The Use of a Mesoscale Numerical Model for Evaluations of Pollutant Transport and Diffusion in Coastal Regions and over Irregular Terrain

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Abstract

A modelling approach is presented that appears to have the potential to provide reliable assessments of pollution concentration in coastal zones and complex terrain, where the assumptions behind current operational air quality models often are inadequate. With the use of a numerical mesoscale model (NMM), physically consistent flow fields can be predicted, thereby providing higher spatial and temporal resolution in the meteorological fields than would be available from a limited number of observation points. These predictions are used to calculate mean trajectories of pollutant parcels, as well as to provide quantitative estimates of pollution concentration using two techniques.

One technique, most relevant for point and line sources, uses mean and fluctuating velocities as derived from the mesoscale model in order to estimate the spread of pollutant, while the second, which is applicable mainly to area sources, utilizes the advection-diffusion equation.

Considering the scarcity of meteorological observational data with adequate spatial and temporal resolution along coastal regions and in irregular terrain, the approach outlined in this paper can be supportive and complementary to the conventional observationally oriented air quality assessments. Additionally, this technique can be utilized as a guide in the estimation of the optimal spatial resolution required in applied and research-oriented air quality observation networks.

1. Introduction

The use of various forms of dispersion models (e.g., Haugen, 1975) is a routinely applied technique used to evaluate pollutant transport (AMS, 1978). Such model assessments have formed a crucial component in estimating potential concentrations of specific air pollutants due to such human activities as the construction of new industrial facilities and urbanization.

Unfortunately, techniques currently applied to evaluate air quality suffer from the availability of only sparse, and sometimes nonrepresentative, meteorological measurements, which mostly are available only immediately above the ground. Operational dispersion models, therefore, generally do not have sufficient meteorological input data and are forced to neglect features such as horizontal and vertical variations in wind direction and vertical motion. This loss of resolution is especially serious in coastal areas and over irregular terrain, where the temporal and spatial inhomogeneities of the wind and turbulence fields can be substantial (e.g., Pielke (1974); Carpenter (1979); Mahrer and Pielke (1977)) and limited observations are too sparse to resolve the local meteorologically-pertinent fields.

In this paper, we report on the development of methods that have the promise of adding realism to air quality assessments in coastal areas and complex terrain. The basis of these methods is the use of a prognostic dynamic model employing mathematical representations for the conservation of mass, momentum, heat, and water in order to simulate the land/sea or mountain/valley circulations. The observed data needed for the initialization of the dynamic model are negligible compared with the amount of data needed for the spatial and temporal observational descriptions of these circulations. The ability to use only limited data in the initialization is due to the fact that the mesoscale features simulated in this study are primarily forced by the underlying terrain.

In the examples that follow, the numerical mesoscale model (NMM) developed and improved as reported in Pielke (1974), Mahrer and Pielke (1977), Segal and Pielke (1981), and McNider (1981), is used as the dynamic model to simulate the 3-dimensional circulations. The mesoscale model usually is applied over horizontal domains of up to several hundred kilometers on a side, with grid intervals from 1 km to 10 km. With use of available observations, the accuracy of the model has been evaluated (e.g., Segal and Pielke (1981), Segal *et al.* (1982), Pielke and Mahrer (1978), and Mahrer and Pielke (1976)) and found to produce realistic simulations of mesoscale circulations. Radiosonde data from one or two sites were used in these studies for the model initialization.

Meteorological fields predicted by such a model can be used to provide refined estimates of pollution concentrations over the model domain from point, line, and area sources. The model also can be applied using a 2-dimensional spatial representation when the terrain is sufficiently uniform in one of the horizontal coordinate directions.

2. Qualitative evaluations of pollutant transport

a. Trajectory analyses over coastal areas

Figures 1–3 give examples of several meteorological fields

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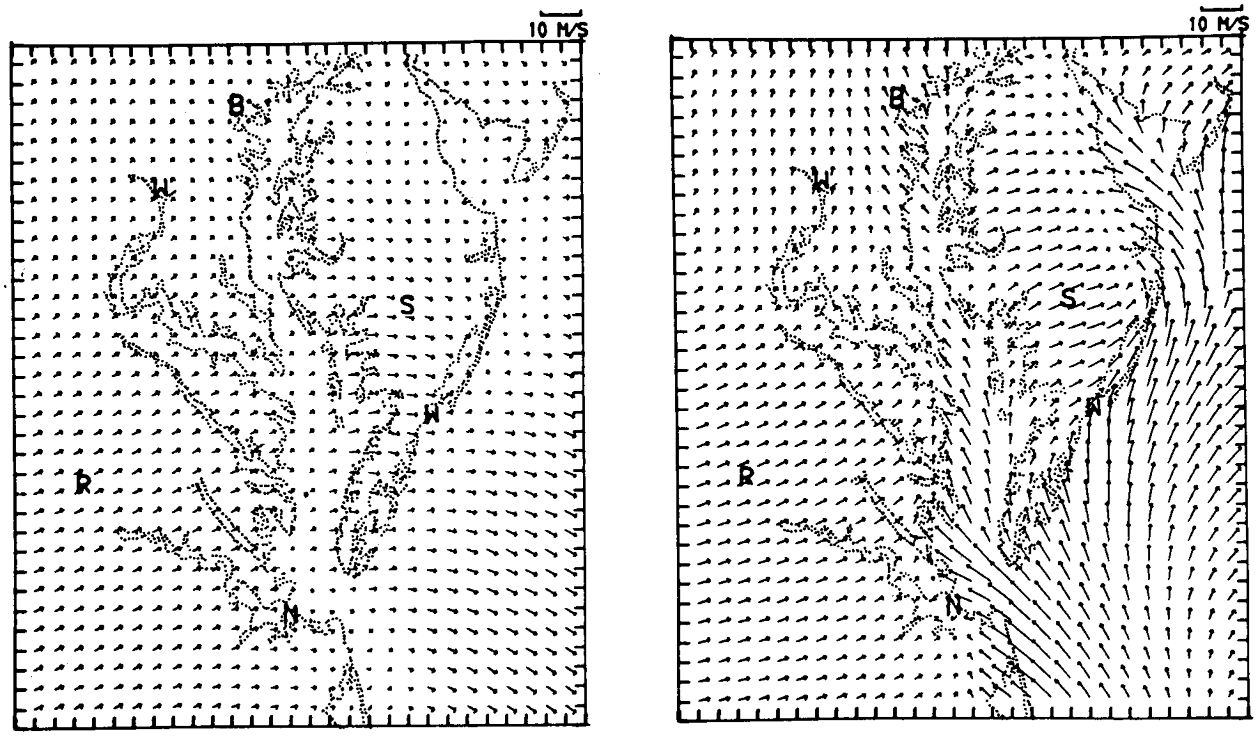

FIG. 1. The NMM predicted horizontal winds at 15 m at 0900 LST (left) and 1600 LST (right) on 21 July 1978, over the Chesapeake Bay Region (from Segal *et al.* (1982)).

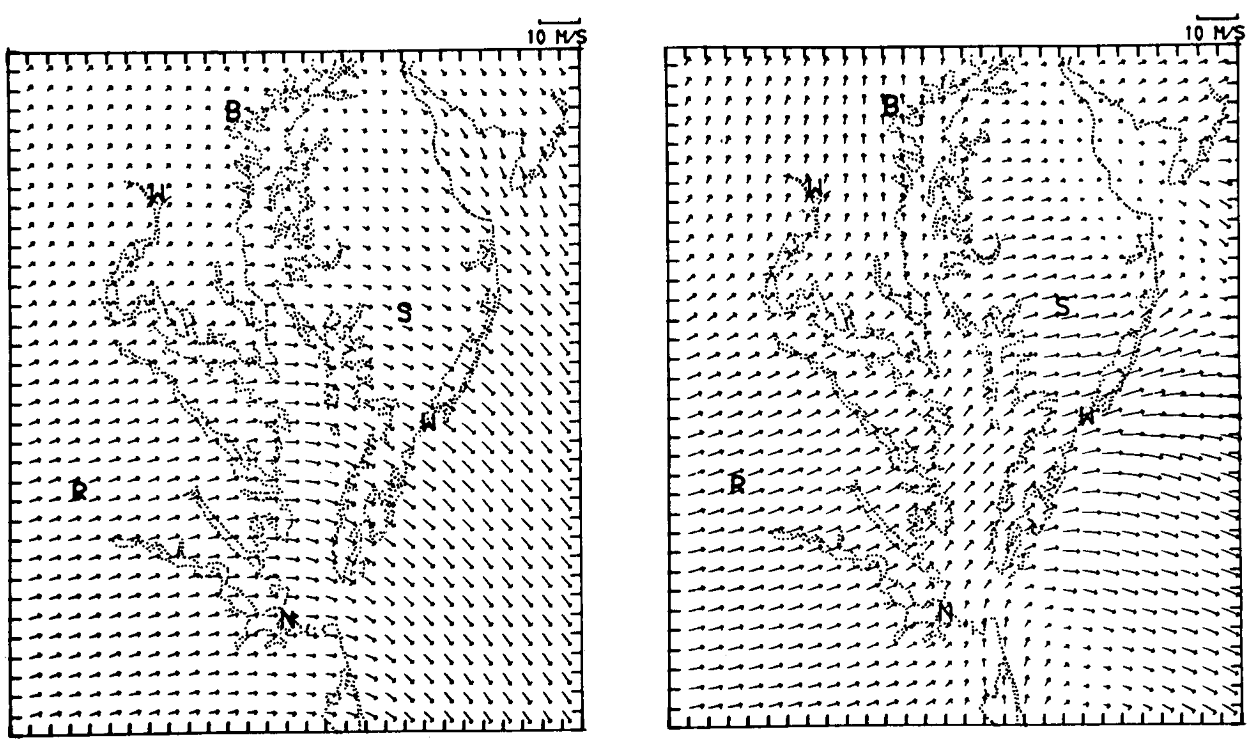

FIG. 2. The same as Fig. 1, except for 500 m.

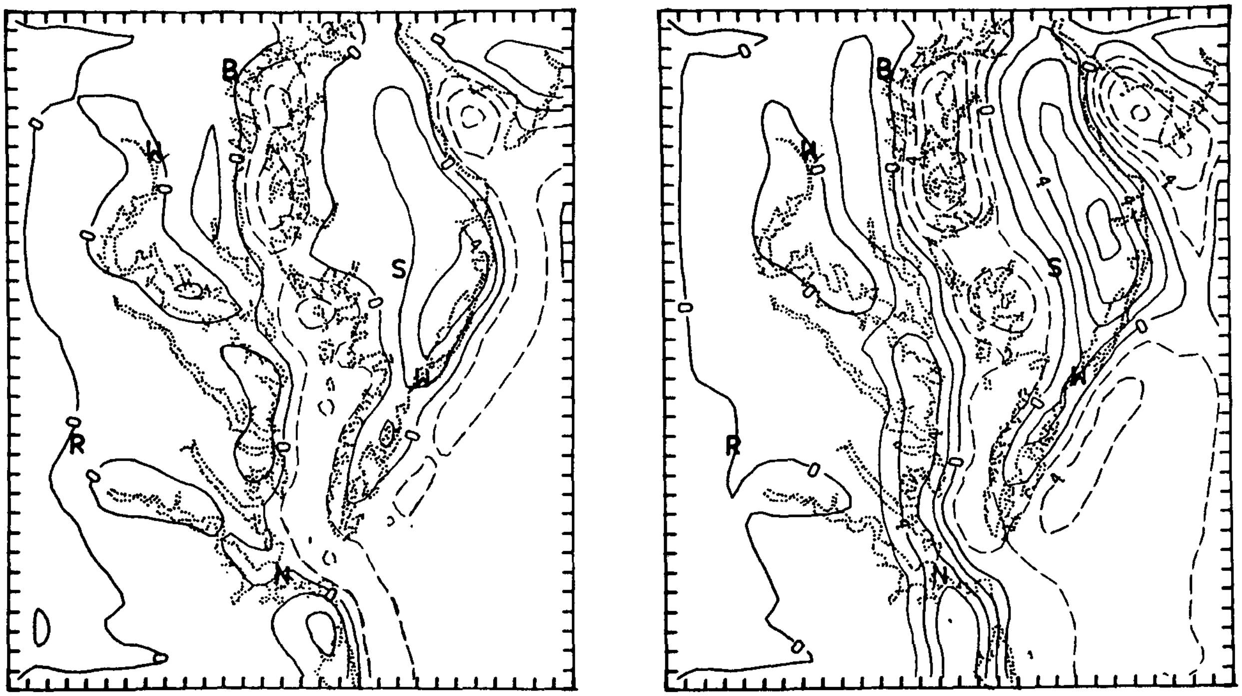

FIG. 3. The same as Fig. 2, except for vertical velocity (cm/s) at 1100 LST (left) and 1600 LST (right). Contour interval is 2 cm/s; dashed lines indicate negative vertical velocity.

predicted by this model. For this case, corresponding to 21 July 1978, the NMM-predicted horizontal winds at 15 and 500 m at 0900 LST and 1600 LST, and the vertical motion field at 500 m at 1100 LST and 1600 LST, are presented for the Chesapeake Bay Region.[4] The spatial and temporal wind variations shown developed in response to the differential heating rates between the land and water during the daylight hours and interacted with the prevailing synoptic flow. For this situation, the large-scale flow was assumed southwesterly over the left-hand portion of the domain, veering to northwesterly farther east. This synoptic wind pattern, along with the initial thermal stratification used in the model, is typical of the Bermuda High, humid weather often observed in the Middle Atlantic states during the summer. Figure 1 illustrates the diurnal development of the sea-breeze near the surface. Among the results, well-defined regions of calm wind were calculated within the sea breeze convergence zones, while the veering of the sea breeze during the day along the coastal area due to the Coriolis effect was significant. The interaction of the sea breeze circulation with the synoptic flow was well pronounced at the 500 m level, as illustrated by the horizontal wind pattern (Fig. 2). The daytime evolution of the pattern of ascent and descent is given in Fig. 3. Additional details of the meteorological model calculation for this day, along with a comparison against observational information, are given in Segal and Pielke (1981) and Segal *et al.* (1982).

[4] In this simulation, the meteorological fields were resolved on 13 vertical levels with a 10 km horizontal resolution.

With use of the wind field and boundary layer structure predicted by NMM, trajectories and dispersion characteristics can be estimated over this region. Figures 4 and 5, reproduced from Segal *et al.* (1982), illustrate the use of predicted winds to calculate expected particle locations (in this case without considering turbulent diffusion) over the Chesapeake Bay Region at 1600 LST on 21 July 1978. The trajectories of these particles were computed using predicted wind velocities from the NMM meteorological simulation. For this situation, simulated pollution particles were released at 10 min intervals, beginning at 0800 LST, from 15 m, 300 m, and 700 m above the ground. Streak lines representing the movement of the released particles are given in horizontal plain views and vertical cross sections showing the x-y and the x-z distributions of the particles at selected times. Following the particles simultaneously in both cross sections provides their 3-dimensional locations. Particles that move to within one grid interval from the domain boundary are abandoned. For a detailed description of the trajectory analysis methodology, see McNider (1981).

The sites of the releases corresponded to the geographic locations of Norfolk (N), Richmond (R), Wallops Island (WL), and Washington (W). Inland, away from the coast at R, the simulated particles spread laterally with height, due to the reduction of ground friction higher up. For this location, which is typical of flat, homogeneous terrain, the assumption of a uniform wind direction with height within the lowest few hundred meters of the ground during sunny days is reasonable. This result, consistent with the conclusion of AMS (AMS, 1978), suggests that, for this type of geographic location (i.e., homogeneous, flat terrain), meteorological meas-

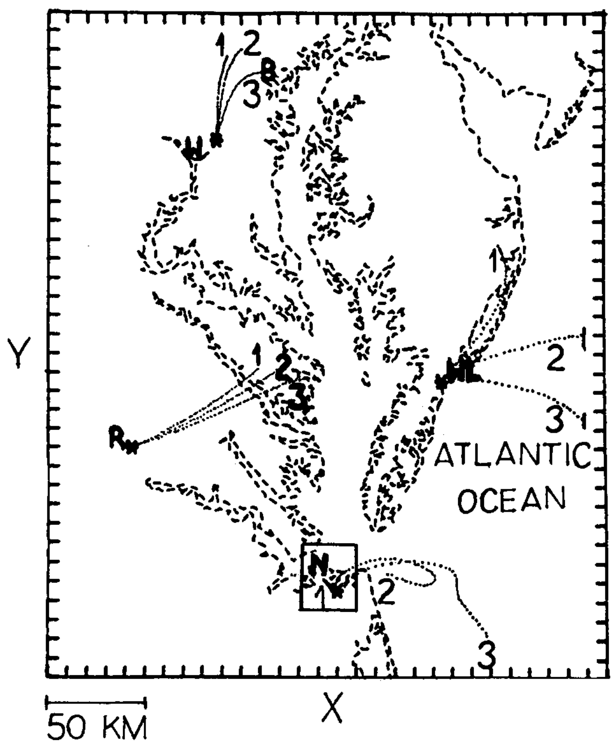

FIG. 4. Plane view showing the predicted x-y distribution at 1600 LST of particles emitted, beginning at 0800 LST on 21 July 1978, at 15, 300, and 700 m heights (indicated by 1, 2, and 3, respectively) from sources situated at the geographic locations corresponding to Norfolk (N), Richmond (R), Wallops Island (WL), and Washington (W). The movement of these particles was determined using the wind predictions from NMM (from Segal *et al.* (1982)).

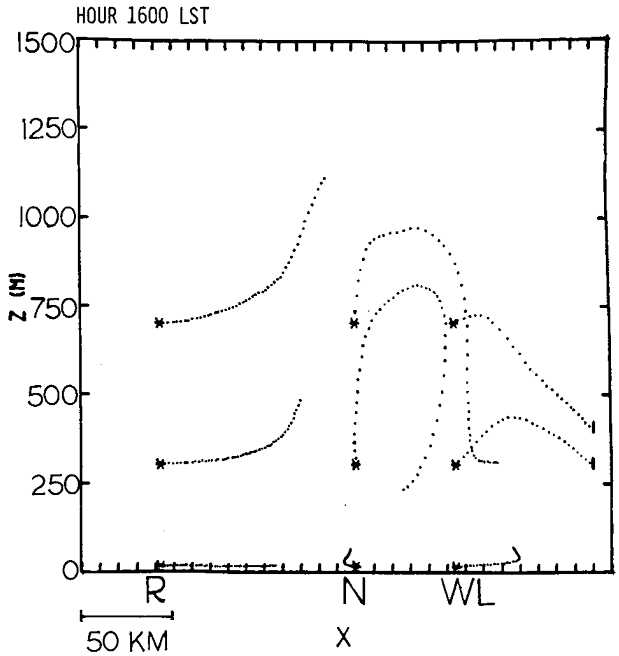

FIG. 5. Vertical view, looking northward, showing the x-z distribution of particles emitted at 15, 300, and 700 m heights from the first three locations listed in the caption to Fig. 4 (from Segal *et al.* (1982)).

urements at one location may be sufficient for use in one of the operational dispersion models.

In the coastal area, however, it is clear that the wind pattern is quite complex. Hence, the use of wind data from a single observation site in a dispersion model may lead to serious errors in estimating transport and diffusion even over relatively short distances. At N, for example, the lowest-level emission stagnates in the location of release and slowly ascends during the simulated day, due to the convergence of the sea breeze wind. Meanwhile, at 300 m, larger upward motion at that level has transferred the particles upward, then eastward, in the prevailing synoptic flow. Subsequently, these particles sink offshore in the subsidence generated by the sea breeze and begin to be advected westward towards the source region. Such recirculations of pollutants (which have been observed, e.g., Lyons and Cole (1976)) can cause an increase in pollution concentrations onshore. At 700 m, on the other hand, the offshore sinking of pollution particles does not reach low enough to be dominated by the lower-level sea breeze, and they are advected eastward by the synoptic flow. Thus, because of such complex mean trajectories, the practice of estimating upper-level winds by a power law extrapolation from surface observations is insufficient to accurately assess air quality in coastal regions, since wind direction changes with height. Additionally, in the evaluation of the transport of pollutants, vertical motion should be considered in coastal regions.

b. Trajectory analyses within mountainous areas

Complicated trajectories also are expected in rough terrain. The topographic situation illustrated in Fig. 6 was chosen to present an example of mean trajectories calculated from the application of NMM to a nocturnal drainage flow simulation as reported in McNider (1982). The meteorological information used to perform the trajectory calculation was obtained from a 3-dimensional version of the model, with 1 km horizontal grid intervals over the 19 km wide by 1.9 km deep valley presented in Fig. 6. In this simulation, pollution particles released 8 m above the ground along the side wall of the valley moved downslope with the cold drainage flow into the valley and then were transported outward from the valley (Fig. 7). As with the sea breeze simulation, this change of direction of pollution transport could not be estimated using a single observation site.

3. Quantitative evaluations of pollutant transport and dispersion

The calculations of mean trajectories alone from the mesoscale dynamic model illustrate serious shortcomings with the use of surface observations, or even a limited set of more extensive vertical soundings, to estimate air quality transport in coastal regions and over irregular terrain. Although mean trajectory calculations provide estimates of average pollution transport, they ignore the effects of turbulent diffusion on the development of pollutant concentration patterns. Two methodologies are being developed in order to obtain

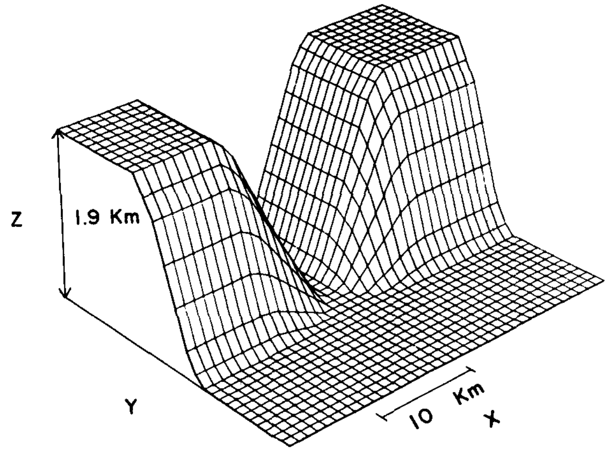

FIG. 6. A 3-dimensional perspective view of the terrain input to NMM. The NMM-simulated nocturnal drainage winds were used to advect the particles shown in Fig. 7 (from McNider (1981)).

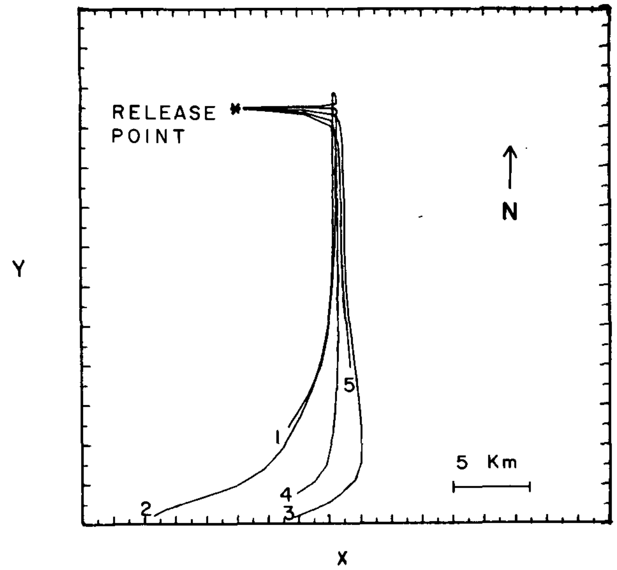

FIG. 7. Horizontal view showing the x-y trajectories of particles emitted, one particle per hour beginning at sunset (numerated consecutively at the end of each trajectory), from 8 m above the ground along the valley side wall (shown by an asterisk). The height of the particles above the ground in kilometers, 5.5 h after sunset, are 0.23 for particle 1; 0.17 for 2; 0.16 for 3; 0.14 for 4; and 0.15 for 5 (from McNider (1981)).

quantitative information concerning the concentration fields. Both utilize predicted winds and boundary layer structure from NMM to estimate transport and diffusion.

a. Pollutant transport and dispersion from point sources

This technique to estimate dispersion using the NMM prediction is designed for point and line sources. As described in McNider (1981), a large number of particles are input sequentially, and advected and diffused in response to mean and turbulent winds obtained from NMM. The location of these particles at subsequent times then are determined from

$$\begin{aligned} x(t+\delta t) &= x(t) + [u(t) + u'(t)]\delta t \\ y(t+\delta t) &= y(t) + [v(t) + v'(t)]\delta t \\ z(t+\delta t) &= z(t) + [w(t) + w'(t)]\delta t, \end{aligned} \qquad (1)$$

where the u, v, and w components of velocity are calculated directly from the mesoscale model, and u', v', and w' are turbulent velocity fluctuations parameterized statistically in terms of the mesoscale model-predicted boundary layer parameters.

The turbulent velocities are based upon a Markov process, as described by Hanna (1979) and Reid (1979). For the w component, for example, they are represented by

$$w'(t) = w'(t-\delta t)R(\delta t) + w'', \qquad (2)$$

where $R(\delta t)$ is the Lagrangian autocorrelation function at lag time δt and w'' is a random component with a Gaussian distribution with a mean of zero and variance defined by the local turbulent variance, σ_w^2. The parameters needed to close the statistical scheme, σ_w and $R(\delta t)$, are deduced from the NMM boundary layer parameters, as described in McNider (1981). This procedure permits the turbulent velocities to be related to the predictions of the mesoscale model.

Figure 8 illustrates the predicted distribution of 1300 pollution particles A) 200 s, B) 600 s, and C) 1000 s after their release for the drainage flow simulation described earlier in this paper. The tabulation of the number of particles per unit volume would provide the expected concentration in relation to the input rate of the particles.

b. Pollutant dispersion from area sources

This technique, described in Segal *et al.* (1980), interpolates the meteorological fields from NMM to a smaller-scale domain with finer grid resolution. The concentration pattern of pollutants then is calculated from a 3-dimensional advection-diffusion equation of the form

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - w\frac{\partial C}{\partial z} + \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + S_c. \qquad (3)$$

In this expression, C is the concentration; u, v, and w are components of velocity in the east-west (x), north-south (y), and vertical (z) directions; K_x, K_y, and K_z are the turbulent exchange coefficients and represent the diffusion of the pollutant as a function of thermodynamic stability; and S_c, a function of space and time, can represent the sources and sinks of the pollutant, including those due to source emissions and chemical changes. A similar modelling formulation has been used by Dieterle and Tingle (1976) and Bornstein and Runca (1977). One major restriction in using Eq. 3 is that the spatial scale of the polluted air mass must be at least two times the grid interval used to numerically represent

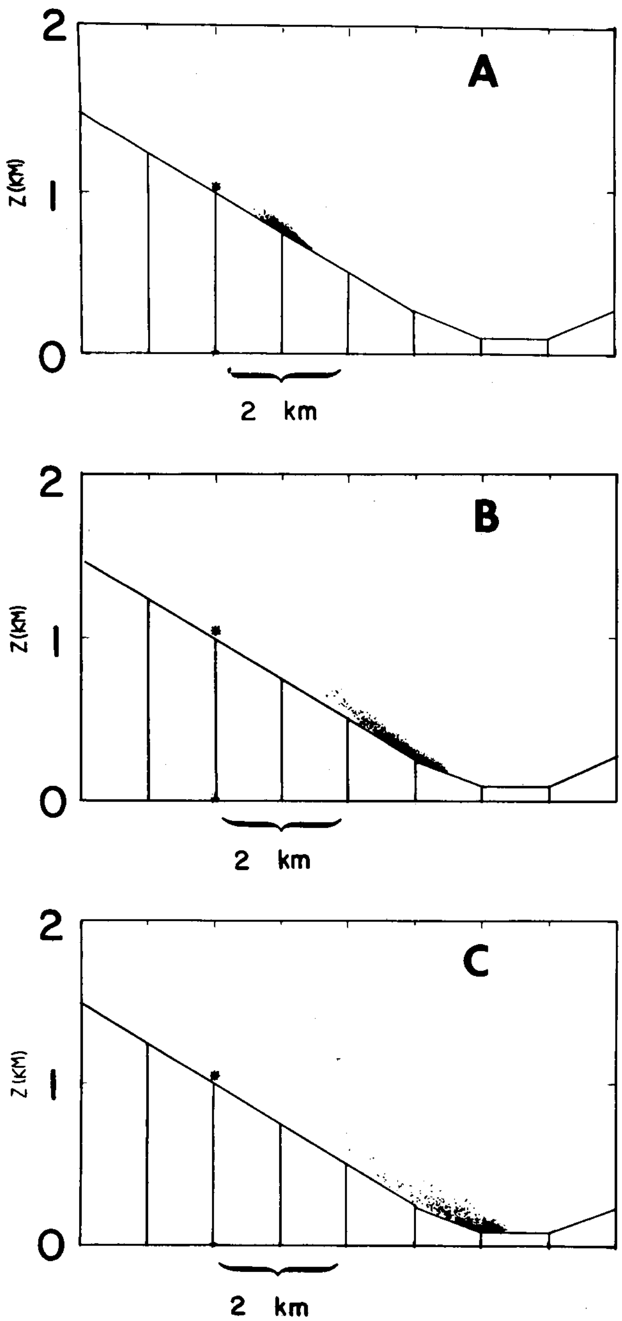

FIG. 8. A cross section view; about halfway up the valley shown in Fig. 6, looking north, showing the spread of 1300 particles due to mean and fluctuation velocities as obtained from the NMM nocturnal drainage flow simulation A) 200 s, B) 600 s, and C) 1000 s after their release. The particles were released at 8 m at two hours after sunset (from McNider (1981)).

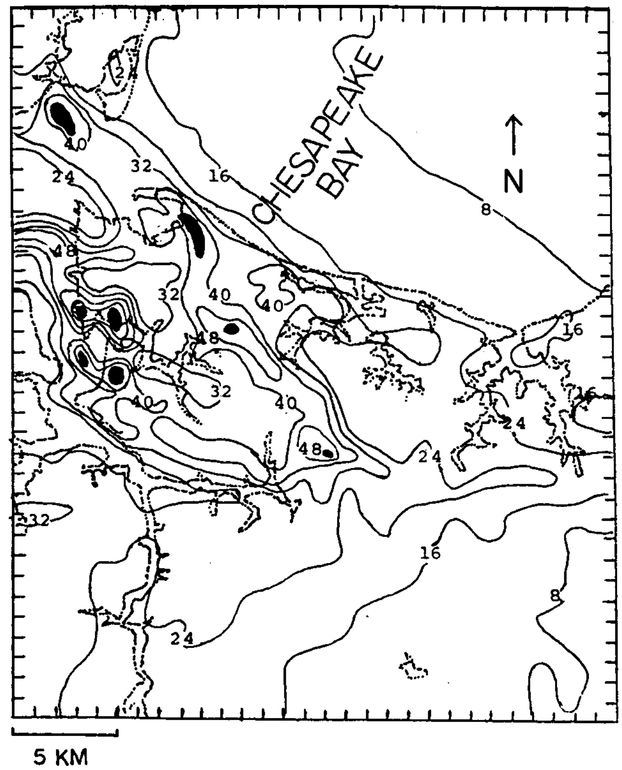

FIG. 9. The CO concentration field at 10 m height at 1700 LST obtained using model results for 21 July 1978 (e.g., see Figs. 1–3), with wind and turbulence characteristics interpolated from NMM to a fine grid domain around Norfolk (N) (illustrated in Fig. 4). Dots indicate shorelines. Contour intervals are in units of $8 \cdot 10^{-3}$ mg/m^3, with peak concentration areas shaded (from Segal *et al.* (1980)).

this equation[5]. Otherwise, the use of an exchange coefficient causes neighboring grid points to receive pollution, due to mixing, too quickly. Equation 3, therefore, is most useful when applied to areal sources where pollution is input over a relatively large scale.

Figure 9 illustrates a predicted field of carbon monoxide (CO) at 1700 LST over the Norfolk area (from Segal *et al.* (1980)) using the NMM predictions over the Chesapeake Bay, as discussed previously in this paper[6]. In the application of the advection-diffusion equation, a 1 km horizontal grid interval and a variable 13-level vertical mesh (with finest resolution as small as 5 m near the ground) were used. Predictions from NMM were introduced to the advection-diffusion equation grid (which covered a domain of 30 × 36 km) via an inverse-distance weighting interpolation formula with vertical exchange coefficients determined separately for land and water points within the fine mesh, as described in Segal *et al.* (1980). When applying Eq. 3 in this case, the horizontal diffusion terms have been omitted due to the dominance of spatial and temporal changes of advection in the horizontal direction in dispersing pollution. The field of CO concentration shown in Figure 9 developed from a daily area source inventory over the Tidewater region of Virginia (Brewer *et al.* (1979)), and evolved in response to the advection and vertical

[5] In order to achieve a reasonably accurate numerical representation, however, better spatial resolution is required (e.g., at least four times the grid interval).

[6] The domain used in Fig. 9 is indicated by the rectangle around Norfolk (N) in Fig. 4.

diffusion predicted from Eq. 3. This equation was solved using 60 s time steps. Since zero CO background concentration was assumed, and only daily average CO source emissions were available to input to the model, only a very preliminary comparison with the sparse number of available measured CO concentrations was possible (although the predicted values were reasonable in magnitude (Segal *et al.* (1980)). The southwesterly sea breeze at this hour controlled the concentration distribution, as indicated by the general orientation of the contours (peak concentration areas are shadowed).

4. Conclusions

The techniques presented in this paper use the meteorological output from a mesoscale model so that, in contrast to air quality evaluations based on a limited set of observations, a more detailed representation of spatial and temporal variations of the flow and turbulence fields is achieved. This improvement is most applicable to coastal regions and irregular terrain. Dense meteorological observational networks with high vertical, horizontal, and temporal resolution would be optimal, of course. The high cost in manpower and dollars of sampling adequately vertically and horizontally, however, makes that approach prohibitively expensive for most situations.

Although further tests and refinements are needed, the methods outlined in this paper could complement observational and simpler model assessments of long-term air quality in regions where complex flow patterns exist. The methods would be most useful where a seasonal persistence of synoptic conditions occur and where the mesoscale circulations contribute significantly to the local climatology, such as in southern California and in the southeastern United States. Additionally, these methods perhaps could be used to estimate the transport and diffusion of accidental, dangerous emissions from specific sites during an emergency by using simulations performed earlier for a series of expected scenarios. Such procedures also could provide a method for the evaluation of pollution concentrations in such adverse air quality episodes as dynamic fumigation near shorelines and plume impingement in elevated terrain. These techniques also might provide guidance for the siting of air quality monitoring stations.

Acknowledgment. The authors gratefully appreciate the support of grants from the Environmental Protection Agency (Grant #R810471), the Atmospheric Science Section of the National Science Foundation (Grant #81-0732-02), and the United States-Israel Binational Science Foundation. Computer calculations reported in this paper were performed at the National Center for Atmospheric Research, which is supported by the National Science Foundation. The authors also wish to acknowledge Ann Gaynor and Sara Rumley, who provided their usual outstanding editorial and secretarial support.

Although the research (or other work) described in this article has been funded wholly or in part by the U.S. Environmental Protection Agency under assistance agreement number R-810471 to Colorado State University, it has not been subjected to the Agency's required peer and administrative review and, therefore, does not necessarily reflect the view of the Agency and no official endorsement should be inferred.

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