

Modeling of Atmospheric Pollutant Dispersion in Complex Terrain – Part II: Development, Validation and Comparison of a Higher-Order Closure Dispersion Model

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1 Introduction

Many of our air-quality related problems are concerned with pollutant transport and diffusion in complex terrain. However, modeling pollutant dispersion in such areas is a difficult task because of the associated complex flow and turbulence. The conventional Gaussian and Eulerian K-theory models are inadequate for modeling dispersion in complex terrain. Alternatively, Lagrangian particle models and higher-order closure models are usually used for this purpose, e.g., Yamada (1985) and Enger and Koracin (1995).

This paper presents a higher-order closure dispersion (HOCD) model, suitable for modeling dispersion in complex terrain. A brief description of the model is presented in the next section. The model has been applied to simulate dispersion in a convective boundary layer (CBL). Comparison of the results with those from tank experiments is done in section 3. The model has also been used to simulate tracer transport and dispersion in the complex terrain, discussed in Part I. The model results are compared with available measurements in section 4.

2 Model Description

The present model is an Eulerian diffusion model, which starts from the mass continuity equation

$$\frac{\partial C}{\partial t} = -U_j \frac{\partial C}{\partial x_j} - \frac{\partial \overline{u'_j c'}}{\partial x_j} + S \quad (1)$$

The corresponding equations for the turbulent fluxes, if we neglect molecular terms and the effect of Coriolis forces on the covariances, are

$$\frac{\partial \overline{u'_i c'}}{\partial t} = -U_j \frac{\partial \overline{u'_i c'}}{\partial x_j} - \overline{u'_i u'_j} \frac{\partial C}{\partial x_j} - \overline{u'_j c'} \frac{\partial U_j}{\partial x_j} - \frac{\partial \overline{u'_i u'_j c'}}{\partial x_j} - \frac{1}{\rho_0} \overline{c'} \frac{\partial p'}{\partial x_i} - \frac{g_i}{\Theta_0} \overline{\theta' c'} \quad (2)$$

The equation for the covariance, $\overline{c' \theta'}$, is

$$\frac{\partial \overline{c' \theta'}}{\partial t} = -U_j \frac{\partial \overline{c' \theta'}}{\partial x_j} - \overline{u'_j \theta'} \frac{\partial C}{\partial x_j} - \overline{u'_j c'} \frac{\partial \Theta}{\partial x_j} - \frac{\partial \overline{u'_j c' \theta'}}{\partial x_j} - D \quad (3)$$

The pressure covariance terms in equation (2) are parameterised according to Enger (1986) as

$$\frac{1}{\rho} \overline{c'} \frac{\partial p'}{\partial x_i} = \alpha_1 \frac{q}{\lambda} \overline{u'_i c'} - \frac{1}{3} \frac{g_i}{\theta_0} \overline{c' \theta'} \quad (4)$$

where α_1 is a constant, and λ is a master turbulent length scale.

The vertical transport term is parameterized using a gradient diffusion approximation according to Donaldson (1973) and Mellor (1973). The molecular destruction term D is parameterized according to Lumley (1975) as

$$D = \alpha_2 \frac{q}{\lambda} \overline{c' \theta'} \quad (5)$$

The values for the constants, α_1 , and α_2 , are 0.3465 and 0.144, respectively. The formulations of the master length scale, λ , are described in Enger (1990). A finite-difference numerical method is used to solve the set of model equations. The model uses an expanding telescoping grid mesh with its origin at the source. This means that we get a more dense grid mesh near the source, where the plume is narrower than further downstream. The prognostic equations in the dispersion model are solved by using a third-order advection scheme, described in Enger and Grisogono (1997). The diffusion is solved with a semi-implicit scheme with weight 0.75 on the future time step. The Arakawa staggered C-grid is used for the model structure. The following boundary conditions are applied at the top of the model

$$\frac{\partial C}{\partial z} = \frac{\partial \overline{w'c'}}{\partial z} = \overline{u'c'} = \overline{v'c'} = \overline{c'\theta'} = 0 \quad (6)$$

and following at the surface

$$\frac{\partial C}{\partial z} = \overline{w'c'} = \frac{\partial \overline{u'c'}}{\partial z} = \frac{\partial \overline{v'c'}}{\partial z} = \frac{\partial \overline{c'\theta'}}{\partial z} = 0 \quad (7)$$

3 Model Simulations in Horizontally Homogenous CBL

The model is used to simulate the characteristics of plume dispersion in a CBL with point sources at 0.62, 0.25 and 0.5 of the boundary layer height. A one-dimensional version of the MIUU mesoscale model was used to simulate an ideal CBL, used in the dispersion model. The CBL height, obtained as the height of minimum heat flux, is about 846 m, with a mean wind speed of about 2.3 m/s. The convective velocity scale is calculated to 1.1 m/s. The CBL is similar to those used in the Deardorff and Willis tank experiments (Deardorff and Willis, 1975; Willis and Deardorff, 1978, 1981). It satisfies the same criteria, i.e., $1.5 w_* < U < 6 w_*$.

Contour plots (in the x-z plane) of the dimensionless crosswind integrated concentration, simulated by the model with different source heights are presented in Figure 1. The results are compared with results from the tank experiments. We can see, that the simulations show the significant features of dispersion in CBLs, as observed in the tank experiments, remarkably well. The model captures the rise and descend of the plume. Also, the 'rebound' of the plume after striking the surface, or the inversion layer above, is equally well simulated. The maximum and minimum concentration values, including their locations, agree very well with the results from the tank experiments.

4 Model Simulation in Complex Terrain

Moreover, the model was used to simulate pollutant transport and dispersion at Colorado River valley during the period of an intensive field program, the Measurement of Haze and Visibility Experiment (MOHAVE). The topography of the area with the domain, used in the presented dispersion simulation, is shown in Figure 1 of Part I. One of the main objectives of the field experiment was to investigate and identify the possible short- and long-term impacts of atmospheric pollutants from major urban areas and industrial sources (especially from Mohave Power Plant, MOPP) on the Grand Canyon and its vicinity. In the field experiment, PTF ortho-perfluorodimethylcyclohexane (oPDCH) was released continuously from MOPP during 50 days in summer. Forty-five percent of the oPDCH consists of the isomer ortho-cis (oc)PDCH, which was measured at the receptor sites. The tracers are inert, non-depositing, and non-toxic chemicals. The stack height of the power plant is 150 m. The effective source height is calculated to be about 300 m AGL. Thus, for the present study an effective source height of 300 m AGL was used. The average release rate of oPDCH for the period is about 0.042 g/s. Details on the experiment and measurements can be found in Green (1999) and Isakov (1998). The measurements used for model comparison in the present study are obtained from Isakov (1998), but converted from femtoliters per liter (fl/L) to micrometer per unit volume ($\mu\text{g}/\text{m}^3$).

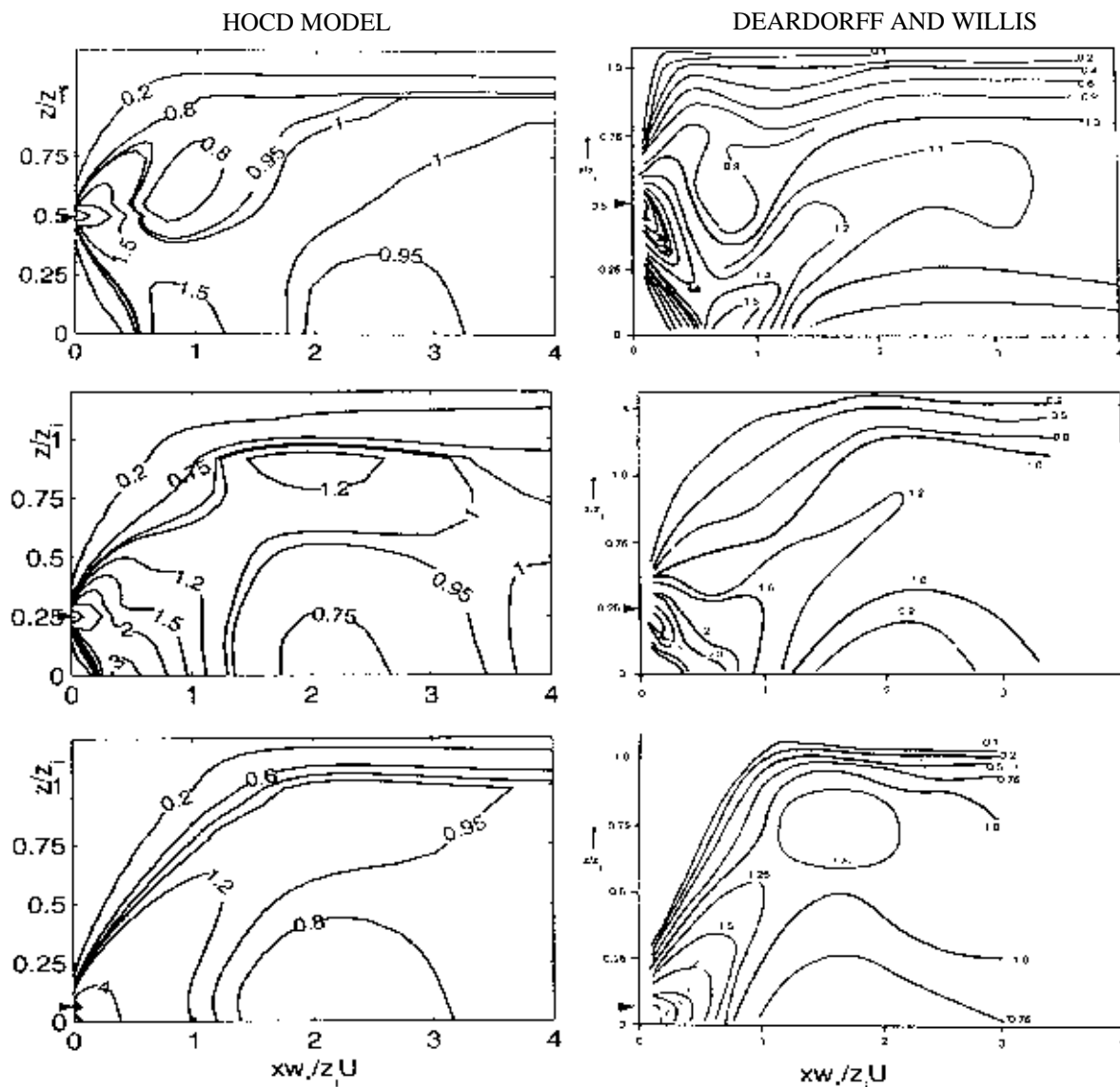


Figure 1 Contours (in x - z plane) of the dimensionless crosswind integrated concentration simulated by the HOCD model (left) and those from Deardorff and Willis (right) for source heights of $0.06 z_i$, $0.25 z_i$ and $0.5 z_i$. Sources are indicated by arrows on the ordinate.

Dynamic flow and turbulence fields over the study area were simulated with the MIUU model for the period 5/8/92 – 14/8/92. The results are discussed and compared with measurements in Part I. For the present study, only the results of the first three days were used. For use in the dispersion model, the MIUU results, which are stored at 1-hour intervals, were firstly interpolated to five-minute intervals. Thereafter, the results were interpolated to the dispersion model grid points. Figure 2a and b show the interpolated horizontal wind vectors at 100 m AGL at 1200 MST (Mountain Standard Time) on 5/8/92 and 1700 MST on 6/8/92. Note that the wind vectors are plotted only at every fifth grid point. Terrain and receptor sites are shown in the background. The results generally show southerly and southwesterly flow in the area. The southerly flow is stronger along the Colorado River valley and follows the bending shape of the valley. Effects of anabatic and katabatic winds along the mountain slopes, due to horizontal pressure gradients created by temperature differences, are visible in the simulated flow at 1200 and 0700 MST, respectively, especially around SPMO and the adjacent mountains.

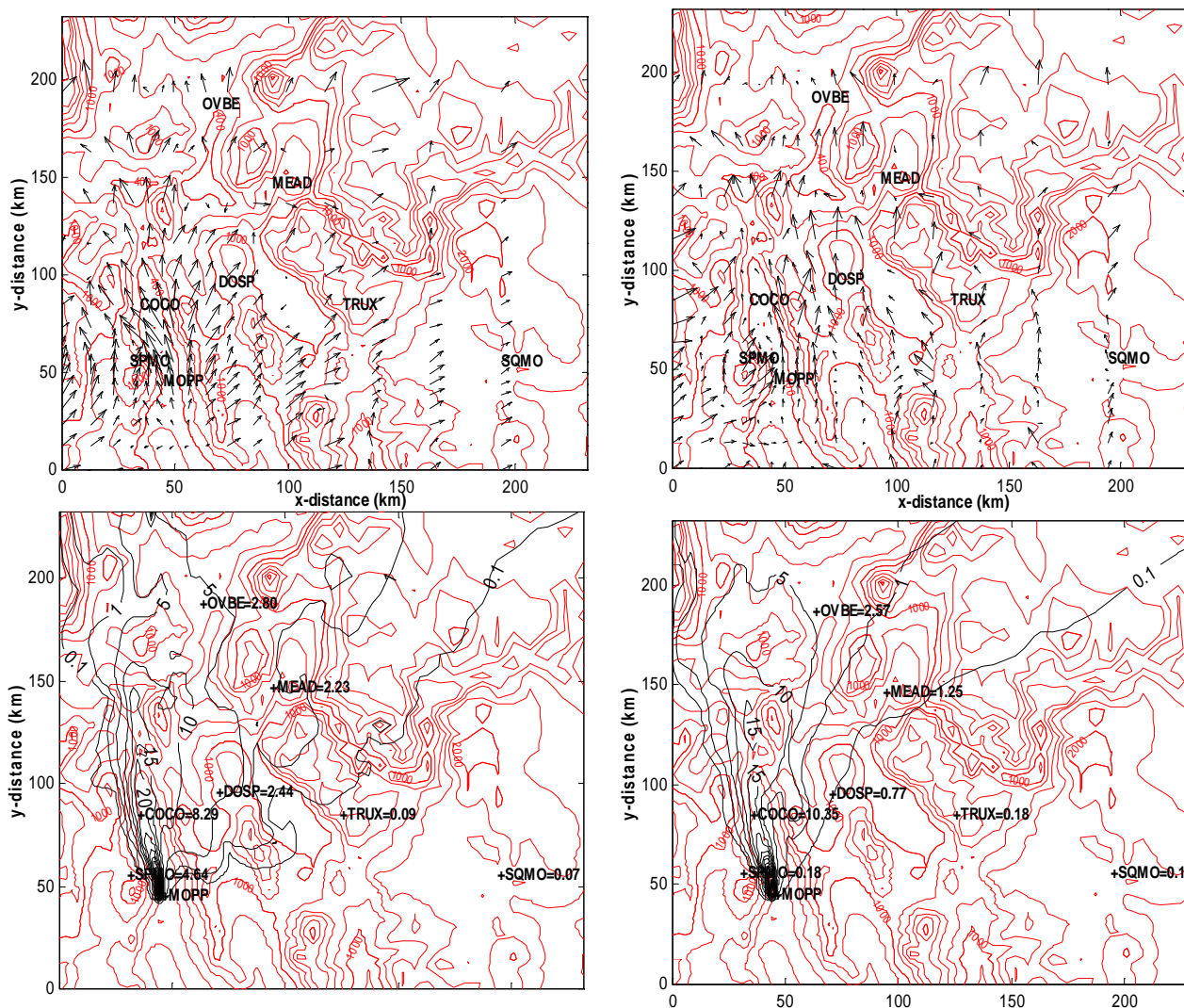


Figure 2 Model simulations in complex terrain (Colorado River valley) during the MOHAVE field program in summer 1992. Panel (a) and (b) show horizontal wind vectors at 100 m AGL interpolated from the MIUU model results at 1200 MST on 5/8/92 and 0700 MST on 6/8/92, respectively. Maximum vector length is 13 m/s and 19 m/s, respectively. Panel (c) and (d) show the HOCD daily mean of the simulated surface concentration at 0700 MST on 6/8/92 and 7/8/92, respectively. Terrain, receptor locations, and mean concentration measurements are shown in the background. The values of both simulated and measured concentrations are in $10^{-5} \mu\text{g}/\text{m}^3$.

Tracer release was represented in the dispersion model by a uniformly distributed area source, extending over the nearest four horizontal and three vertical grid points from the source location. The horizontal grid domain used is 81×81 km, with 1 km resolution close to the source. In the vertical, we use 31 grid points, with 50 m resolution close to the release height. Simulated release started at 1200 MST on the first day and continued until 1200 MST on the third day. The daily-mean simulated surface concentrations at 0700 MST on the second and third day are presented in figure 2(c) and (d), respectively. Terrain, receptor sites, and mean measured concentrations at 0700 MST on the two days are shown in the background. The values of both simulated and measured concentrations are in $10^{-5} \mu\text{g}/\text{m}^3$.

From the figure we can see that the simulated concentrations are in the same order of magnitude as the measured ones. The difference between the concentrations could be due to the fact, that the release of pollutants in the model did not start at the same time as in the field experiment. Also, insufficient spatial resolution of both the mesoscale and the dispersion model can affect the model re-

sults. Nevertheless, the agreement between simulated and measured concentrations is quite good. The model was able to reproduce the spatial pattern of the concentrations over the domain. The model results show, that, during stable conditions, the pollutants are transported aloft few kilometers downwind before reaching the ground surface. During unstable conditions, however, the pollutants reach the ground surface in the vicinity of the release point due to stronger vertical mixing. Moreover, the model simulations show that part of the tracer released from MOPP is transported to Grand Canyon and its vicinity.

5 Conclusions

A higher-order closure model suitable for dispersion in complex terrain is developed. The model-simulated features in CBL-dispersion with different source heights have been discussed. The results are in very good agreement with those from tank experiments. Also, the model is applied over a complex terrain near the US South-West Coast, to study transport and diffusion of tracers released at MOPP during the MOHAVE 1992 field experiment. The simulated pattern and magnitude of concentrations are in good agreement with measurements, made during the experiment. The model results also show, that part of the pollutants released at MOPP is transported to Grand Canyon and its vicinity. The simulations will be refined in the future with higher grid resolution to obtain better results. Also, the dispersion model simulations would be extended to cover the entire period of the field experiment.

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