

Study on the Thermal Internal Boundary Layer and Dispersion of Air Pollutant in Coastal Area by Numerical Simulation^①

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ABSTRACT

In this paper, a scheme on a mesoscale dispersion modeling system was set up. The modeling system was used to study the turbulence structure of TIBL and dispersion features under shoreline fumigation situation. The modeling system has successfully solved the problem of meteorological input of stochastic dispersion models and exploited a new approach to comprehensive application of this kind of dispersion models.

Key words: Atmospheric Dispersion; Thermal Internal Boundary Layer; Numerical Simulation

I. INTRODUCTION

Many power plants, industrial enterprises, nuclear reactors, and other potentially pollutive installations are located in coastal area. The coastal thermal internal boundary layer (TIBL) is one of the most important and interesting atmospheric processes along shoreline, because it has some distinct turbulent features and has great influence on the dispersion of contaminant.

The dispersion model should be able to handle the unique meteorological phenomena in coastal area. Most fumigation models are Gaussian models and assume smooth growth of the TIBL and the instantaneous perfect vertical mixing of an entraining plume. The validity of these assumptions is questionable. The Lagrangian particle dispersion model avoids the above assumptions and has some advantages over other dispersion models. Recently, it was demonstrated by some researchers that the Lagrangian particle dispersion model was suitable to the simulation of fumigation dispersion (Luhar et al., 1990; Hurley et al., 1991).

Firstly, the Lagrangian stochastic model was set up and applied to the fumigation phenomenon over the shoreline area in this paper. The irregular shape of the TIBL profile was considered. Secondly, a mesoscale dispersion modeling system during shoreline fumigation was set up. A second-order closure model provides meteorological wind and turbulence fields, as well as the TIBL profile, for input of the Lagrangian particle dispersion model. Finally, some sensitivity tests were performed.

II. AN APPLICATION OF LAGRANGIAN STOCHASTIC MODEL TO DISPERSION DURING SHORELINE FUMIGATION

In recent years, Lagrangian stochastic modelling has become popular with the simulation of atmospheric diffusion, particularly in complex flows where many other techniques are

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inappropriate or invalid. The model is of simplicity in concept and application, and requires limited programming and computer resource.

In the Lagrangian particle dispersion model applied to dispersion during shoreline fumigation, a number of particles were released from their source continuously. When a particle intersects with TIBL interface, it was entrained into TIBL and was carried to the ground via convection. Then, it was reflected between the ground surface and the TIBL interface continuously. The particle trajectory equations are as follows:

$$X_i(t + \Delta t) = X_i(t) + (v_i + v'_i)\Delta t, \quad (i = u, v, w) \quad (1)$$

where v_i denotes mean wind velocity; Δt is time step; v'_i denotes the turbulence fluctuation velocity which may be obtained from Markov Chain simulation, i.e.

$$v'_i(t + \Delta t) = v'_i(t)R_i + (1 - R_i^2)^{\frac{1}{2}}\sigma_i\gamma + (1 - R_i)T_H\frac{\partial\sigma_i^2}{\partial z}\delta_{3i}, \quad (i = u, v, w) \quad (2)$$

where R_i ($i = u, v, w$) is auto-correlation coefficient and it is taken simply as exponential form; σ_i is the standard deviation of fluctuation velocity; γ is a Gaussian random number, T_H is the Lagrangian time scale. The last term is drift correction to the vertical velocity (Legg and Raupach, 1982). δ_{3i} is Kronecker denotation.

The TIBL interface generally increases parabolically to inland from the shoreline until an equilibrium height is reached. However, it was found in the experiment that the TIBL interface presented local fluctuation. So this feature might have important influence on dispersion. According to Deardorff and Willis (1982), the variation of Z_i (the top of TIBL) is

$$\Delta Z_i = \left(0.2 + 4\frac{W_e}{W_*}\right)Z_i, \quad (3)$$

where W_e is entrainment rate and W_* is the scale of convection velocity. It was assumed that the particles intersected with variable TIBL interface in an equal probability during the modeling.

The parameterizations of σ_i and T_H ($i = u, v, w$) are one of the key problems in the random walk model. Out of the TIBL, stable stratification is assumed. Within TIBL, air is in convective state. The different fitting formula (Hanna, 1982) was used in the model. The variable time step $\Delta t = 0.1T_{iw}$ was used and then the statistical numbers of the particles in the different grid cells were calculated to obtain the pollutant concentration. Complete reflection on ground surface and at the top of the TIBL was imposed.

Some relevant data of Nanticoke Shoreline Fumigation Project on the Northern Shore of Lake Erie (16:00 June 6, 1978) was inputted to present model. The distribution of ground level centerline concentration of SO_2 was simulated (see Fig. 1). The figure also shows the field observations[1] and results of some fumigation dispersion models, such as the Misra model[2], the modified Misra model[3] and Deardorff and Willis model[4]. It shows that the maximum is in accordance with observation, except for the location of the maximum. The performance of the model is superior to other fumigation dispersion models, so that the Lagrangian stochastic approach is suitable for simulation of fumigation dispersion in shoreline regions.

III. A MESOSCALE SIMULATION SYSTEM OF FUMIGATION DISPERSION IN SHORELINE AREAS

1. Control Experiment and Its Validation

In Section II, a set of fitting formulas of σ_i ($i = u, v, w$) was used as input of the Lagrangian stochastic model. However, these fitting formulas were inappropriate in complex terrain. One of the most feasible approaches is to use a prognostic PBL model for simulating the flow fields and the TIBL structure under the sea-breeze condition. Meanwhile, the PBL model can offer the wind and turbulence parameters needed for a dispersion model. In the past decades, a mesoscale atmospheric dispersion modeling system has been used successfully (Segal et al., 1988a, b; Jiang et al., 1990). However, the use of a K -model to study the turbulence structure and dispersion would be inappropriate due to the complication of the turbulence features under the TIBL condition and the somewhat coarse resolution.

Our modeling system was composed of two numerical codes, a second-order closure PBL model and a Lagrangian particle dispersion model. Detailed discussion of the formulation and preliminary applications of the PBL model can be found in Jiang's papers (Jiang et al., 1992, 1993). The meteorological wind and turbulence fields were provided by the PBL model. After Kao and Yamada(1988), the standard deviations of the fluctuation velocities were presented as follows:

$$\sigma_u = (\overline{u'^2})^{\frac{1}{2}} + C_H \Delta X \left| \frac{\partial u}{\partial x} \right|, \quad (4a)$$

$$\sigma_v = (\overline{v'^2})^{\frac{1}{2}}, \quad (4b)$$

$$\sigma_w = (\overline{w'^2})^{\frac{1}{2}}, \quad (4c)$$

where $C_H = 3$ is an experimental constant. Height of the TIBL profile was determined by calculated potential temperature field from the prognostic model.

The dispersion modeling system has been run to estimate pollutant concentration from an elevated point source posited on the shoreline in fumigation situation under typical onshore flow condition.

Simulated results from the PBL model show that there are obvious fluctuation and changing slope on the top of the TIBL (Jiang et al., 1992). It is in accordance with some observed profiles (Fritts, 1980). It is believed that the spread of the particles in the TIBL will be under the influence of this feature seriously. Fig. 2 presents the profiles of $\overline{u'^2}$, $\overline{v'^2}$, $\overline{w'^2}$ at

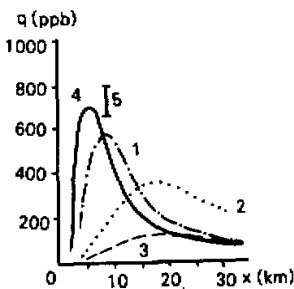


Fig. 1. The distribution of surface centerline concentration (16:00, June 6, 1978).

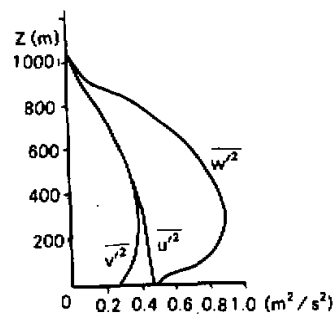


Fig. 2. The distribution of $\overline{u'^2}$, $\overline{v'^2}$ and $\overline{w'^2}$ at 20 km from shoreline.

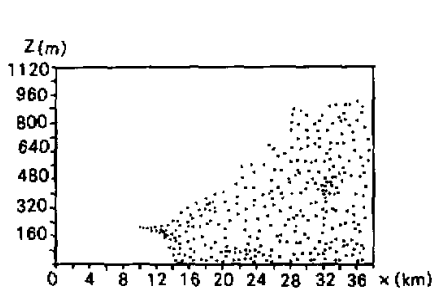


Fig. 3. Calculated particle distribution projected on the $X-Z$ plane (14:00).

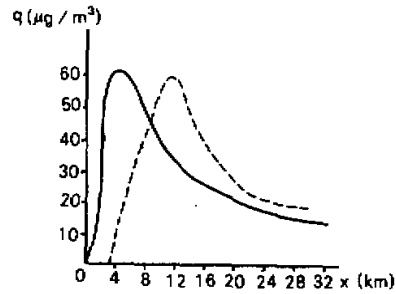


Fig. 4. Distribution of surface center-line concentrations at 14:00 (solid line: Lyons model; dashed line: present model).

20 km inland. It is seen that $\overline{u'^2}$ and $\overline{v'^2}$ reach their maximums near the surface due to stronger wind shear. However, $\overline{w'^2}$ reaches its maximum at the height of 300 m or so, resulting mainly from buoyancy effect. Below 500 m, $\overline{u'^2} > \overline{v'^2} > \overline{w'^2}$ and over 500 m, $\overline{u'^2}$ and $\overline{v'^2}$ tend to be equivalent, however, $\overline{w'^2}$ is greater than $\overline{u'^2}$ and $\overline{v'^2}$ obviously because it is in convective boundary layer condition (Wyngaard et al., 1974).

Some dispersion features during developing stage of the TIBL on shore was revealed by the distribution of particles in $X-Z$ plane. At the beginning, the particles travelled in stable layer and the dispersion in vertical was very weak (see Fig. 3). Lately, the particle cluster was intersected by the TIBL and mixed perfectly in the TIBL. At 5 km (11:00) and 6 km (14:00) from the source, it fell on the ground surface. Generally, the fumigation position from the source at 14:00 is nearer than those at 11:00. But the calculated TIBL profile has obvious fluctuation and changing slope resulting in this local singularity.

Despite the limitation in applying a Gaussian model based evaluation in this study, it is worth comparing the magnitude of the concentrations predicted by using a modified Gaussian dispersion model, such as Lyons et al. (1975), with that obtained by using the more refined approach developed in this paper. Fig.4 illustrates the comparative result of the distributions of surface centerline concentrations. It shows that both values of the maximum surface concentration are very closed but their locations are different. This is probably due to unreasonable assumptions in the Lyons model, such as instantaneous perfect mixing.

2. Sensitivity Analysis of the Modeling System

1) Test 1

If the releasing height of the particle cluster is different, the positions of the intersecting points between the plume and the TIBL profile may be different so that their influence on the surface concentration will be different also. Fig. 5 presents the ground-level centerline concentration for different releasing heights. It is seen that when the releasing height increases from 200 m to 400 m, the maximum of surface concentration decreases from $80 \mu\text{g}/\text{m}^3$ to $59 \mu\text{g}/\text{m}^3$ and the distance of the maximum from the shore increases from 6.2 km to 12.4 km. This analysis supports that the height of plume relative to TIBL is an important factor for the dispersion in coastal area.

2) Test 2

The presence of large scale background wind is an important factor in the formation of sea-land breeze circulation. In this part, a synoptic scale wind along shoreline was taken into account. Under this condition, the front of sea-breeze extends to inland farther, but the vertical extent is greater. The obvious recirculation is revealed. Fig. 6(a),(b) show the distributions of particles projected on $X-Y$ plane under different synoptic flow conditions. It is seen that, in alongshore flow situation, the horizontal bulk spread of the particles is greater than that in onshore flow. This is due to stronger veering of wind in alongshore flow. However, the displacement that the particles travel in stable layer is small. Meanwhile the position of falling on ground level is closer (see Fig. 7 and Fig.3). So it is concluded that the pollutant will accumulate near the shore in alongshore flow situation.

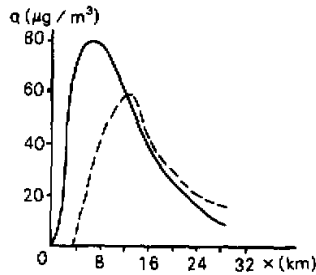


Fig. 5. Distribution of surface centerline concentrations (14:00) (solid line: $H_s = 200$ m; dashed line: $H_s = 400$ m).

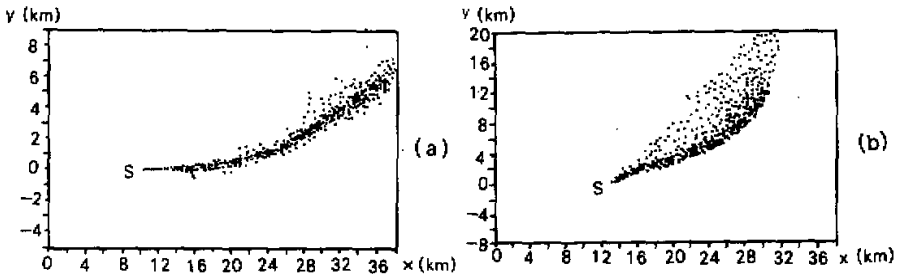


Fig. 6. The distribution of particles projected on $X-Y$ plane at 14:00 (a: onshore flow; b: alongshore flow).

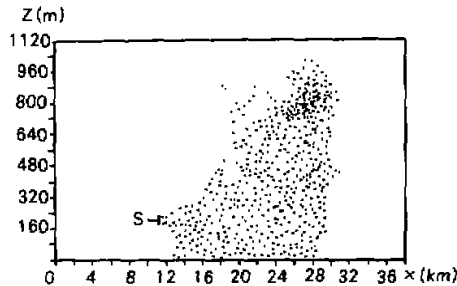


Fig. 7. The distribution of particles projected on $X-Z$ plane in alongshore flow condition.

IV. DISCUSSION AND CONCLUSIONS

A scheme on the mesoscale fumigation dispersion modeling system has been designed and discussed in this paper. The system consists of a second-order closure PBL model and a Lagrangian particle dispersion model and it has been used to make the estimation of a realistic fumigation condition. The modeling effort has successfully solved the problem of meteorological input of the stochastic dispersion model and exploited a new approach for comprehensive applications of this kind of model.

It is clear from this work that the scientific significances of this scheme for mesoscale modeling system developed in this paper are as follows: (1) The temporal and spatial variation of the TIBL structure and the PBL meteorological fields are simulated with the higher-order closure PBL model; (2) Because of the complexity of the atmospheric dynamic and thermodynamic, PBL structure under sea-breeze and TIBL conditions, it is demonstrated that the modeling methodology described in this paper may be a suitable approach for assessing mesoscale dispersion; (3) The particle dispersion model is Lagrangian type and does not need more assumptions so that it is more reasonable than other models based on the Gaussian type. Preliminary results and numerical tests indicate that the performance of the modeling system is well. The field experiments over mesoscale areas are necessary to assess quantitatively its ability to predict concentration field.

REFERENCES

- Fritts T.W., F.J. Straheim and D.J. Deihl (1980), A Formulation for Defining the Development of the TIBL in Sea Breeze Flows, Preprint, *Second Conf. on Coastal Meteorology, AMS*, 147-151.
- Hanna S.R. (1982), Applications in Air Pollution Modeling in *Atmospheric Turbulence and Air Pollution Modeling*, chapter 7, (edited by F.T.M. Nieuwstadt and H. Van Dop), *Reidel, Dordrecht*, 275-310.
- Hurley P. and W. Physick (1991), A Lagrangian Particle Model of Fumigation by Breakdown of the Nocturnal Inversion, *Atmos. Environ.*, **25a**: 1313-1325.
- Jiang W.M. and Wu X.M. (1990), A Linked Three-Dimensional PBL and Dispersion Model in Coastal Regions, *Boundary-Layer Meteorology*, **53**: 43-62.
- Jiang W.M., Wu X.M. and Zhou J.N. (1992), A Higher Order Closure Model Applied to Research on the Structure of the Thermal Internal Boundary Layer (TIBL), *Boundary-Layer Meteorology*, **61**: 301-307.
- Jiang W.M. and Zhou J.N. (1993), Numerical Simulation of the TIBL Structure on Land over Coastal Area, *China Environmental Sciences* (in Chinese), **13(1)**: 28-35.
- Kao C-Y.J. and T. Yamada (1988), Use of the CAPTEX Data for Evaluations of a Long-Range Transport Numerical Model with a Four-Dimensional Data Assimilation Technique, *Mon. Wea. Rev.*, **116**: 293-306.
- Legg B.J. and M.R. Raupach (1982), Markov-Chain Simulation of Particle Dispersion in Inhomogeneous Flows: the Mean Drift Velocity Induced by a Gradient in Eulerian Velocity Variance, *Boundary-Layer Meteorology*, **24**: 3-13.
- Luhar A.K. and R.E. Britter (1990), An Application of Lagrangian Stochastic Modeling to Dispersion during Shoreline Fumigation, *Atmos. Environ.*, **24a**: 871-881.
- Lyons W.A. (1975), Turbulent Diffusion and Pollutant Transport in Shoreline Environments in *Lectures on Air Pollution and Environmental Impact Analysis*, Chapter 5, 136-207.
- Segal M., R.A. Pielke, R.W. Arritt et al. (1988a), Application of a Mesoscale Dispersion Modeling System to the Estimation of SO₂ Concentrations from Major Elevated Sources in Southern Florida, *Atmos. Environ.*, **22(7)**: 1319-1334.
- Segal M., Yu C.-H., Arritt R.W. et al. (1988b), On the Impact of Valley / Ridge Thermally Induced Circulations on Regional Pollutant Transport, *Atmos. Environ.*, **22(3)**: 471-486.
- Stunder M., S. Sethuraman, P.K. Misra et al. (1986), Downwind Non-Uniform Mixing in Shoreline Fumigation Processes, *Boundary-Layer Meteorology*, **34**: 177-184.
- Wyngaard J.C., O.R. Cote and K.S. Rao (1974), Modeling the Atmospheric Boundary Layer, *Adv. Geophys.*, **18a**: 193-212, Academic Press, Inc, NY.