The use of Mesoscale Models on Air-Pollution Studies in Industrial Installations

G. Kallos
Department of Applied Physics, Meteorology Laboratory, University of Athens, Ippocratos 33, Athens 10680, Greece

ABSTRACT
This paper discusses the combined use of a mesoscale numerical model and a Lagrangian particle dispersion model in order to derive useful conclusions on the possible environmental impacts in the area around the site of a new industrial installation or in larger areas. This procedure is recommended for cases with complicated flow patterns over irregular terrain or for areas near coastlines. In such cases the dispersion and transport of pollutants could not be achieved with the classical Gaussian models because they are not able to handle important local features accurately. Local circulations such as sea-land breezes or slope flows can influence the dispersion and transport of pollutants in different ways. The results presented in this paper are part of a detailed study for the possible environmental impacts in the Eastern Corinthian Gulf in Greece where an alumina plant will be built. Experimental data, a synoptic classification scheme, and model simulations will help to take all the appropriate measurements during the design of the plant in order to minimize the environmental impacts during its operation.

KEYWORDS: Air pollution, Gaussian model, Mesoscale model, Lagrangian particle dispersion model, Dispersion, Diffusion, Transport

SOFTWARE AVAILABILITY
Colorado State University Mesoscale Model and Lagrangian Particle Dispersion Model original codes are available from Professor R. A. Pielke, Colorado State University, Department of Atmospheric Science, Fort Collins, CO 80523, USA. Modifications for these codes as well as the plotting routines for CALCOMP plotting packages and plotters are available from the author of this paper.

INTRODUCTION
Having advance knowledge of the microclimate, other specific characteristics and the flow behaviour which would lead in pollution episodes of the area where a new plant will be erected, will assist us to take all the appropriate measurements to avoid significant environmental damage from the released air pollutants. In almost all cases, an environmental study for the plant design employs Gaussian type models to study the dispersion of pollutants. The shortcomings however of such models are well known, and in several cases the results are considered unreliable. The reliability of such methods is even lower in cases where the site is characterized by a highly varying topography or is near the coast. In such cases the wind fields in the area are very complicated and the spatial and temporal variations are significant. In these cases an accurate description of the wind fields and detailed description of the dispersion of pollutants is necessary. Following this approach, Pielke, McNider and their collaborators have carried out a number of studies for different areas in U.S.A., Arritt and Pielke [1] had investigated the role of topographically induced mesoscale circulations in pollutant transport in Shenandoah Valley. Yu and Pielke [2] had studied the layered haze phenomenon in the Lake Powell area, Segal et al [3] have studied the impacts of the air pollution from the urban areas of South Florida to the neighboring National Parks. Physick [4] had studied the dispersion characteristics in the Grand Canyon region under various wind and stability regimes while Pielke et al [5] discussed various tools which can be applied on emergency cases, such as accidental toxic or radioactive releases as well as nowcasting air pollution episodes.

In this study some preliminary results from a numerical investigation of the mesoscale circulation and pollutant transport in the area of the Eastern Corinthian Gulf in Greece are presented. The pollutant source is in the area of Thisvi near the northern coast of the Gulf from the proposed alumina plant. The pollutants, mostly sulfur dioxide, result from petroleum combustion. The combusted quantity is estimated to 150 - 170 tons per day. The initial estimate of the stack height is about 100m above the ground level and 130m above the sea level. The topography around this area is very complex and the site is about 1.3km from the coast. To the North of the site, there is a small valley of an elliptical shape with the smaller axis of about 3km and the larger of about 6km. Further to the North there is Mount Elikon with its peak at approximately 1500m. There are also three small populated areas in a distance of 3-5km from the site in the northern end of the small valley. Some other populated areas...
are located from 5-20 km away. The southern coastline of the Corinthian Gulf is also populated, with the largest city of Corinth. The possible transport of pollutants toward south or north when the sea-breeze is the dominant mechanism in the area during the summer is examined. The sea-breeze circulation dominates in this area for a considerable number of days during the summer months. As seen in Figure 1, the coastline has an East-West orientation thus the sea-breeze circulation is expected to have a significant component perpendicular to the coastline.

For this study a two-stage procedure was employed: In the first stage the two-dimensional version of the Colorado State University Mesoscale Model (CSU-M) was used to predict the meteorological fields for the vertical cross-section along the axis shown in Figure 1 by the thick line. In the second stage, a Lagrangian particle dispersion model described by McNider [6] and Pielke et al [7] was used. A brief description of the two models is given below while the capability of this procedure to describe such complex phenomena is briefly discussed.

MODEL DESCRIPTIONS

a. Mesoscale Model

The mesoscale model used in this study was originally developed by Pielke [8] and modified later by Mahur and Pielke [9]. The CSU-M is a hydrostatic, prognostic model based on the primitive equations of motion, energy, continuity, and water content. It uses the terrain-following coordinate system and exchange coefficients for parameterization of the turbulence exchange processes. For the Planetary Boundary Layer (PBL) a detailed parameterization is included where short and long-wave radiative contributions are included in the surface energy balance calculations. The depth of the convective boundary layer is computed from Deardorff’s [10] prognostic equation with Businger’s [11] similarity theory used for the surface layer. The exchange coefficient profile in the PBL was specified by O’Brien’s [12] cubic polynomials. For the case of stable stratification, the local exchange coefficient scheme based on local gradient Richardson number calculations is used. At the uppermost four levels of the model, an absorbing layer is applied to avoid reflections of the generated gravity waves.

b. Lagrangian Particle Dispersion Model (LPDM)

This model uses as input the predicted fields from the mesoscale model described previously. It is a Lagrangian type dispersion model on which the motions of discrete mass elements (which represent the pollutants) are tracked inside the model domain. The position of each particle at time \( t \) is given by

\[
X_i(t+\Delta t) = X_i(t) + (u_{oi} + u_i' + u_i''(t)) \Delta t ,
\]

where

\( \Delta t \) is the time step

\( X_i \) are the spatial coordinates of each particle

\( u_{oi} \) are synoptic-scale wind components

\( u_i' \) are mesoscale wind components

\( u_i'' \) are microscale velocity components (turbulent)

The microscale velocity component \( u_i'' \) is computed from the Markov process

\[
u_i''(t+\Delta t) = R_{ii} u_i''(t) + (1-R_{ii})^{1/2} u_i'(t) + \delta_3(1-R_{ii}^{1/2})W_d
\]

with

\[
R_{ii}(\Delta t) = \exp(-\Delta t/T_{ii})
\]

\( W_d = T_{ij} \lambda \delta / \chi_j \) (\( \delta_j^2 \))

\( R_{ii} \) is the Lagrangian velocity autocorrelation in the \( i \)-th direction

\( T_{ii} \) is the Lagrangian integral time scale for each direction

\( u_i''(t) \) is a random velocity component

\( \delta_3 \) is the Kronecker delta

\( W_d \) is the drift velocity correction

\( r \) is a normal random variate (with 0 mean and 1 variance)

\( \sigma_i \) is the standard deviation of the \( i \)-th microscale velocity component

Synoptic and mesoscale wind components are these calculated directly from the mesoscale model while the turbulent components are deduced from the mesoscale model closure scheme. A more detailed description of this technique is presented in McNider [6], Arritt [13], and Pielke et al [14].

DATA USED

During the period from July 31 to August 3, 1987 a program of extensive measurements in the surface as well as in height was performed in the area near the site of the plant. Model simulations were performed for August 3. During this day the synoptic conditions were favorable for the formation of sea-land breeze circulation in the area. The data used for the initialization of the model were local tethered balloon observations at 02:00 LST for the lowest 1000 m and above this level, the radiosonde observations from Athens airport (located approximately 40 km SSW from the site) at 02:00 LST. These profiles were interpolated to obtain the appropriate data at the model levels. Initial profiles and additional data used for this simulation are shown in Table 1. For more details about the experimental data for this day see Helmis et al [15]. The simulation starts at 02:00 LST and the first three hours were used for dynamic initialization.
...tion, allowing the initial fields to adjust to the terrain before sunrise where the heating of the surface begins. The model coordinates were rotated 90 degrees counterclockwise, therefore in the following figures the left corner corresponds to the South while the right to the North. Terrain data were obtained from maps 1:50000 and were smoothed appropriately.

Table I. Model input data used for simulation of August 3, 1987 case.

<table>
<thead>
<tr>
<th>Height (m)</th>
<th>Potential Temp. (K)</th>
<th>Specific Humid. (g/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>295.20</td>
<td>0.0137</td>
</tr>
<tr>
<td>10</td>
<td>295.21</td>
<td>0.0136</td>
</tr>
<tr>
<td>15</td>
<td>295.40</td>
<td>0.0104</td>
</tr>
<tr>
<td>150</td>
<td>297.00</td>
<td>0.0099</td>
</tr>
<tr>
<td>300</td>
<td>297.90</td>
<td>0.0089</td>
</tr>
<tr>
<td>500</td>
<td>298.22</td>
<td>0.0085</td>
</tr>
<tr>
<td>700</td>
<td>299.50</td>
<td>0.0064</td>
</tr>
<tr>
<td>900</td>
<td>300.50</td>
<td>0.0073</td>
</tr>
<tr>
<td>1100</td>
<td>301.45</td>
<td>0.0070</td>
</tr>
<tr>
<td>1300</td>
<td>302.20</td>
<td>0.0061</td>
</tr>
<tr>
<td>1500</td>
<td>302.75</td>
<td>0.0059</td>
</tr>
<tr>
<td>1800</td>
<td>304.10</td>
<td>0.0057</td>
</tr>
<tr>
<td>2100</td>
<td>305.90</td>
<td>0.0051</td>
</tr>
<tr>
<td>2500</td>
<td>306.15</td>
<td>0.0045</td>
</tr>
<tr>
<td>3000</td>
<td>310.84</td>
<td>0.0029</td>
</tr>
<tr>
<td>3500</td>
<td>314.75</td>
<td>0.0027</td>
</tr>
<tr>
<td>4000</td>
<td>317.10</td>
<td>0.0024</td>
</tr>
<tr>
<td>4500</td>
<td>320.05</td>
<td>0.0022</td>
</tr>
<tr>
<td>5000</td>
<td>323.96</td>
<td>0.0019</td>
</tr>
<tr>
<td>6000</td>
<td>326.94</td>
<td>0.0009</td>
</tr>
<tr>
<td>7000</td>
<td>328.99</td>
<td>0.0005</td>
</tr>
<tr>
<td>8000</td>
<td>331.89</td>
<td>0.0007</td>
</tr>
<tr>
<td>9000</td>
<td>332.99</td>
<td>0.0007</td>
</tr>
</tbody>
</table>

Additional data:
- Albedo: 0.20
- Roughness length: 15 cm
- Surface pressure: 1012. mb
- Sea-surface temperature: 298 K
- Initial PBL height: 350 m
- Horizontal grid interval: 1000 m
- Time step: 10 sec
- Geostrophic wind speed: 3 m/s
- Geostrophic wind direction: 335 deg.
- Soil density: 1.5 g/cm^3
- Soil specific heat: 0.3 cal/degK
- Wetness of the soil: 0.0005
- Soil thermal conductivity: 0.003 cal/cmKs
- Time start: 1200 LT
- Grid points horizontal: 80
- Grid points vertical: 23

**DISCUSSION**

As highlighted above, the modeling area is characterized by a complex terrain and frequent changes from land to sea. In Figure 1 the coastline is oriented along the E-W axis in both sides of the Gulf, so the main features of the sea-breeze mechanism could be represented in two-dimensional runs along a N-S axis. In sea-breeze cases, it is possible to have recirculation of the air-pollutants (Lalas et al. [16], Christidis [17], Pielke et al. [7]). The synoptic flow in this run was 3m/s from NW which is blocked by Mount Elikon in the North. During the morning hours, where the sea-breeze circulation started with a northward orientation near the ground in the northern coast and a southern in the South. In the center of the domain a shallow convergence zone is formed over the mount Gerania, because of the sea-breeze cells developing in both sides of the mount. The sea-breeze cell in the northern side is intensified by the slope flow developed at Mount Elikon because of its orientation. This is the main reason why the vertical development of this cell is extended up to 2Km in this region during the afternoon hours. The return flow is merged with the synoptic circulation, and an intensification in the upper levels is observed. Figures 2a-c display the horizontal wind field component through the N-S axis with positive direction toward North, the vertical velocity field, and the potential temperature field respectively for 14:00 LST, when the sea-breeze mechanism is at its peak. During the night, when the sea-breeze ceases, a slope flow is developed in the slopes of the mountains. In Figures 2a-c the flow and potential temperature fields at 01:00 LST are shown.

The LPDM was used to simulate the movement of 500 particles released at the alunina plant stack. The release was at a fixed time once from a height of 150m above the ground level. The particles served as tracers for the illustration of the combined effects of advection by the wind field resolved from the mesoscale model and the subgrid-scale turbulence. After the release, the positions of these particles were plotted at fixed time intervals. Several releases were performed at different day and night hours for releases at different day and night hours were performed. For releases during the morning hours, when the sea-breeze is developing, the particles moved northward, where a portion impacted onto the slopes of the mountain while the rest of them moved toward South with the return flow. Figures 4a and 4b show the position of the particles one and five hours respectively after the release at 05:00 LST. Because the release occurred at a time where the sea-breeze started to develop, and the flow in the lower levels is relatively weak with small vertical extend, the particles moved initially toward the slopes of the Mount Elikon. Later they moved southward because the return flow from the sea-breeze circulation and the synoptic wind component are from North during the morning hours. The sea-breeze circulation in the lower levels is from North while in the southern is from the South. In the coast of Northern Peloponnese the sea-breeze is fres North. A convergence zone develops over Gerania. Over the sea the stable layer is forming during the day hours. (see Figure 2). Therefore the particles released from the site of the plant and moved in this area followed a complicated path. A portion of them moved toward Peloponnese while the others, trapped within the stable layer over the sea, moved later toward North with the aid of the sea-breeze (Figure 4b). Particles released later dig into the nor during the day moved quickly northward over the slopes of Elikon and later southward with the return flow, reaching the heights of 2-3Km (not shown here). Particles released a few hours before sunset moved initially toward the slopes of the Mount Elikon. Later when the sea-breeze weakens, these particles remain near the slopes of the mountain and start moving downslope toward their release point at a small distance from the ground (see Figure 4c). This is because of the downslope flow developed near the ground during the night hours. For releases during the night hours when the atmosphere becomes more stable, the transport and dispersion of the particles occur in a smaller scale than during the day. The particles remain for longer time around the area of release and moved slowly toward South over the sea. Figure 4d shows the release at 2500 m above the sea level. This is due to the light winds near the surface and the stronger winds aloft. The land-breeze mechanism is not strong enough to maintain its classical configuration and the northern flow dominates in the area. During the morning hours of the next day, the particles remaining near the sea-surface move northward after the sea-breeze mechanism starts again.

**CONCLUSIONS**

This paper briefly discusses the combined use of a mesoscale atmospheric model with a Lagrangian particle transport and dispersion model to study some of the dispersion and diffusion characteristics of pollutants released from a complex stack of a large industrial installation. In such complex terrain the flow fields show temporal and spatial variations and therefore the dispersion characteristics are very significant cannot be described with simple numerical models such as the Gaussian. With the aid of mesoscale models and Lagrangian trajectories we are able to describe accurately the complicated flow fields as well as the dispersion and diffusion of pollutants on an accurate manner. This strategy with the aid of synoptic classification and...
Figure 2. Predicted fields of (a) u component in m/s (interval 1 m/s), (b) w component in cm/s (interval 25 cm/s), (c) potential temperature in degrees K (interval 1 deg.K) at 14:00 LST for 3 August 1987. Only the domain between the grid points 20 and 70 is shown. Broken lines show negative velocities.

Figure 3. As in Figure 2 but for 01:00 LST at 4 August 1997. Contour interval for w is 10 cm/sec.
Figure 4. Particle locations at (a) 1 hour, (b) 5 hours after the release at 08:00 LST, (c) 3 hours after the release at 19:00 LST, (d) 3 hours, (e) 7 hours after the release at 21:00 LST. The release point is marked by an asterisk.
micrometeorological observations can be used to study the dispersion characteristics in order to guide the design of the factory. The conclusions will be used to minimize the environmental impact from the industrial operations. It is obvious that three-dimensional simulations are more appropriate in such cases but even the two-dimensional ones provide useful informations. For the present study, based on these results, several three-dimensional simulations will follow in the near future. Such a procedure can be obviously applied also in the case of accidental toxic releases.

ACKNOWLEDGEMENTS

Support for work reported in this paper was provided by the Hellenic Alumina Industry Inc. I would like to thank my collaborators D.N. Asimacopoulos, C. Helmis, G. Varotsos and D. Deligiorgi for their work on collecting and processing the experimental data in this site and N. Moran for his help on model simulations. I would like also to thank R. Pielke for his support during my visit at Colorado State University during the winter of 1988. Part of these simulations were performed on the NCAR CRAY-XMP computer (NCAR is sponsored by the NSF). Most of the model computations were performed on the CDC CYBER-930 computer at the Control Data Greece Inc computer facilities.

REFERENCES


