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A NUMERICAL MODEL STUDY OF PLUME FUMIGATION DURING NOCTURNAL INVERSION BREAK-UP

MORDECAY SEGAL, YTZHAQ MAHRER† and ROGER A. PIELKE
Department of Environmental Sciences, University of Virginia, Charlottesville, Virginia 22903, U.S.A.

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Abstract—The elimination of the ground based nocturnal inversion during the morning hours may be associated with very high surface pollutant concentrations, as elevated plumes fumigate into the developing mixed layer. The common approach of studying this phenomenon is based on the application of Gaussian plume model concepts using prescribed meteorological data. Such a methodology, however, is deficient during fumigation when the meteorological fields are spatially and temporally non-homogeneous. In the present study a more appropriate approach is suggested. A three-dimensional numerical solution of the advection–diffusion equation in a fine mesh grid has been carried out for an elevated source. The dispersion data is provided by a numerical boundary layer meteorological model. A simulated fumigation event is illustrated and discussed.

1. INTRODUCTION

The elimination of the ground based nocturnal inversion, as the planetary boundary layer* (PBL) with its turbulence develop following sunrise, may be associated with a temporary increase of surface pollutant concentrations as elevated concentrated plumes fumigate the growing PBL. Although this phenomenon must be considered when evaluating air quality patterns from tall stacks, relatively little research attention has been focused on it compared with other plume dispersion topics. This relative lack of study may be due to the difficulty of investigating unsteady boundary layers as they grow rapidly during the early morning hours. Accurate representations of fumigation, however, require a precise description of the non-steady PBL, in addition to an air pollution model with the capability to respond to changes in PBL structure.

Early quantitative tall stack fumigation studies which are reviewed by Gifford (1968), as well as more recent ones, such as the comprehensive observational study of Thomas *et al.* (1970), and Wang (1977), are based on the application of Gaussian plume model concepts in which prescribed or measured meteorological data are used. The variability of the spatial and temporal dispersion conditions during such an episode, however, is in disagreement with the requirements of vertical homogeneous structure within the PBL and of steady state conditions of the Gaussian models. Consequently, a major simplification of actual atmospheric dispersion properties results when adopting this methodology.

Our current status of understanding of air pollution dispersal [e.g. as discussed by Hanna *et al.* (1977)] has indicated the need for much more theoretical and experimental work regarding the accurate assessment of the fumigation process. Besides the need for more physical understanding, high resolution observed meteorological data is also required for the accurate description of this process. Such information is generally lacking.

The present study involves a realistic and comprehensive approach to study the fumigation process, where a three dimensional numerical solution of the advection–diffusion equation on a fine mesh grid has been carried out for an elevated source plume. The meteorological data is provided by a one dimensional numerical mesoscale model with a relatively sophisticated and accurate representation of the PBL structure. Based on this approach, preliminary simulated results illustrating the dispersion and ground level concentration patterns when fumigation occurs during nocturnal inversion break-up, are reported and discussed.

2. THE METEOROLOGICAL MODEL

The University of Virginia numerical mesoscale model (Pielke, 1974) with its last published modifications as reported by Mahrer and Pielke (1978), has been adopted for providing the dispersion data. In the current model, a more realistic approach to the determination of the vertical exchange coefficient, K_z,

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* Same as the so-called mixing layer.

† Present address: Department of Soil and Water Sciences, The Hebrew University of Jerusalem, Israel.

during the nocturnal regime has been introduced (McNider and Pielke, 1981). As reported in that paper, calculation of K_z values, which are dependent on the local gradient Richardson number, the critical Richardson number, the mixing length and the local wind shear is adopted when surface heat fluxes are positive (i.e. when the surface layer atmosphere is stably stratified). When heat fluxes change sign after sunrise, K_z calculations switch to the original profile formulation given in Pielke and Mahrer (1975).

In the preliminary experiments reported here, the numerical meteorological equations are integrated using a one dimensional version of the model (i.e. horizontal homogeneity of terrain and forcing functions are assumed), while in the vertical, 26 layers at 0, 10, 22.5, 40, 62.5, 87.5, 112.5, 137.5, 162.5, 187.5, 225, 275, 325, 375, 425, 475, 550, 650, 750, 850, 1050, 1350, 1750, 2500, 4000 and 5000 m are used. Starting at 2000 LST (following sunset) the model is integrated for the next 12 h using a 45 s time step. The predicted meteorological data, namely the vertical profiles of velocity, eddy diffusion coefficients and temperature have been used as input for the dispersion model simulation. The initial profiles of the temperature and humidity are typical of midsummer over central Israel where the occasional merging of the nocturnal surface inversion and low based upper layer inversion creates a deep stable layer. A geostrophic wind, $U_g = 2.8\,\mathrm{m\,s^{-1}}$; $V_g = 0$, is used for the initialization of the flow. A roughness parameter, $z_0 = 4\,\mathrm{cm}$, has been adopted.

3. THE DISPERSION MODEL

The dispersion model is based on the three dimensional advection–diffusion equation:

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} + \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + S \quad (1)$$

where C is concentration, K_x, K_y and K_z are the eddy diffusion coefficients and S is the source intensity (K_z corresponds to the eddy exchange coefficient for heat in the meteorological model). In the present stage of simulations, only the u-component of the horizontal wind has been used for the advection, although the v-component formed due to the Ekman veering could have some effect on the concentration field. The diffusion term in the flow direction has been omitted since it is small compared with the advection term. Hence, the model in this study is composed of a unidirectional flow in the x-direction associated with lateral, y, and vertical, z, diffusion.

The advection term is solved by using a cubic spline scheme which, as reported by Pepper *et al.* (1979), is an accurate representation for the advection of pollution. Their suggested horizontal filter with a coefficient of $\delta = 0.01$ has been used to eliminate aliasing associated with the numerical representation of the nonlinear components of (1). A modification of the Crank-Nicholson scheme suggested by Paegle *et al.* (1976) is adopted for the diffusion terms.

3.1 *Boundary conditions*

In the vertical: $C = 0$ at the model top and

$$K_z\frac{\partial C}{\partial z} = 0 \text{ at } z = 0. \quad (2)$$

These boundary conditions assume negligible concentrations at the top and a reflective surface with zero flux at the bottom.

The domain lateral size has been specified so as to contain most of the plume. Nevertheless, care must be given to the choice of boundary conditions on the lateral boundary in order to avoid reflection or absorption relating to the diffusion term, mainly at large distance from the source. Based on the steady state solution of the advection–diffusion equation [e.g. Sutton (1953)] we have approximated the diffusion fluxes on the lateral boundary as follows:

$$\left(K_y\frac{\partial C}{\partial y}\right)_B = \left(K_y\frac{\partial C}{\partial y}\right)_{B-1}\cdot\frac{y_B}{y_{B-1}} \times \exp\left[-\frac{u}{4xK_y}\cdot(y_B^2 - y_{B-1}^2)\right] \quad (3)$$

in which y_B is the distance of the lateral boundary from the plume axis; and $y_{B-1} = y_B - \Delta y$, where Δy is the lateral grid interval. At the longitudinal boundaries

$$\frac{\partial C}{\partial x} = 0. \quad (4)$$

3.2 *General aspects*

In order to resolve the plume, a fine grid is needed in the direction where diffusion is dominant. Grid intervals of $\Delta y = 50\,\mathrm{m}$ were used in the y direction while in the vertical the meteorological model resolution is adopted. In the x direction, dominated by advection, a 1000 m grid interval has been chosen. The model lateral and longitudinal domain sizes are 2000 and 28000 m, respectively. The integration time step is 45 s.

A continuous source has been located at 325 m height to approximate an effective stack height of a medium utility power plant under the prevalence of thermally stable conditions. However, when the PBL exceeds this height during the morning hours, the source elevation has been increased, correspondingly, in order to approximate an effective height which is in agreement with the new thermal stratification. The vertical exchange coefficients, K_z, for the advection–diffusion model are predicted by the meteorological model, while the lateral exchange coefficients, K_y, are determined from the K_z values as a function of the thermal stratification.

Sensitivity simulations with different functional forms relating K_y to K_z of the form given in Fabrick *et al.* (1977), have indicated possible changes of surface

Table 1. K_y/K_z as function of vertical thermal gradient (from Fabrick *et al.*, 1977)

$\Delta T/\Delta Z$ (°C/100 m)	< -1.9	-1.9 to -1.7	-1.7 to -1.5	-1.5 to -0.5	-0.5 to 1.5	> 1.5
K_y/K_z	0.5	0.75	1.05	1.4	1.7	2.0

concentration by a factor of 2 at long distances, depending on the functional form chosen. These differences, however, decrease toward the source. We have adopted the K_y/K_z values as recommended in that paper (see Table 1).

4. RESULTS

No data are available to verify the meteorological and the advection–diffusion model for this specific situation. However, boundary layer predictions using this meteorological model (in its one dimensional version) have been compared with observations in other situations, as reported, for example, by Pielke and Mahrer (1975), Mahrer (1979) and McNider and Pielke (1981). These studies have demonstrated that the meteorological model yields accurate prediction of velocity and temperature within the PBL. Two and three-dimensional versions of this meteorological model on the mesoscale have, also, been applied and objectively validated as reported, for example, in Pielke and Mahrer (1978) and Segal and Pielke (1981).

Advection diffusion models considering emissions from elevated sources have been shown in validation studies to be a reasonable tool for a quantitative evaluation of pollutant dispersion (e.g. Shir and Shieh (1974), Runca *et al.* (1975), Fabrick *et al.* (1977), Marziano *et al.* (1979)).

4.1 *Meteorological patterns*

At sunrise (0500 LST) the nocturnal surface temperature inversion is about 140 m deep, merging with an upper stable layer which is capped aloft by a second inversion (Fig. 1). By 0700 LST and 0730 LST, a well-defined adiabatic layer is predicted from the surface to the source elevation, indicating an intensive inversion break-up process. The vertical profile of the u-component is presented in Fig. 2. A low altitude and slight nocturnal jet at 0500 LST is converted to a constant u-profile above 150 m at 0700 LST, while some wind shear persists in the lower 150 m surface layer. The changes in both profiles is controlled by the magnitude of the exchange coefficients for heat and momentum as illustrated for several selected times in Fig. 3 (in this figure K_z is that of heat). The determination of K_z within the PBL is highly dependent on the PBL depth and is altitude dependent with a maximum at about one third of the PBL depth. The PBL depth growth rate, which is about 20 m per 10 min preceding its arrival to the level of the base of the upper layer inversion (around 0700 LST), slows for a period of time after attaining that height (Fig. 4).

4.2 *Surface concentration*

The dispersion model has been initialized by the meteorological predictions obtained 1 h before sunrise. Using these meteorological data, the advection–diffusion model is integrated for 5 h in order to obtain a steady-state nocturnal plume representation. The calculated Richardson number around the plume elevation was larger than the critical Richardson number, indicating that negligible eddy diffusion effect has been predicted by the meteorological model. As a result, a thin and longitudinal homo-

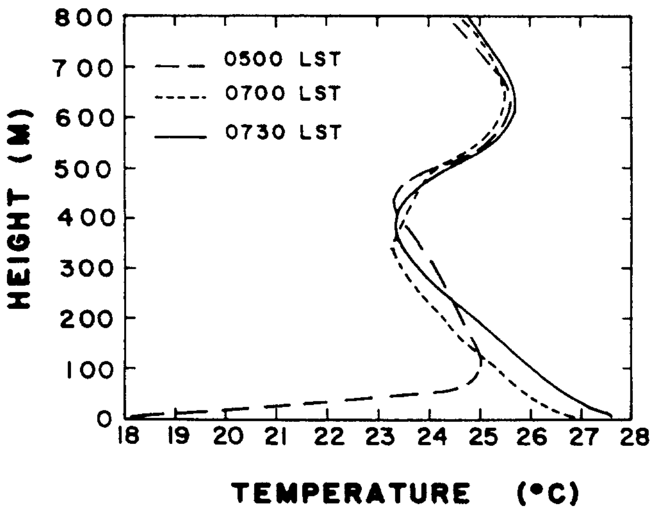

Fig. 1. Vertical profiles of the predicted temperature at three selected times.

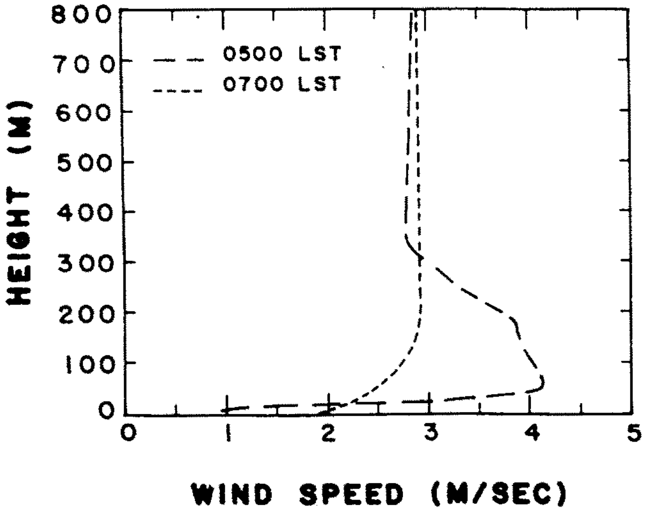

Fig. 2. Profiles of the u-component of wind velocity at sunrise (0500 LST), and while the mixing layer is developing (0700 LST).

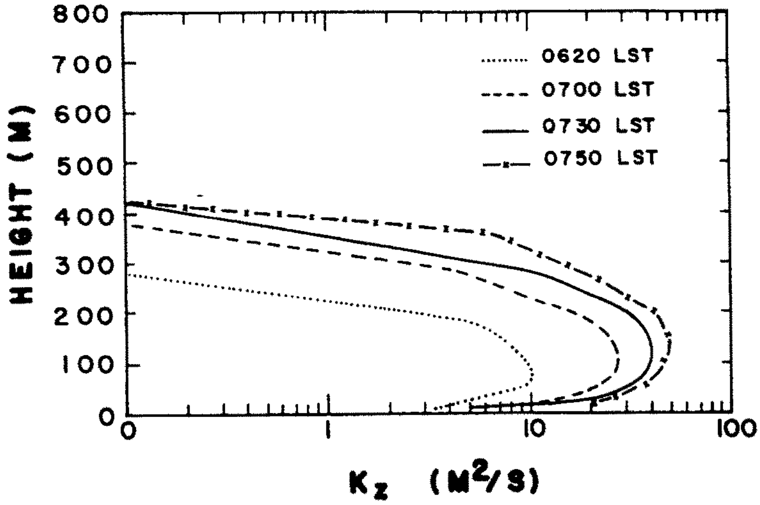

Fig. 3. Profiles of the predicted heat exchange coefficient, K_z, at several selected times.

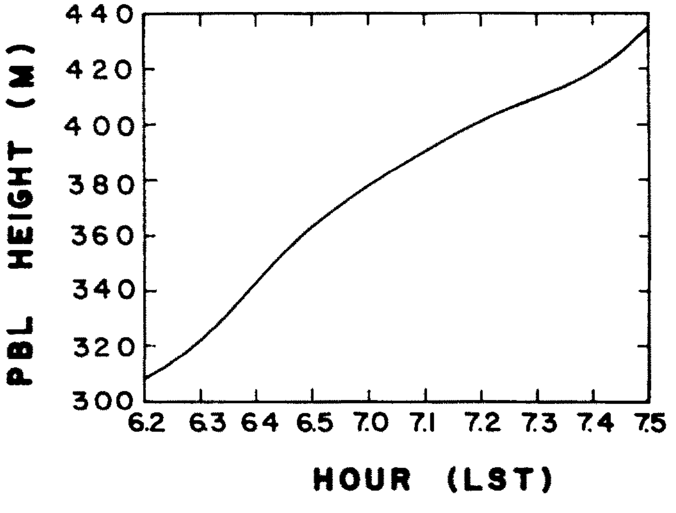

Fig. 4. The PBL height during the morning hours (beginning at 0620 LST).

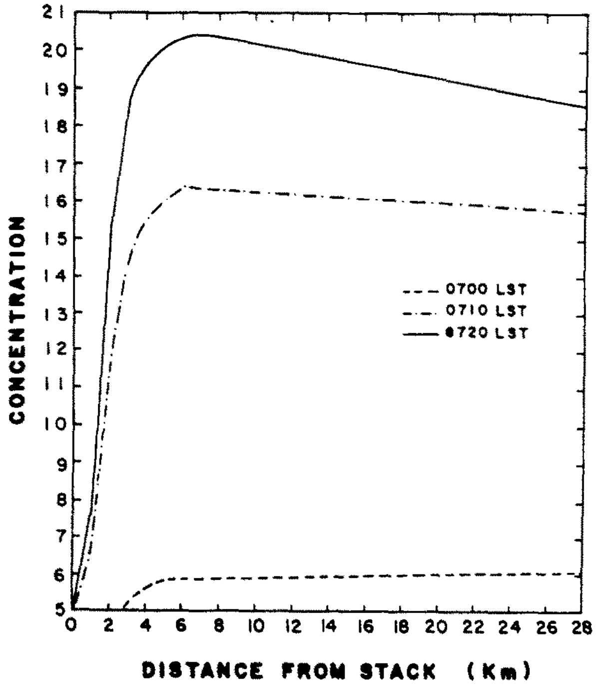

Fig. 5. Surface concentrations along the plume axis for several selected times (a relative concentration of 10 corresponds to $1000\,\mu g\,m^{-3}$ if the source intensity is $10^9\,\mu g\,s^{-1}$).

geneous plume with no surface concentration developed when initializing the dispersion model. This homogeneous structure is approximately conserved during the fumigation process as illustrated in Fig. 5. The peak of the surface concentration occurred at 0720 LST, about 6 km from the stack, followed by only a slight reduction with distance. The duration of the fumigation peak was about 600 s.

While analyzing the results the following points have to be considered:

(i) Veering of the wind height is not represented in the plume model; however, as indicated by the observational study of Johnson and Uthe (1971), it can play an important role in the determination of fumigation surface concentrations from tall stack plume.

(ii) The adjustment of the source height to the changing thermal stratification, while interpreting its elevation as an effective stack height, was estimated conservatively, as no stack emission parameters have been considered. Generally, an earlier adjustment of source elevation to higher levels would lead to lower peak values of concentrations and their locations would be shifted downwind. This would not be the case, however, when the nocturnal jet maximum is above the plume elevation at sunrise. (According to the Gaussian methodology, e.g. Carpenter *et al.* (1971), the calculation of the surface peak concentrations due to fumigation are based on the evaluation of trapping of the advected plume which existed when the inversion break-up reaches the top of the stack. Although this approach is logically reasonable when the flow is vertically homogeneous, it fails when positive vertical wind shear dominates aloft, because advected plumes which originated at higher levels at later times could fumigate in the same location as the original plume)

(iii) Changes of the surface roughness parameter (z_0) will affect eddy diffusion.

Although further study is needed regarding these points, we have considered the effects of thermal stratification and vertical shear of the longitudinal wind at the plume elevation at the prefumigation period as primary influences to be analyzed. These factors, since they influence the Richardson number and therefore the K_z values, will affect the degree of conic spread of the plume during the nocturnal period, consequently affecting the longitudinal concentration distribution when fumigation does occur. Meteorological model simulations with slight changes in the initial thermal stratification and some initial vertical shear of the horizontal wind at source levels have indeed indicated the occurrence of intensified eddy diffusivity there.

To test this effect we have used the meteorological model data as input; however, the predicted K_z values as used in the dispersion model have been limited to be no lower than a specified minimum value in order to examine the sensitivity of dispersion to such factors as slight changes in the vertical gradient of potential temperature or of increasing the wind shear. Figure 6 illustrates the plume development using K_z

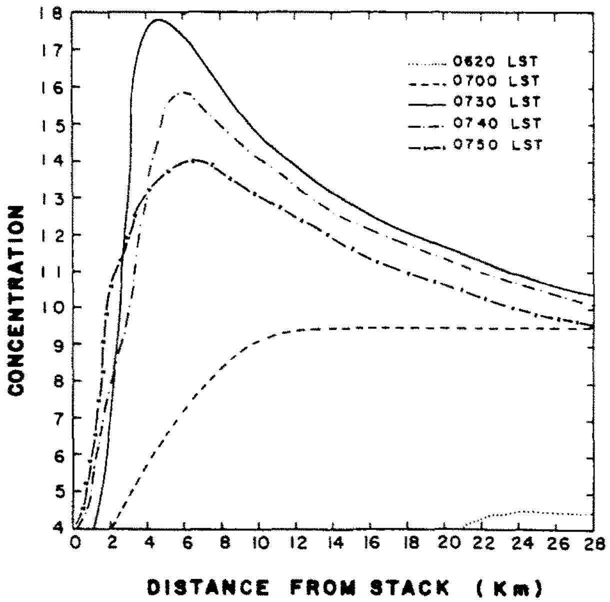

Fig. 6. Same as Fig. 5 except for the modification imposing K_z to be no lower than 0.5 $m^2 s^{-1}$.

= 0.5 $m^2 s^{-1}$ as a limiting value (the plume itself may generate some turbulence, and therefore enhanced dispersion, due to its different radiative properties). With this change, at 0620 LST far enough downwind from the stack, the conic shaped plume is close enough to the ground to be entrained in and mixed downward in the growing PBL, leading to increases in surface concentration there. As the mixed layer develops further, the enhancement of eddy diffusivity and its continued vertical penetration is accompanied by additional increases of concentrations. The locations of maximum surface pollution also spread in the upwind direction (0700 LST). At 0730 when the PBL is already about 90 m above the elevated plume core, the large values of eddy diffusivity intensity along with the length of time of mixing have been sufficient to cause substantial fumigation with a peak value about 4.5 km from the stack. The duration of the high level concentration (~18 units) was for about 600s. Subsequent increase in turbulence intensity (affecting also the lateral spread of pollutants) as well as the deepening of the PBL reduces the maximum values as they are shifted downwind due to the advection effect (0740, 0750 LST).

As the plume acquires a larger conic spread compared with the previous simulation, fumigation begins earlier and the peak concentrations are closer to the source. A series of sensitivity runs with lower limiting values than $K_z = 0.5\ m^2 s^{-1}$ have indicated the gradual transfer from the longitudinal highly inhomogeneous surface concentration patterns as described in Fig. 6 to the essentially uniform pattern shown in Fig. 5.

5. CONCLUSIONS

Although further evaluation experiments are needed, the present modeling approach provides an appropriate methodology to describe the fumigation during nocturnal inversion break-up. Preliminary simulations have implied possible effects of vertical wind shear (i.e. from the large scale flow; or from a mesoscale induced intensive nocturnal jet) and vertical temperature gradient during the night hours on the longitudinal surface concentration distribution as fumigation occurs. The results suggest, however, that although the longitudinal distribution of surface concentrations can significantly vary due to small changes in these parameters, the peak values of the concentrations are almost unaffected.

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