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USE OF METEOROLOGICAL MODELS AS INPUT TO REGIONAL AND MESOSCALE AIR QUALITY MODELS — LIMITATIONS AND STRENGTHS

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Abstract—The importance of meteorological variability and uncertainty is described and discussed in the context of dispersion and chemistry of air pollution. Synoptic, mesoscale, and turbulent scales are defined in relation to pollution dilution. Spatial variability effects due, for example, to synoptic baroclinicity, propagating synoptic and mesoscale features, and surface-forced atmospheric circulations are described. Temporal variability resulting from diurnal and seasonal effects are discussed and examples presented. Among the questions addressed is the importance of differential advection relative to horizontal diffusion at different space and time scales. The concept of delayed diffusion is presented. Among the conclusions is that regulating agencies such as the EPA and NPS have generally not taken sufficient advantage of regional and mesoscale meteorological model-generated wind and turbulence fields, nor used the limits on the accuracy of these models to provide an upper limit to the skill of air quality models. Part of this failure is due to the poor communication by scientific researchers, of model capabilities and limits to the agencies and other users of meteorological model output as part of air quality assessments. © 1998 Elsevier Science Ltd. All rights reserved.

Key word index: Dispersion, long-range transport, terrain-induced, mesoscale modeling, boundary layer.

1. INTRODUCTION

The need to accurately describe the wind and turbulence fields for input into air quality assessment models should be obvious (e.g., Physick *et al*., 1992; Pielke *et al*., 1983, 1991; Tucker, 1993; Svensson, 1996a; Kallos, 1996; Berkowitz and Fast, 1996; Physick, 1995; Yamada, 1996; Mueller *et al*., 1996; Millán *et al*., 1996; Liu and Carroll, 1996; Schayes *et al*., 1996; Bornstein *et al*., 1996; Sharan *et al*., 1996; Nowacki *et al*., 1996; Banta, 1990). Otherwise, how could the transport, deposition, and dispersion of a chemical effluent and resultant concentration fields and chemical reactions be accurately represented. Sistla *et al*. (1996), for example, show the influence of meteorological uncertainties with respect to ozone control strategies. Al-Wali and Samson (1996) illustrate the sensitivity of the Urban Airshed Model to the placement of boundary layer measurements with respect to the location of emissions. Svensson (1996b) demonstrated that relative errors in meteorological variables simulated in a model may be larger than the uncertainties in chemical rate constants. That paper emphasized the importance of understanding how errors in the meteorological fields affect the results (and conclusions) from the air quality model. Hanna (1992) discusses the effects of data limitations on the ability to improve short-range dispersion models. Kahl (1996) presents a paper on the prediction of trajectory error.

In this paper we discuss this need with particular emphasis on the mesoscale and regional scale. The limitations and strengths of using meteorological models to obtain wind and turbulence information is presented, as well as uncertainties in the atmospheric flow field analyses. These uncertainties will place limits on what accuracy is achieved in estimating chemical concentration fields from air quality models.

2. REVIEW OF MODELING APPROACHES

Meteorological models have been used in a diagnostic form or in prognostic version (Pielke, 1985; Kumar and Russell, 1996; Zannetti, 1990; Ratto *et al*., 1994). Prognostic models permit nonlinear terms (e.g., advection) to create a flow field that contains information not present in the observational analysis used to initialize the model. Diagnostic models are constrained by available observations, topographic terrain and linear conservation formula (e.g., the conservation of mass) such that they are unable to

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obtain spatial and temporal structure smaller than the available input data. Hybrid models exist also where a prognostic model ingests observed data and nudges the simulated field towards the measured observations (e.g., see Hoke and Anthes, 1976; Bigler-Engler *et al.*, 1996; Ching and Pleim, 1996). This analysis procedure is referred to as four-dimensional data assimilation (4DDA) (Fast, 1995). Hariharan and Venkatram (1996) illustrate errors that result when mass conservation is not retained in air quality models. McNider *et al.* (1996) demonstrate the values of 4DDA even when a reasonably complete prognostic model formulation is used.

This paper focuses on modeling of atmospheric flow and turbulence using prognostic models. It should be pointed out that turbulence characteristics required by air pollution models (i.e., eddy diffusivities, wind velocity variances, Lagrangian time scales) are usually not provided directly by meteorological models but must be derived from their output using wind and temperature fields and often some additional fields such as turbulent kinetic energy, turbulent length scales, mixing height or parameters of the atmospheric surface layer. Ideally, the same turbulence parameterization scheme should be used for this purpose as one applied in the meteorological model, otherwise, these calculations may introduce additional sources of errors. The turbulence parameterizations used in recent mesoscale and regional meteorological models are reviewed by Uliasz (1994).

Contemporary air quality models taking into account atmospheric chemistry and removal processes may also require additional meteorological input including radiative and/or water fields (i.e. water vapor, cloud, and precipitation fields). The current state and future directions of tropospheric chemistry and transport models are discussed by Peters *et al.* (1995).

In most modeling approaches atmospheric chemistry and dynamics are effectively decoupled allowing one to use an off-line approach where the meteorological model is applied independently from the air quality model. It is possible to simulate different emission scenarios or to run different dispersion models using the same meteorological fields without necessity to repeat the meteorological simulations. However, the output from meteorological models must be stored for this purpose quite frequently. A modeling domain of the mesoscale/regional meteorological models is often much larger than the domain used in air pollution simulations and it may be covered by multiple nested grids. As a consequence, a huge volume of data must be produced in the case of long-term simulations. Therefore, an additional processing of meteorological fields may be useful to extract only these fields from the meteorological output which are required by the air pollution model and to reduce size of the modeling domain. An example of this procedure is described by Uliasz *et al.* (1996) for the 1 year simulation of air pollution transport in the southwestern United States.

The on-line modeling approach must be used in order to investigate feedback effects between air chemistry and atmospheric dynamics. Therefore, more advanced modeling systems must contain both chemical and meteorological components and allow interaction between the two.

In addition to continuous meteorological simulations, an alternative approach may be considered for practical applications as proposed by Enger (1990). First, a data base with a thousand or more wind and turbulence fields is created by running a prognostic mesoscale model for a typical diurnal cycle with different directions and speeds of the geostrophic wind. To simulate the dispersion, the data base is searched for the meteorological fields which are the closest to the actual observations in the area and these fields are used as input to the dispersion model. This approach was applied in a moderately complex terrain for both operational and long-term dispersion simulations.

3. METEOROLOGICAL VARIABILITY

The dispersion of chemical effluent from point, line and area sources is the result of differential wind advection and turbulent diffusion. Differential wind flow results from time- and space-varying winds, which in the context of a numerical model or observational analyses are those winds that are resolved. The winds are three-dimensional including horizontal and vertical components. The term turbulence is used to describe those scales of flow that are smaller than the model or analysis resolution. As discussed by Pielke (1991), models are able to resolve features reasonably only when the spatial scale is at least four grid increments in each of the three directions.

The resolved scales can be separated into two categories — the synoptic scale where the flow is in near gradient wind balance above the planetary boundary layer and the mesoscale where the flow deviates significantly from the balance even in the free atmosphere. Both synoptic- and mesoscales are close to hydrostatic balance. Turbulent flows can be considered as deviating significantly from hydrostatic balance; thus, cumulus clouds including thunderstorms are one type of turbulence.

Dilution of chemical effluent occurs due to turbulent diffusion, and because of wet and dry deposition to the ground. This dilution reduces the chemical concentration of a chemical species in the absence of additional effluent or chemical reaction (e.g., due to photochemical effects) which creates more of the chemical than is being diluted. Differential advection, in the absence of deposition and chemical reactions, can only result in the vertical and horizontal displacement of a chemical but will not result in dilution until turbulent diffusion occurs. If there is a time lag between differential advection and when diffusion occurs, this is referred to as delayed dispersion (Moran, 1992).

3.1. *Spatial effects*

3.1.1. *Synoptic and larger scales.* Meteorological variability on this scale is directly associated with baroclinic effects (i.e., vertical shear of the horizontal wind), propagating synoptic features, and large-scale ascent/descent patterns. Bluestein (1992) and Carlson (1991) provide recent texts on the dynamics of these synoptic effects.

On the synoptic scale, vertical wind shear is a direct result of a horizontal temperature gradient. Since such gradients are a feature of the polar front and extra-tropical cyclones (e.g., see Pielke *et al.*, 1987), this mechanism of differential wind transport will always occur near these weather features. The movement of these weather features is what creates ascending and descending air with magnitudes up to tens of centimeters per second over thousands of square kilometer areas. Figure 1 shows how even a horizontal synoptic wind field differential wind flow can deform an area of pollution.

Examples of papers that discuss this effort are Artz *et al.* (1985), Stocker *et al.* (1990).

3.1.2. *Propagating mesoscale systems.* Squall lines, frontal circulations, cumulus convection embedded in stratiform systems and mesoscale convective systems are examples of atmospheric features of hundreds of kilometers in scale that move through the atmosphere. When deep cumulonimbus occurs with these features, rapid and extensive, horizontal and vertical

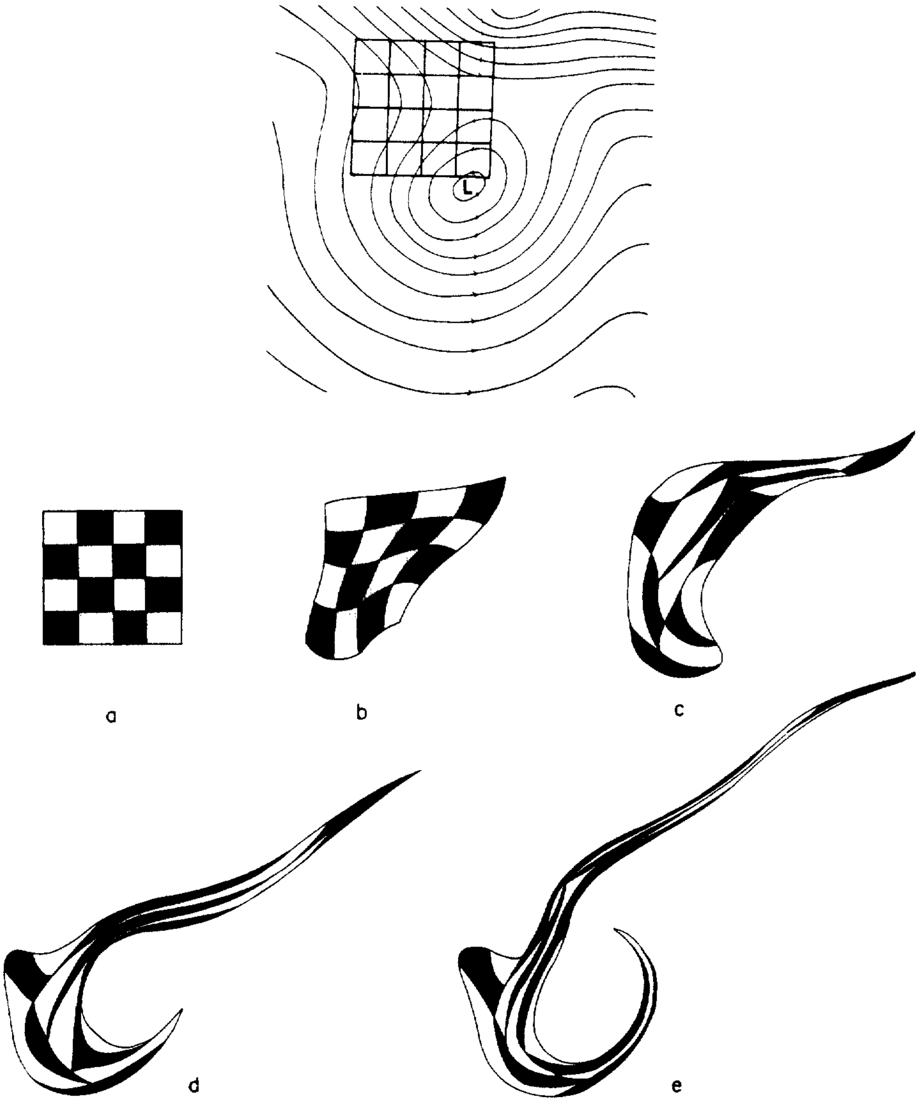

Fig. 1. Horizontal deformation of a large-scale parcel by two-dimensional incompressible flow at 500mb as predicted by a barotropic numerical model after a time period of: (a) 0 h; (b) 6 h; (c) 12 h; (d) 24 h; and (e) 36 h. The initial streamline pattern is shown at the top. The sides of the colored grid squares are 300 km (Welander, 1955; as reproduced by Moran, 1992).

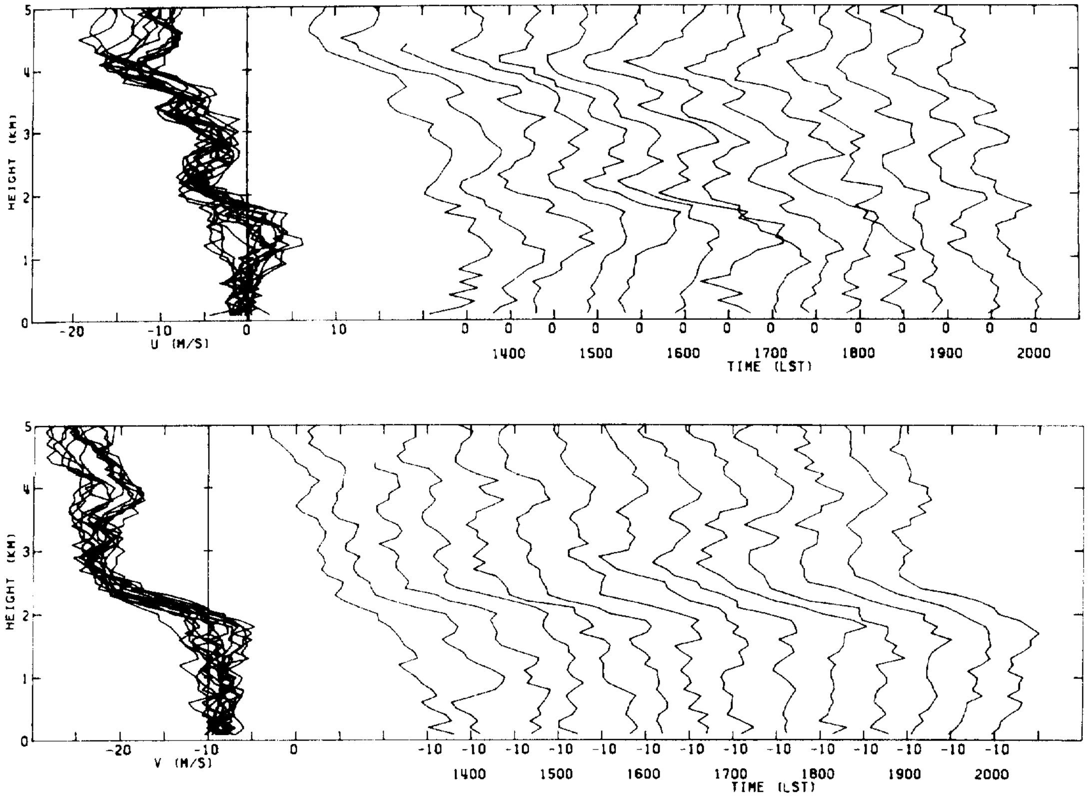

Fig. 2. Sequential vertical profiles (height above the ground) of the east–west (upper panel) and north–south (lower panel) velocity component winds from 14 balloon launches over a 6 h period on 31 March 1976 at St. Cloud, Minnesota (from Gage and Jasperson, 1979; as reproduced by Moran, 1992). The profiles on the right-hand side of the figure are collapsed on top of each other on the left side, to better illustrate the temporal variability. Positive values correspond to westerly and southerly components, respectively.

differential winds and turbulent diffusion will result in considerable dilution. Scavenging of aerosols and water soluble chemical species and resultant wet deposition can further dilute the chemical concentrations. In addition to scavenging, deep cumulus convective clouds vertically transport chemical species from near the surface to higher altitudes (Cotton *et al.*, 1995; Lyons *et al.*, 1986).

3.1.3. *Mesoscale surface effects.* Sea and land breezes, mountain–valley winds, and winds generated due to other types of land surface variability (e.g., urban–rural differences, snow–no snow cover variability, vegetated areas adjacent to less vegetated regions, etc.) also contribute to differential wind and turbulence fields. These mesoscale features develop due to horizontal surface gradients in surface sensible and latent turbulent heat fluxes. These atmospheric features are described in a wide variety of sources including (Atkinson, 1981), and Pielke (1984). Avissar (1996) illustrated the importance of vegetation in the urban environment on the dispersion of pollutants in which turbulent mixing is strongly influenced by the relative partitioning of turbulence into sensible and latent fluxes by the plants, as contrasted with non-vegetated surfaces.

Even if the differences in surface turbulent fluxes are not strong enough to create a distinct mesoscale circulation, they can significantly affect vertical structure of the atmospheric boundary layer and in turn atmospheric dispersion. These effects were demonstrated by simulating atmospheric dispersion over a series of land patches with different soil water content (Pielke and Uliasz, 1993).

3.2. *Temporal effects*

The variability of wind speed and direction, turbulence intensity and precipitation rates will also influence the dilution of chemicals. Even in the free atmosphere, winds are not steady but undergo variations on all time scales (Fig. 2).* McNider *et al.* (1988) shows how inertial oscillations due to the Coriolis effect, synoptic vertical shear, and decoupling and recoupling of the planetary boundary layer with the volume of the chemical species of interest will

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* Figure 2 indicates that the routine release of radiosonde balloons at 12 h intervals by the operational weather centers around the world, introduces an appreciable error in the ability to account for dispersion due to time changes in wind speed and direction.

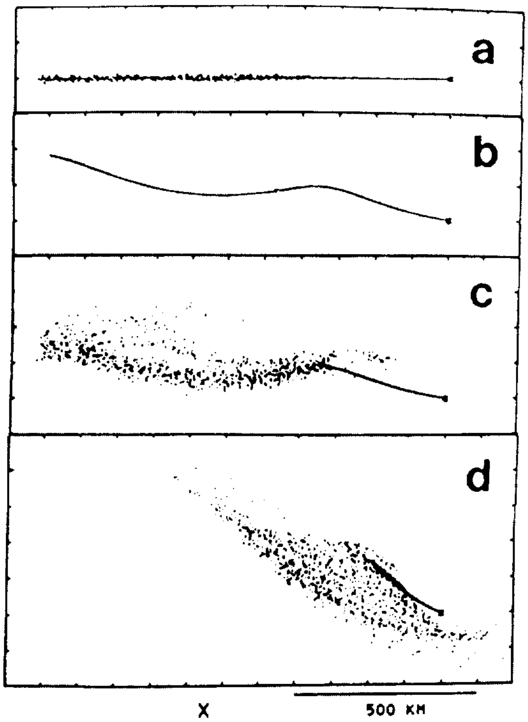

Fig. 3. Instantaneous depiction of plume release after 42 h from Mt. Isa smelter in Australia. (a) Only planetary boundary layer (PBL) turbulence but no PBL shear and no Coriolis force. (b) Including Coriolis force but no PBL turbulence. (c) Includes PBL turbulence, PBL shear and Coriolis force. (d) Same as (c) except for baroclinic case which includes geostrophic shear. The data correspond to particles released from the smelter stack 300 m altitude at 600 s intervals starting at 1115 Local Standard Time. The low-level wind was from right to left (easterly) in the southern hemisphere. The "solid" appearing line is actually the superposition of particles which remain close to each other (from McNider *et al.*, 1988; see that reference for more details on this experiment).

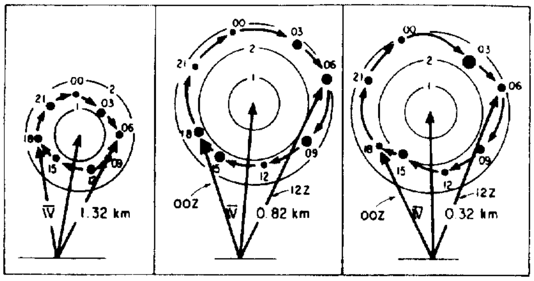

Fig. 4. Hodographs of the summertime diurnal wind variation for three levels at Fort Worth, Texas including the mean wind vector and the wind vectors at the two standard synoptic observing times (0000–1200 UTC). Speeds indicated by the concentric circles are in meters per second. The size of the solid circles for each observing time (shown as CST) is proportional to the magnitude of the probable error in determining the deviation vector at that time (adapted from Bonner and Paegle, 1970 and reported in Moran, 1992).

directly influence dispersion (Fig. 3). Figure 4 shows how the inertial wind variation in the U.S. Great Plains creates a time-varying horizontal wind, as well as what is missed because the routine synoptic observations are only made at 12 h intervals.

On the longer time scale, seasonal differences in the structure of synoptic and mesoscale systems, in surface-based turbulence, and precipitation type and intensity will also result in different magnitudes of dilution.

4. EXAMPLES OF UNCERTAINTY

4.1. *Due to spatial resolution*

Increasing spatial resolution of a meteorological model allows one to include more mesoscale motions in its numerical solution. The higher resolution meteorological fields used in the dispersion model with corresponding resolution will in turn lead to lower concentrations simulated on a regional scale, i.e., a given receptor will experience lower contribution from distant emission sources. This effect is illustrated in Fig. 5 on an example of passive tracer transport between the Los Angeles basin and the Spirit Mountain receptor (located about 350 km NE from Los Angeles) (Uliasz *et al.*, 1996). The meteorological simulations were performed with the Colorado State University Regional Atmospheric Modeling System (CSU RAMS) using two nested grids with spacing 60 and 12 km, respectively. Dispersion was simulated by Lagrangian Particle Dispersion model using the output from both RAMS grids (RAMS) and the output from the coarse grid only (RAMS-1). The output from the coarse grid #1 does not really represent an independent coarse resolution simulation since there is a two-way interaction between nested grids in RAMS. Nevertheless, concentration plots in Fig. 5 demonstrate an evident and important difference between these two sets of particle simulations. The coarse grid particle simulations provide much higher concentration values in comparison to the simulations where input from both nested grids was used. Mesoscale motions simulated on the finer grid #2 cause much more intensive dispersion of the tracer. This figure shows also that concentrations simulated by the ATAD (Atmospheric Transport and Diffusion) model are higher than those predicted by the RAMS-LPD simulations which take into account more mesoscale motions. The ATAD model is a tool commonly used by the National Park Service (NPS) for a trajectory analysis. In this model, a 2-D wind field (u, v) is interpolated from rawinsonde and pibal data. The wind field is averaged within a transport layer determined from a temperature inversion height.

There are a number of papers that illustrate how the spatial resolution in a model influences how realistically transport is represented. For example, Fig. 6 from Lyons *et al.* (1995) shows how vertical motion associated with a sea breeze at Kennedy Space Center is not accurately represented until the horizontal grid intervals are reduced to 1 km. Banta *et al.* (1996)

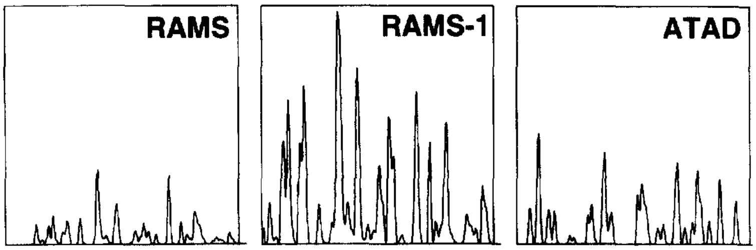

Fig. 5. Concentration of a passive tracer at Spirit Mountain during a three-month period (July–August) as simulated for the Los Angeles source by two versions of RAMS/LPD simulations and an ATAD model analysis (concentrations presented at the same scale).

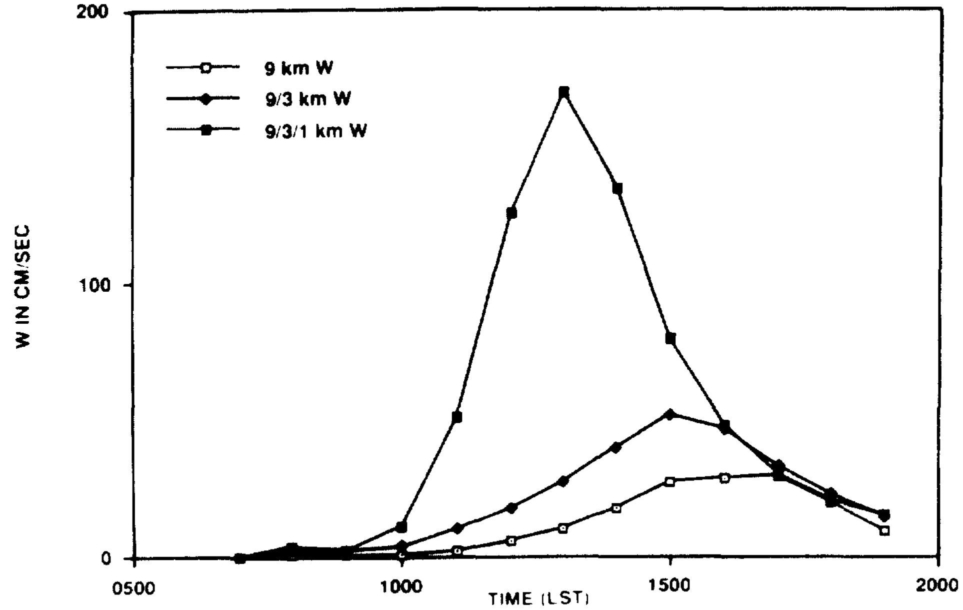

Fig. 6. Maximum model-predicted upward vertical motions w (cm s^{-1}) in the sea breeze convergence zones around the Kennedy Space Center region, 7 November 1988, as a function of the size of the model grid cell (9 km; a two nested run with the smallest grid increment of 3 km; a three model run with the smallest grid increment of 1 km; from Lyons *et al.*, 1995).

discusses the implications of small-scale flow features to modeling dispersion over complex terrain. Portela and Castro (1996) illustrate important (in the context of dispersion) atmospheric features that are missed in synoptic analyses and forecasts from the European Centre for Medium-Range Weather Forecasts (ECMWF) over the Iberian peninsula. Byun (1996) illustrates the influence of the number of vertical levels in the Mesoscale Model Generation 4 (MM4) meteorological model on planetary boundary layer height.

4.2. *Due to model type*

Mesoscale and regional models have different numerical formulations and parameterization schemes. Pielke and Pearce (1994) recently report on several mesoscale models and their capability in two case study simulations. Schlünzen (1994) overviews several German mesoscale models. Eastman *et al.* (1995) compares a prognostic model with an EPA-approved diagnostic model for the western shore of Lake Michigan (Fig. 7). The observed tracer data agreed much more with the simulated tracer behavior using the prognostic model. Figure 8 illustrates how the additional physics in the prognostic model resulted in a more realistic behavior of the simulated tracer movement. Lagoivardos *et al.* (1996) contrasts two prognostic models over Greece. Moran and Pielke (1996a, b) contrast a prognostic model with several diagnostic models for a tracer release from Norman, Oklahoma (see Fig. 9). Grossi *et al.* (1996) recommends the use of output from different meteorological models to assess the sensitivity and the robustness of simulated air quality concentrations.

Several research groups have utilized wind fields from the NGM model to run their dispersion or chemistry models, e.g. Schichtel and Husar (1994); Venkatram *et al.* (1994). The NGM model is a

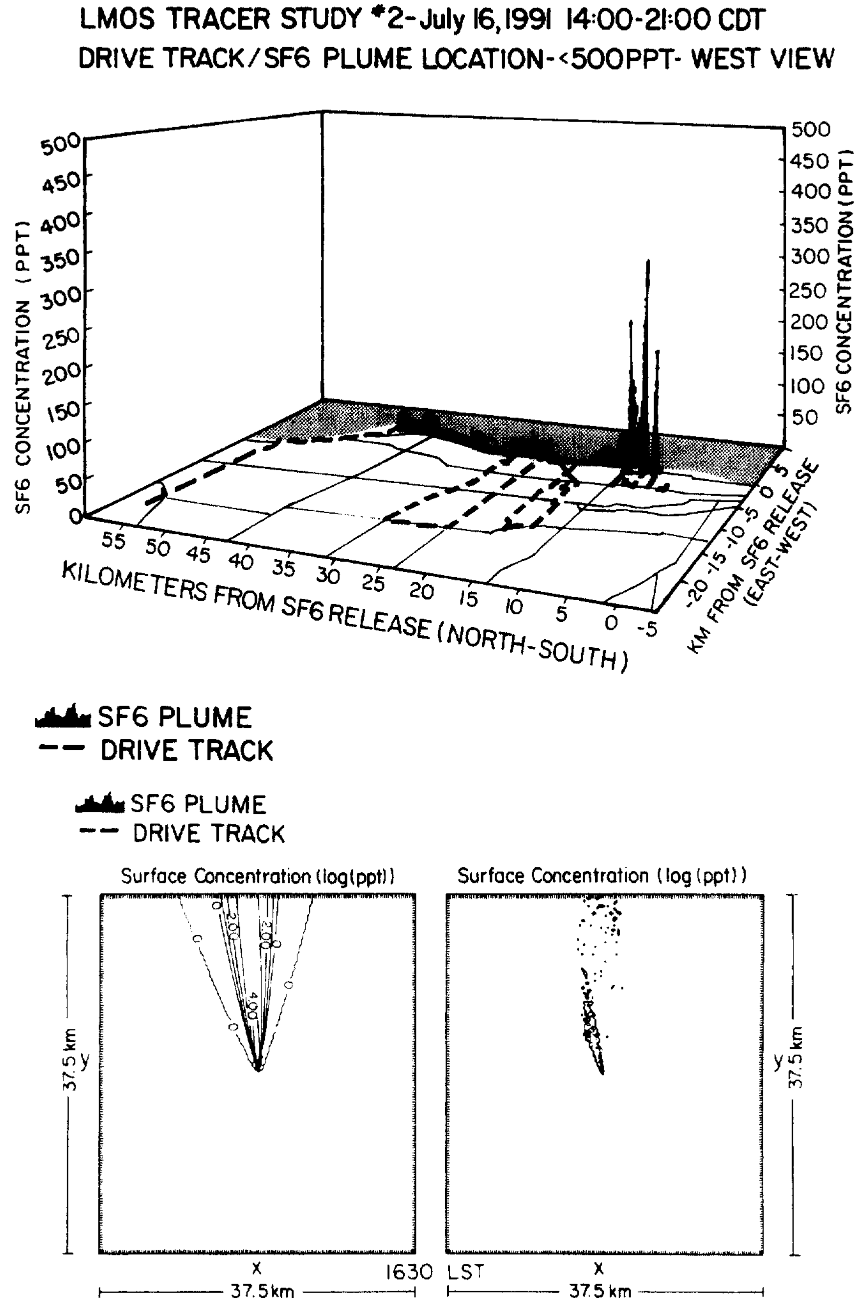

Fig. 7. Perspective view of (a) observations from a mobile van from 1300 to 2000 LST. Values are in ppt (Wilkerson, 1991). (b) Surface isopleths in log (ppt). Left (ISCST); right (LPDM). The two panels taken at 1600 LST. Domain size is 37.5 km × 37.5 km (from Eastman *et al.*, 1995).

hydrostatic primitive equation hemispheric model used operationally by the National Weather Service. Availability of archived NGM output is very attractive since it allows one to perform a multi-year transport study when combined with a rather simple dispersion model. However, these meteorological fields have low time and space resolution: $\Delta x \approx 80$ km (archived with $2\Delta x$ spacing), vertical grid spacing: $\Delta z \approx 150$ m close to the surface. Therefore, the representation of terrain topography is very crude.

Regional transport simulations in the southwestern United States have been validated using a tracer of opportunity—methylchloroform released mostly in the Los Angeles area and measured in three receptors in the vicinity of the Grand Canyon National Park (Uliasz *et al.*, 1996). While correlations between observed and simulated methylchloroform concentrations are within the range of 0.3–0.8 for different months of 1992 for the results from RAMS/LPD modeling, the correlations for results from dispersion

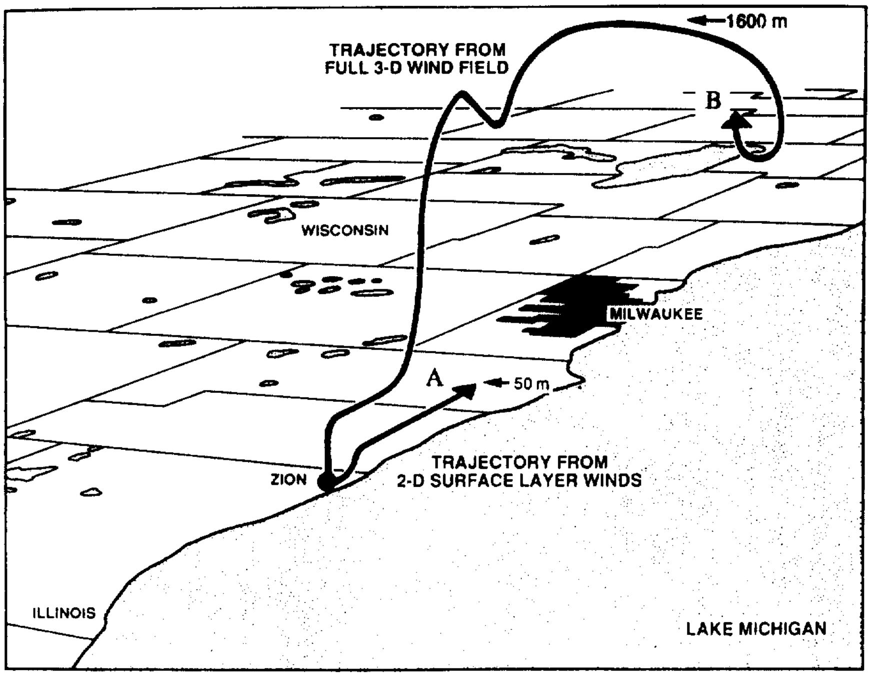

Fig. 8. Typical plume trajectories, calculated from the prognostic model output by utilizing only surface layer winds (trajectory A) which stay at 30 m altitude and the complete 3D wind field (trajectory B) which rises to heights of 1600 m (from Lyons *et al.*, 1995).

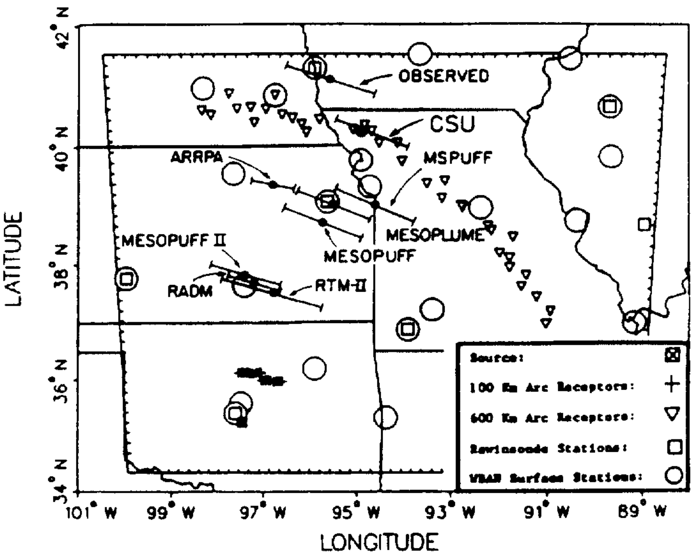

Fig. 9. Schematic showing perfluoromonomethylcyclohexane (PMCH) cloud centers (indicated by solid black dots) and approximate cloud widths (indicated by bars passing through cloud centers) predicted by eight mesoscale atmospheric dispersion models for the first 3 h sampling period of the Great Plains experiment (0800–1100 UTC 9 July 1980). Note that RADM corresponds to the radom-walk advection and dispersion model. The Colorado State University modeling system result corresponds to the baseline experiments (experiment 4b). An estimate of the actual tracer puff position is also shown based on an extrapolation of 600 km arc sampler measurements since it is impossible to tell from the measurements when the tracer material first arrived at this arc. The 3 h release of perfluorocarbon tracer took place at Norman, Oklahoma (lower left-hand corner) beginning at 1900 UTC 8 July 1980 (from Moran and Pielke, 1996b).

models driven by NGM output are always negative (Uliasz *et al.*, 1994; Schichtel and Husar, 1994). It seems that the NGM model is not able to reproduce summer monsoonal flow in southern California due to a lack of sufficient initialization data in this area and coarse resolution. It is interesting that the same

NMC analysis data were used to initialize the RAMS simulations which were much more successful due to better resolution and physics.

4.3. *Due to averaging time of the meteorological model simulated fields*

It is often assumed that longer averaging time of the model output of winds and turbulence will necessarily reduce the error and uncertainty of the dispersion field. However, this is only true if the shorter-term variability were random. If there are systematic features of the atmospheric flow (e.g., surface-forced mesoscale flow, etc.) that are not resolved by the meteorological model, averaging of the simulated data will be unable to properly represent atmospheric dispersion.

Figure 10 compares observed and simulated methylchloroform concentrations in the southwestern United States with the aid of spectral analysis (Uliasz *et al.*, 1996). The presented coherence is derived from a cospectrum calculated for two time series and varies between 0 and 1 (e.g. Sirois *et al.*, 1995). It may be interpreted as a correlation between these time series expressed as a function of frequency or wavelength. The simulated concentrations at three receptors Spirit Mountain, Meadview and Long Mesa in the vicinity of the Grand Canyon National Park were obtained from RAMS/LPD modeling as a contribution from the Los Angeles basin emission. The coherence between the simulated and observed time series of methylchloroform concentration varies significantly with wavelength (time scale) but have similar features for each receptor site. All cospectra show that simulated time series are to some extent coherent with the observed ones for the time scale longer than about 3 days. For the shorter time scale, the cospectra become very noisy. The maximum coherence (between 0.6 and 0.8) appears at time scales between 150 and 180 h at Spirit Mountain and Meadview. This corresponds to the weekly cycles in methylchloroform concentrations related to the fact that this anthropogenic emission is shut down during weekends. It should be noted that the maximum value of coherence for Meadview is lower than that of the two other sites. The Meadview receptor is located at a mouth of Grand Canyon in a much more complex terrain than other receptors. The horizontal grid spacing of the CSU RAMS in these long-term simulations performed over the entire year of 1992 was 12 km on a finer grid. This spatial resolution is obviously not sufficient to correctly represent terrain features in both source and receptor areas. Although it was possible to correctly simulate long-term episodes (3 days) of the observed methylchloroform, the much higher resolution of meteorological fields would be necessary to reproduce shorter-term episodes strongly affected by local and mesoscale circulations in complex terrain.

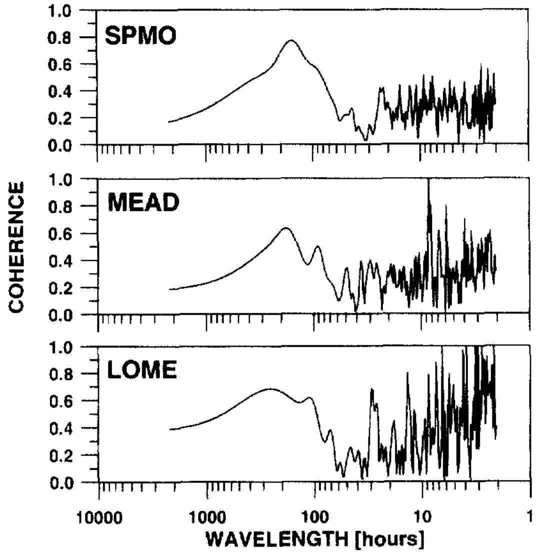

Fig. 10. Cospectra of the observed methylchloroform concentrations and simulated Los Angeles contribution for three receptors (from Uliasz *et al.*, 1996).

5. WHAT NEEDS TO BE DONE

There are opportunities to improve the accuracy of differential wind and diffusion for use in air quality models. These include the use of research and operational meteorological models. For example, since the United States National Weather Service runs an Eta model twice daily every day, why not use the output of that model (archived at half-hourly time periods) to input to a dispersion model?

There are also a number of questions that need to be answered. How can model output (which is a grid-volume representation) be most accurately compared with observed data (which is usually point data)? What effect does ensemble average parameterization representations for turbulence and other physical processes in meteorological models influence the limitation on estimating natural uncertainty? What value-added would be achieved, and what uncertainty range would result from ensemble regional and mesoscale simulations for use as input into air quality models?

Can dispersion models fully utilize and take advantage of information provided by a mesoscale or regional meteorological model? Lagrangian particle models can easily handle meteorological fields of any resolution as input. Lagrangian puff models may have problems with more complicated wind fields (puff splitting techniques try to overcome some difficulties). Eulerian grid models usually have quite poor resolution, especially, in the vertical.

Also, what is the value of advanced meteorological modeling when there is a huge uncertainty in emission data? It is a problem not only with uncertain emission rates but also with uncertain parameters characterizing stack emission. The effect related to uncertainty in plume rise (effective stack height) calculations may be enhanced when meteorological fields with a detailed vertical structure of the atmospheric boundary layer are used in regional dispersion simulations instead of a mixing layer concept.

The level of accuracy imposed on meteorological models by computer and data limitations needs to be explored. For example, model resolution is constrained by computer memory, while initialization and boundary condition information limits model skill. There is a need, for example, for better land cover and soil moisture data.

6. SUMMARY

In this paper we have sought to address the value of meteorological models as input to regional and mesoscale air quality models. Unfortunately, up to the present, regulating agencies such as the U.S. EPA and National Park Service have generally failed to take full advantage of meteorological model-generated wind and turbulence fields, nor used the limits on the accuracy of these models to provide an upper limit to the skill of air quality models. Work is underway in this direction by the EPA (Dennis *et al.*, 1996) and this effort should be strongly supported by the air quality community. Moreover, the EPA minimum recommended performance evaluation procedures (EPA, 1991) need to be extended to meteorological model evaluation as suggested, for instance, by Wheeler (1996).

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