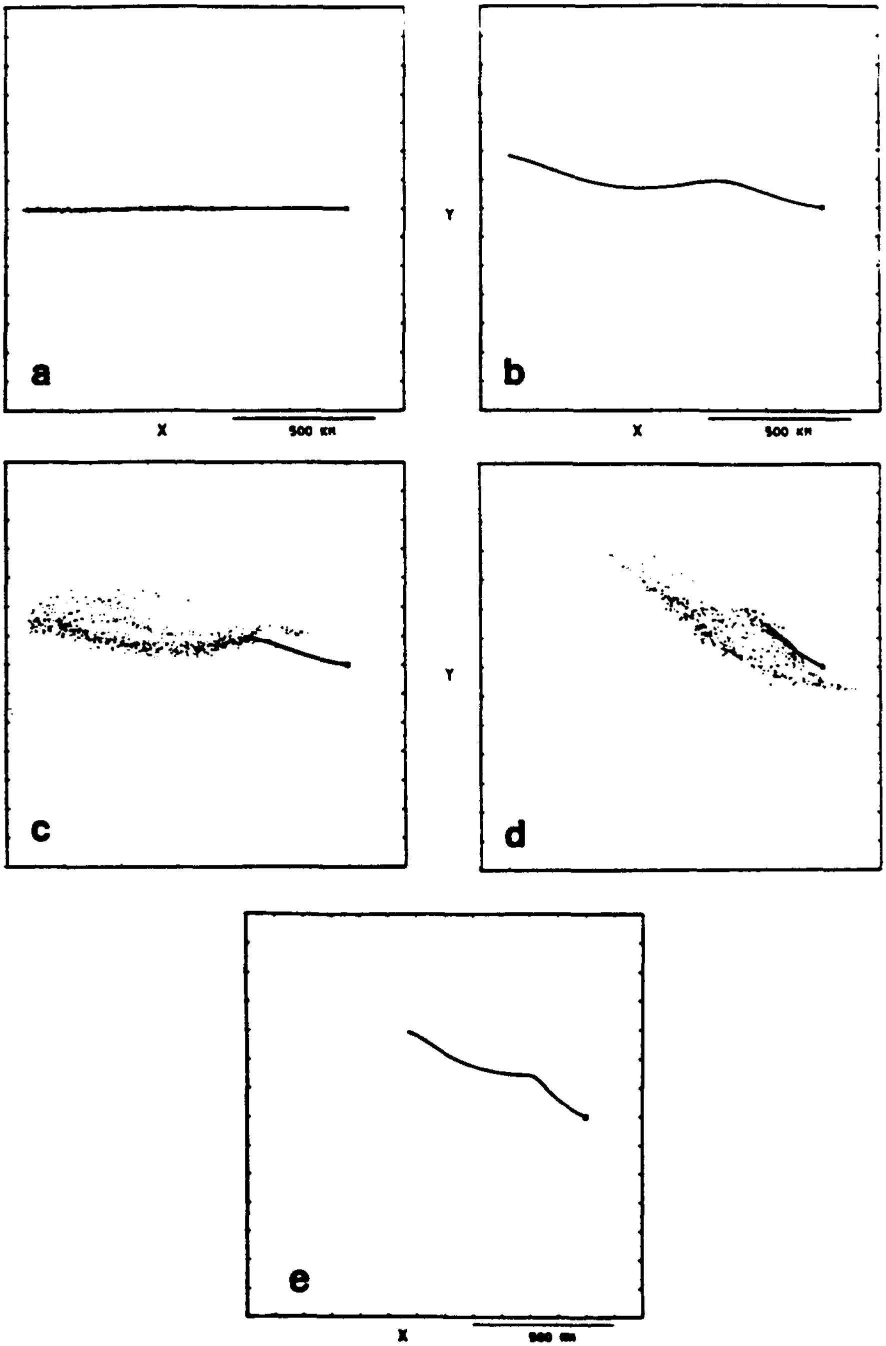

Figure 3. Model simulations (a) through (e) as defined in the text. Panels are plan views; grid spacing is 100 km in both X and Y directions.

The five simulations represent:

a) Horizontal plume diffusion due to u", v", and w" only. A steady, vertically uniform background flow was specified (i.e., $u_o = v_o$ = constant, $w_o = 0$).

b) Horizontal plume meandering due to temporal changes in u_o and v_o as a result of diurnal changes in the right side of equation 4a. Diffusion by u", v", and w" is not included (i.e, u" = v" = w" = 0).

c) Horizontal plume dispersion due to both u", v", and w" and temporal changes of u_o and v_o which result from diurnal changes in the right-hand side of equation 4a.

d) Horizontal plume dispersion when a westerly thermal wind (i.e., $\frac{\partial u_o}{\partial z}$; $\frac{\partial v_o}{\partial z}$) of about 5.5 $ms^{-1}km^{-1}$ up to 2500 meters (with an easterly geostrophic wind of 6 ms^{-1} at 300 m) is assumed. Plume diffusion due to u", v", w" is also included. Non-zero values of w" are important since vertical advection transports a parcel to a level with a different advecting velocity in this synoptic baroclinic environment.

e) Same as (d) except plume diffusion is not included (i.e., u"= v" = w" = 0).

These experiments, demonstrate i) the importance of synoptic baroclinic effects on plume dispersal, ii) the interaction of diffusion with differential transport as a result of synoptic wind shear, and iii) temporal meandering of a plume as a result of diurnal changes in coupling between the boundary layer and the free atmosphere above. A more detailed discussion may be found in McNider et al. (1987).

3.2 Influence of Mesoscale Motions on Dispersion

Using a two-dimensional version of the meteorological model with a horizontal grid interval of 5 km to simulate the thermally-forced circulations in the Lake Powell area of Utah (U.S.A.) associated with the daytime heating of elevated terrain in the summer, Segal et al. (1986a) performed a set of experiments in which an initially uniform mass of pollutant (as represented by particles in the Lagrangian particle model) was transported into the region and subsequently dispersed by the mesoscale flow. Figures 4 - 8 present one set of these simulations where the synoptic flow, u_o and v_o, is across the valley in the figures and w_o = 0. Representative meteorological fields in the simulated cross section for the nighttime (0500 LST) and daytime (1400 LST) are given in Figure 4. The geostrophic flow is from right to left in the figure at 2.5 ms^{-1}.

Of particular relevance to the interpretation of the dispersion of pollution parcels shown in Figures 5 - 8 are: i) the development of well defined regions of mesoscale ascent and descent (with velocities of up to 21 cm s^{-1}); ii) the deepening of the boundary layer up to 2.5 km by convective turbulence as illustrated by the potential temperature field; and iii) the large spatial variability in the mesoscale horizontal velocity, u'.

The dispersion of particles in Figures 5 - 8 represent the following cases:

(1) Dispersion as a result of u', v', and w' only. Transport by u_o and v_o included. Particles are released at 0900 LST (Figure 5).

(2) Dispersion as a result of u', u", v', v", w', and w". Transport by u_o and v_o is included. Particles are released at 0500 LST (Figure 6).

(3) Same as (1) except particles are released at 1100 LST (Figure 7).

(4) Same as (2) except particles are released at 2100 LST (Figure 8).

The major results of this study, as reported in more detail in Segal et al. (1986a) are i) the trapping of pollutants within the valley; ii) upward and downward venting by mesoscale ascent and descent, w'; iii) slowing of cross-valley transport from that obtained if only u_o and v_o advect the pollutants; and iv) drastically different dispersion characteristics depending on the time of day in which the pollutant particles are released. In a study reported in Moran et al. (1986a), transport times of the center of a mass of pollution across Lake Ontario were slowed up to a factor of 20%, and vertical and horizontal dispersion increased up to a factor of three (i.e., 300%) during daytime traverses of the lake.

3.3 Application of the Regional Atmospheric Meteorology Dispersion Modeling System

Segal et al. (1986b) report on the application of the modeling system with a horizontal grid interval of 11 km to estimate the worst-case impact of coastal power plant emissions in southern Florida on Everglades National Park and the Big Cypress Preserve. There is concern that excessive SO_2 levels could harm susceptible plants such as orchids within the protected areas.

Figure 9 presents a figure from the Segal et al. (1986b) report which shows (a) the simulated horizontal wind field (u_o + u', v_o + v') at 500 m; (b) the vertical velocities w_o + w' at 500 m; (c) a plan view of particle plumes from the four power plant sites; (d) a vertical cross section looking north at the four plumes; and (e) the resultant average concentration fields obtained from the particle density in the lowest 25 meters, averaged over 3 hours. Late afternoon (1600 LST) on

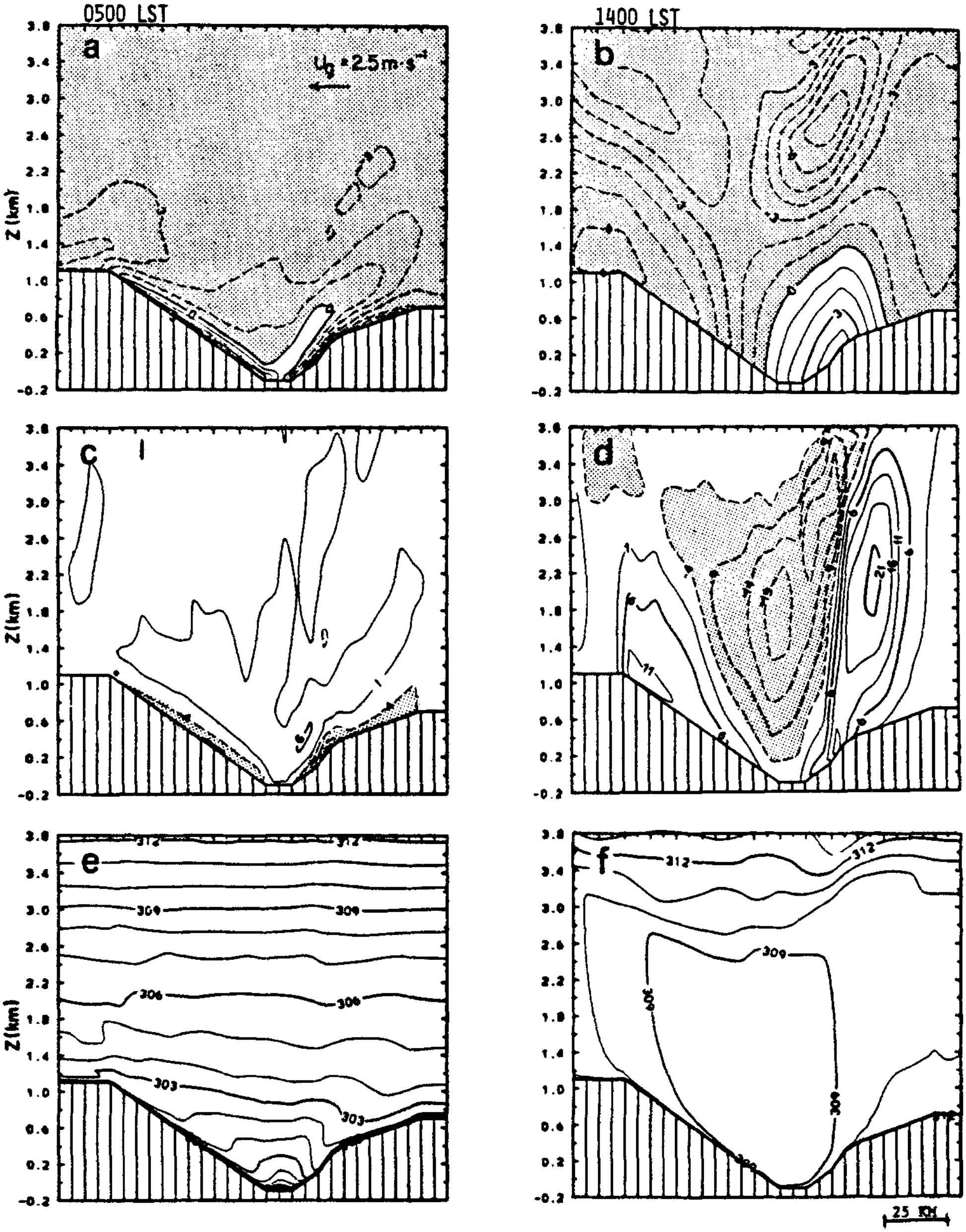

Figure 4. Simulated fields of horizontal velocity (a) and (b) in ms^{-1}; vertical velocity (c) and (d) in cms^{-1}; and potential temperature (e) and (f) in K for the Lake Powell simulation. Shading indicates negative values.

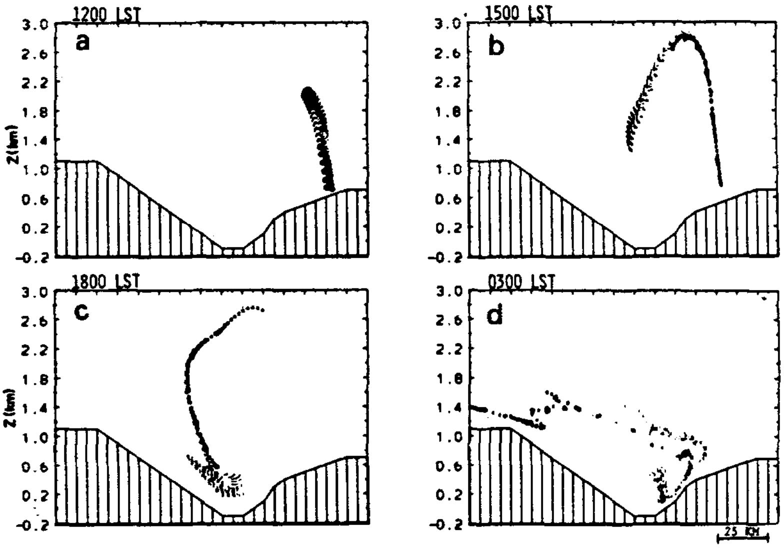

Figure 5. Described in (1) in Section 3.2.

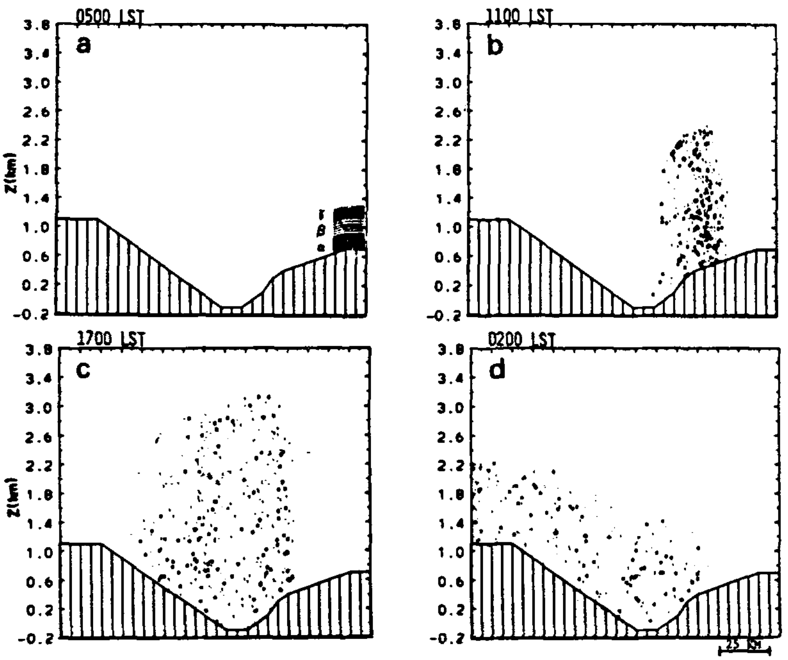

Figure 6. Described in (2) in Section 3.2.

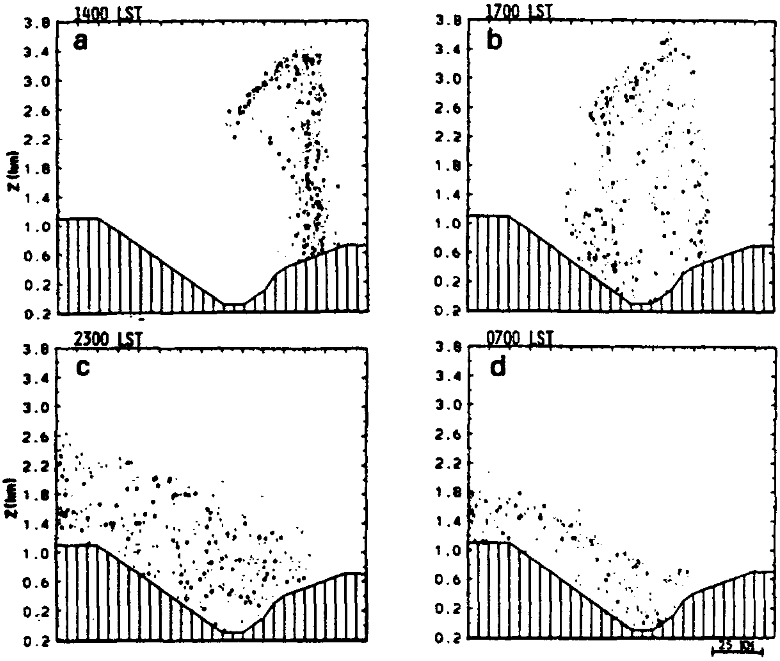

Figure 7. Described in (3) in Section 3.2.

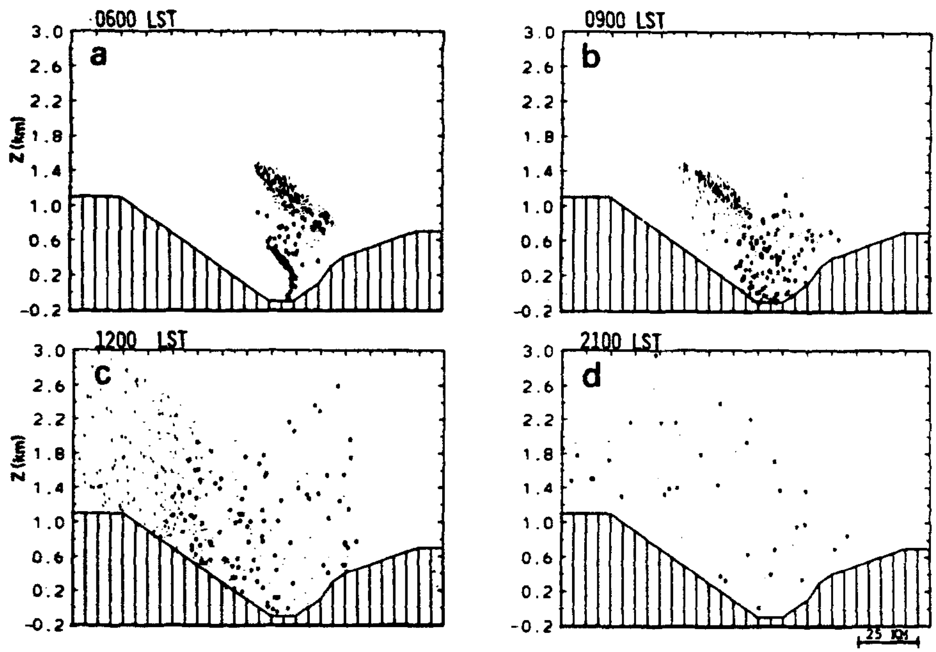

Figure 8. Described in (4) in Section 3.2.

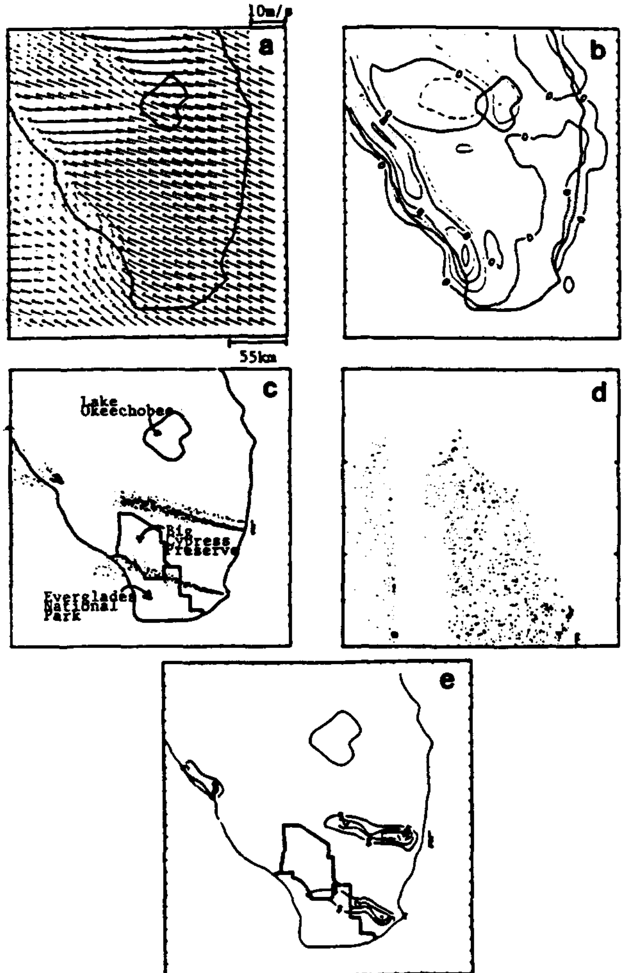

Figure 9. Results from the mesoscale meteorological and Lagrangian particle models for a summertime simulation of SO_2 transport and dispersion over the south Florida peninsula (Segal et al., 1986b). Four major elevated point sources near Miami, Fort Lauderdale, Port Everglades, and Fort Myers were considered. The prevailing synoptic wind was from just south of east at 5.8 m/s, and the horizontal grid resolution used was 11 km.

a. Horizontal wind field at approximately 500 m above sea level (1600 LST).
b. Vertical wind speed field at 500 m above sea level; contour intervals are 4 cm/s; dashed lines denote sinking motion (1600 LST).
c. Plan view of the four particle plumes at 1600 LST (release began at 0800 LST).
d. Side view looking north at the four particle plumes (1600 LST).
e. Mean three-hour-average SO_2 concentrations at ground level (1526 LST).

a summer day was chosen for this illustration. The virtual mass of each particle is weighted by the emission levels from the power plants and an effective stack height which varies diurnally based on the meteorological model output is used to input the particles.

The three-hour-average maximum ground-level concentrations predicted within the Park and Preserve at this time (about 10 ug m^{-3} of SO_2) for the 3 hours centered at 1526 LST are well below even the U.S. 24-hour SO_2 National Ambient Air Quality Standards (NAAQS) of 365 ug m^{-3}. Whether or not these low levels of SO_2 have a deleterious effect on sensitive vegetation, as well as how well observations will verify with the simulated results, of course, are questions which still remain to be answered.

4. CONCLUSIONS

In a mesoscale dispersion model, dispersion results from diffusion by microscale motions and from differential motion on the synoptic- and meso- scales. Vertical changes in horizontal wind speed and direction, and vertical motion cause differential movement of a polluted air mass. Turbulent diffusion permits pollution to move to different vertical levels and horizontal locations, thereby permitting differential advection to directly influence subsequent dispersion.

Meteorological model output of wind velocity and of turbulence intensity can be used as input to a stochastic, Lagrangian particle model in order to simulate the most-likely dispersion characteristics of a pollution plume in complex terrain. Examples of simulation results presented in this paper suggest that dispersion is enhanced by mesoscale circulations and through synoptic vertical shears of the horizontal wind. Transport rates of pollution can also be strongly influenced by mesoscale circulations.

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