A COUPLED MODEL APPLIED TO THE BHOPAL GAS ACCIDENT

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1. INTRODUCTION

The dispersion of methyl isocyanate gas from the Bhopal accident was investigated using two numerical models. A three-dimensional mesoscale meteorological model was coupled with a three-dimensional Lagrangian particle dispersion model. The temporal and spatial variations of the wind and turbulence fields were simulated with the meteorological model. The dispersion characteristics of the accidental release were then evaluated using the Lagrangian particle model.

2. METHODOLOGY

2.1 *Mesoscale meteorological model*

The mesoscale numerical model used in this study has been described in detail by Huang (1990) and Huang and Raman (1991). The model is hydrostatic and anelastic in a terrain-following coordinate system. The governing equations include equations for the horizontal momentum for the east-west and north-south wind components, the thermodynamic equation for the potential temperature, the conservation equations for water vapor, cloud water, and rain water.

The atmospheric planetary boundary layer is treated in two parts as the surface layer and the transition layer. Surface fluxes are based upon surface similarity stability theory using the non dimensional profiles given by Businger et al. (1971). Above the surface layer, a turbulence closure scheme using prognostic equations for the turbulent kinetic energy and dissipation is incorporated with the level 2.5 scheme of Mellor and Yamada (1982) in order to determine the eddy diffusivities in the transition layer.

2.2 *Lagrangian Particle Dispersion Model*

The Lagrangian particle dispersion model used in this study was originally developed by Zannetti (1981, 1986). The model simulates the dispersion of pollutants in the atmosphere by means of large ensemble of particles moving, at each time step, with pseudo-velocities in a terrain-following coordinate system. These pseudo-velocities simulate the effects of two basic dispersion components: transport due to the mean wind and diffusion due to semi-random turbulent fluctuations of the wind components. Hence, the particle movement during a time period is determined from the grid-scale mean wind component obtained from the mesoscale meteorological model output, plus the subgrid scale turbulent wind fluctuations whose statistics are evaluated from the boundary layer formulations used in the mesoscale model. Since the meteorological variables are defined only on the mesoscale model grid mesh, a linear interpolation scheme is used to estimate their values at each particle position at each time step.

3. A BRIEF DESCRIPTION OF THE ACCIDENT AND MODEL PARAMETERS

The Union Carbide plant was licensed to manufacture phosgene, monomenthyl amine, methyl isocyanate and carbaryl with a total output of 22 tons per day and was located in the northern part of the city of Bhopal. The accident occurred under calm wind, clear skies and stable atmospheric conditions around 0030 LST 3 December, 1984 when methyl isocyanate gas escaped through a nozzle at about 33 m height above the ground. Reports indicated that about 40 tons of methyl isocyonate escaped into the atmosphere in about 90 minutes until 0200 LST 3 December, 1984. The estimated source strength was about 7 kg s^{-1}. Meteorological and concentration observations at the site on the day of accident are not available. Therefore, we had to use mean climatological data for Bhopal in our simulations.

A vertical potential temperature gradient of 6 ^{0}C/km is used in the mesoscale meteorological model. Top of the mesoscale model domain is set at 1 km. The horizontal domain includes a matrix of 35 X 30 points with a uniform grid interval of 1 km. The model is integrated for 11 hours after sunset (1800 LST 2 December, 1984) with an integration time interval of 15 s. The initial surface temperatures are based on climatological observations. During the integration, the temperature over the water surface is kept constant. Surface roughness values are assumed to be 12 cm over the city center decreasing to 7 cm towards the suburban area and 4 cm over rural area, while Charnock's relationship is used over the water.

Time-dependent three-dimensional fields of wind and turbulence predicted by the mesoscale meteorological model are stored from 0030 LST to 0500 LST 3 December, 1984 with a time step of 4 minutes and then used as input for the Lagrangian particle model. The concentration fields are evaluated by counting the number of particles in the grid cells finer than those in the mesoscale model. Top of the particle model domain is set at 400 m. The horizontal domain includes a matrix 140 X 120 grid points, with a uniform grid interval of 250 m. The Lagrangian model simulation began at 0030 LST and ended at 0500 LST A total of 35,000 particles are released with 20 s time interval between 0030 LST and 0200 LST. Buoyancy terms were neglected in the present study, assuming that the released particles were nonbuoyant. Source is at 33 m height, with a source strength of 7 kg s^{-1}.

4. DISCUSSION OF RESULTS

A northwesterly flow of about 1 m s^{-1} is used in this simulation. Simulated closed isotherms over the city and the lake (not shown here) caused by differential heating during the day separate these areas from the rural environs. Strong temperature gradient over the city indicates development of the Bhopal urban heat island circulation, while relatively weaker temperature gradient over Upper Lake shows the development of a weak land breeze circulation as the land surfaces become cooler than the water surfaces at night. This temperature contrast between the urban and the surrounding rural and lake areas creates lower pressure regions at the surface of the urban area. Therefore, low-level horizontal winds converge southeast of the city and increase in speed due to the acceleration of the air toward the lower pressure regions (the predicted winds are superimposed on concentration fields in Figs.1 and 2). Later in the night, the convergence area is advected further downwind by the ambient wind. The advection of the convergence area is generally controlled by the magnitude of the ambient wind and the intensity of the total heat input to the air (Boybeyi and Raman, 1992).

Simulated vertical velocities (not shown here) show a region of rising motion over the city and relatively weaker regions of subsidence motion over the surrounding environs in the general direction of the ambient wind. A similar circulation pattern is also simulated by the model over Upper Lake associated with weak land breeze circulation. Later in the night, the intensity of urban heat island circulation decreases, while intensity of land breeze circulation slightly increases by the seventh hour due to radiative cooling at nighttime. The urban boundary layer attains a depth of about 250 m (see wind field in Fig.2) and becomes shallower farther downwind. The simulated mixed layer height is in good agreement with the mixed layer height for Bhopal estimated by Singh and Ghosh (1985).

The Lagrangian particle dispersion model, using wind and turbulence fields from the mesoscale model, is then used to simulate concentration field of accidental gas release of the Bhopal accident. Simulated concentration fields after 90, 150, 210 and 270 min of travel are presented in a finer domain in Fig.1 for a horizontal plane at source height. Advection and the diffusive growth of the gas under the northwesterly ambient winds reflect complex dispersion characteristics of the gas cloud resulting from the interaction of thermally forced mesoscale systems. Concentration values both at the source height and near the surface (not shown) decrease as the gas cloud advects downwind and expands. Rapid decrease in concentration values initially from 90 min to 150 min of travel is later slowed down by the upward mass diffusion via turbulent mixing. The direction of dispersion is also changed due to spatially and temporarily varying meteorological fields simulated by the mesoscale model.

After 90 min of travel, emission of the gas ends. The gas cloud moves towards the city center with little mixing. Simulated concentration values near the surface directly beneath the moving gas cloud (not shown) are thus lower than those at the source height at least until the first 90 min of travel. After 150 min of travel, the gas cloud enters the city center and expands due to more turbulent mixing caused by weaker stability over the city center as compared to both the suburban and the rural areas. Fumigation resulting from this weaker stability leads to significant increases in the computed near-surface concentrations as compared to those at the source height. At 210 min of travel (3.5 hours after release), the influence of the urban heat island circulation on the concentration fields is even more pronounced. After 270 min, advection of the concentration fields both at the source height and near the surface have been slowed and the gas cloud is trapped by the local circulations caused by the urban heat island as illustrated from the simulated wind fields. In the later hours, the particles get recirculated within a limited region instead of being advected further downwind by the ambient wind (not shown). One important feature is that the gas cloud stays over the city for a significant time and disperses very slowly, affecting

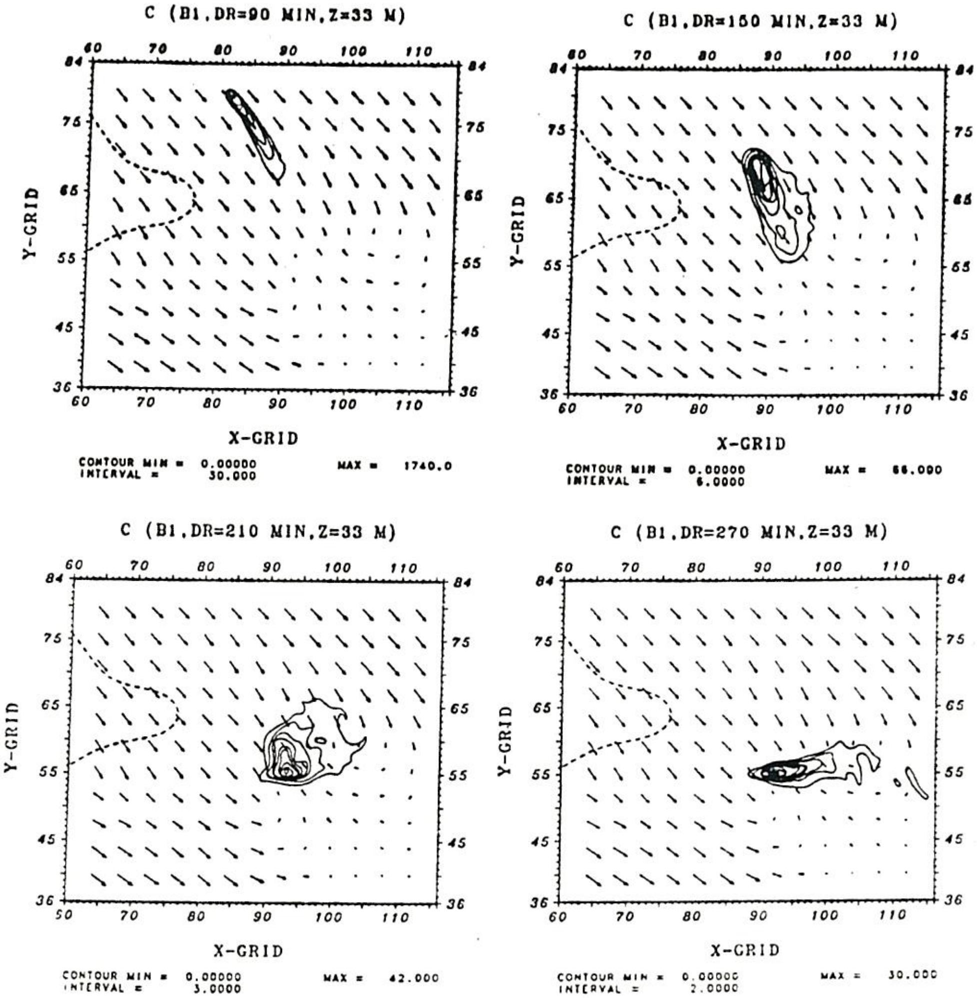

Fig.1 Stack height concentration C (10^3 μg m^{-3}) distributions after 90, 150, 210 and 270 min of travel with northwesterly winds

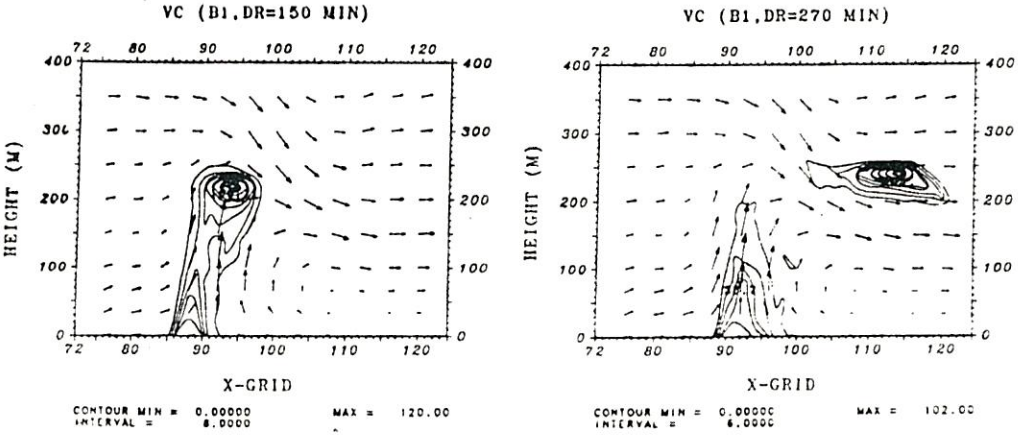

Fig.2 Lateral vertical concentration VC (10^3 μg m^{-3}) distributions after 150 and 270 min of travel with northwesterly winds

the areas in the eastern, southeastern and southern directions from the plant as available observations indicated.

Lateral vertical cross sections of concentration distributions taken through the regions where high concentrations were located in Fig.1 after 150 and 270 min of travel are shown in Fig.2. The results illustrate that little vertical mixing occurs at 90 min of travel (not shown). High concentrations are seen within the relatively shallow layer near the surface. In the later stages, more mixing of the gas cloud takes place as the gas is advected into less stable urban boundary layer. For example, 150 min after release, the concentration field has been mixed upward due to the growth of the urban boundary layer. As a consequence of growth of the internal boundary layer over the city, the location of maximum concentration increases in height with time. This increase is also due to the fact that the dispersion of the gas is significantly retarded at the top of the mixed layer by this hour due to the stability of the inversion layer aloft. This causes accumulation of particles and hence high concentration values at the top of the mixed layer. Later, the gas cloud axis is tilted downstream at the top of the mixed layer height, resulting in advection of the cloud at the top of the mixed layer at a different rate, as illustrated by the simulated wind fields.

5. CONCLUSIONS

Three-dimensional numerical simulation of mesoscale circulations and associated dispersion of the gas related to the Bhopal gas accident were carried out using the coupled model. Results suggest that the complex dispersion characteristics of the gas at Bhopal result from the interaction of thermally forced mesoscale systems. Urban heat island circulation produced by the presence of the Bhopal urban area causes a convergence region in the southeastern part of the city to trap the pollutants with the particles recirculating within a limited region instead of being advected farther downwind. This resulted in the gas cloud to linger over the city. Occurrence of the accident during calm northwesterly winds, clear skies and stable nighttime atmospheric conditions caused the cloud of accidentally released menthyl isocyonate gas to be advected and dispersed slowly, affecting mostly eastern, southeastern and southern parts of the city as available observations and media reports indicated. Simulated low mixing layer height also significantly retarded the dispersion of pollutants.

Most importantly, the results have shown the need for a realistic assessment of mesoscale dispersion. The modeling technique described in this paper may be a suitable tool for studies of air pollution episodes under complex meteorological conditions from accidental or routine releases.

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REFERENCES

Boybeyi Z. and Raman S. (1992) A three-dimensional numerical sensitivity study of convection over the Florida peninsula. *Boundary Layer Met.* **60**, 325-359.

Businger J. A., Wyngaard J. C., Izumi Y. and Bradley E. F. (1971) Flux-profile relationships in the atmospheric surface layer. *J. Atmos. Sci.* **28**, 181-189.

Huang C. Y. (1990) A mesoscale planetary boundary layer model for simulations of topographically induced circulations. Ph.D. dissertation, North Caroline State University.

Huang C. Y. and Raman S. (1991) Numerical simulation of January 28 cold air outbreak during "GALE" II, the mesoscale circulation and marine boundary layer. *Boundary Layer Met.* **56**, 51-81.

Mellor G. L. and Yamada T. (1982) Development of a turbulence closure model for geophysical fluid problems. *Rev. Geophys. Space Phys.* **20**, 851-875.

Singh M. P. and Ghosh S. (1985) Perspectives in air pollution modeling with special reference to the Bhopal gas tragedy, CAS. Tech. Report IIT, New Delhi.

Zannetti P. (1984) A new Monte-Carlo scheme for simulating Lagrangian particle diffusion with wind shear effects, *Applied Mathematical Modeling* **8**, 188-192.

Zannetti P. (1986) Monte-Carlo simulation of auto- and cross-correlated turbulent velocity fluctuations (MC-LAGPAR II Model), *Environmental Software* **1**, 26-30.