1352–2310(95)00031–3

BHOPAL GAS LEAK: A NUMERICAL SIMULATION OF EPISODIC DISPERSION

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(First received 13 January 1993 and in final form 12 December 1994)

Abstract—A mesoscale meteorological model coupled with a Lagrangian particle dispersion (LPD) model was used to simulate the Bhopal methyl isocyanate (MIC) gas leak. A simple two layer K-closure version of the Pielke primitive equation meteorological model was used to produce the wind and turbulence fields in the planetary boundary layer (PBL). Initialized by a single 3 m s⁻¹ geostrophic wind, the PBL model produced a low wind speed stable surface layer capped by a 250 m high nocturnal inversion. The results compared well with limited meteorological observations. However, the LPD model failed to produce enough vertical and horizontal mixing to match the extent of the affected area which was derived from the mortality statistics. Recommendations to improve the model physics to accommodate enhanced mixing in urban areas and to treat MIC thermodynamics and chemistry are suggested.

Key word index: Mesoscale model, Lagrangian dispersion, Bhopal gas leak, stable boundary layer.

I. INTRODUCTION

The Bhopal gas tragedy is one of the worst industrial air pollution disasters that has ever occurred in the world. The count down for the disaster started around 0030 IST when untreated vapors of methyl isocyanate (MIC) were seen escaping through a nozzle of 33 m high atmospheric vent-line, from the Union Carbide (UC) plant located at Bhopal (India), in the early hours of Monday, 3 December 1984.

The sequence of events are as follows: storage tank 610 contained 41 t of MIC. The temperature in the tank increased markedly due to the exothermic reaction of MIC with water that had earlier seeped into the tank. The presence of abnormally high concentration of chloroform caused corrosion in the tank. The iron produced as a result of corrosion catalyzed the concurrent exothermic trimerization of MIC. The rapid increase in pressure and temperature inside the tank resulted in the opening of the safety valve. About 40 t of MIC escaped into the atmosphere in 90 min. The area involved was about 50 sqkm and nearly 200,000 people were affected due to the gas leak. Singh and Ghosh (1985) used a modified version of Gaussian plume model to simulate the Bhopal gas tragedy. In Fig. 1 we have reproduced the concentration contours based on their model computations. The results match the extent of the affected area (Table 1) that were derived from mortality statistics. However, as the meteorological fields were not available during the episode, the element of speculations could not be avoided in such a simulation.

1.1. Biological aspects of MIC

MIC is extremely toxic. It affects all living beings including vegetation. MIC is an unbearable lachrymator. The isocyanates have been known to attack respiratory system, eyes and skin (Singh and Ghosh, 1985). In fact, most of the deaths resulting from the episode were attributed to various forms of respiratory distress. In some cases, the gas caused such massive internal secretion that their lungs became clogged with fluid. In other cases, spasmodic constrictions of bronchial tubes led to suffocation and eventually to death. The standard recommended level of MIC is 0.02 ppm averaged over 3 h (Singh and Ghosh, 1985). This threshold limit defines the upper value above which the gas may harm human beings.

1.2. Modelling the gas leak

The existing models for the dispersion of air pollutants may be broadly classified into two groups: (i) analytical models such as Gaussian plume/puff and (ii) numerical models.

The Gaussian type of dispersion models which assumes that the winds are constant in space and time may fail in an urban environment. Most of the modifications to incorporate the changes in wind speed and direction with height, are based on ad hoc assumptions
Fig. 1. Map of Bhopal city: the gas affected areas determined on the basis of mortality statistics are indicated by dots and the concentration of dots approximately represents the extent of the effect. Contours indicate the parts per million isopleths extracted from Singh and Ghosh (1985) and are classified as follows: Zone I, 50 ppm; Zone II, 15 ppm, Zone III, 1.5 ppm and Zone IV, < 10 ppm

<table>
<thead>
<tr>
<th>Zones</th>
<th>Main areas included</th>
<th>Mortality statistics</th>
<th>Area (km²)</th>
<th>Mortality (km⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I Severely affected</td>
<td>J.P. Nagar, Chola, Kazicamp, Nisatpura</td>
<td>1265</td>
<td>1.33</td>
<td>951.1</td>
</tr>
<tr>
<td>II Very badly affected</td>
<td>Khajanchi Bagh, Chandbad, Railway colony, Straw products, Bus stand, Ash Bagh stadium</td>
<td>767</td>
<td>1.95</td>
<td>392.3</td>
</tr>
<tr>
<td>III Moderately affected</td>
<td>Punjabi Bagh, Shah Jahanabad, Sindh colony</td>
<td>270</td>
<td>4.6</td>
<td>58.7</td>
</tr>
<tr>
<td>IV Mildly affected</td>
<td>Firdous Nagar, Jama Masjid, Professor's Colony, Central Library, Central school, Lal Parads ground, Berkhari, Birla Mandir</td>
<td>108</td>
<td>7.5</td>
<td>14.4</td>
</tr>
</tbody>
</table>

Total reported deaths 2410* 166 (in other areas)

* The toll was much higher than the report. Many of the deaths occurred in the slums and went unregistered (Singh and Ghosh, 1985).
and experimental conclusions which at best may be valid at a given time for a specific location. Also, the dispersion parameters required for computing the concentration distribution in Gaussian models have their own limitations, particularly in weak wind and stable conditions.

The planetary boundary layer (PBL) plays a vital role in the diffusion and transport of air pollutants. The structure of PBL shows large temporal and spatial variations which in turn directly influences the dispersion processes. The variations become substantial in coastal areas and over irregular terrain. Numerical models are a good tool to study the structure of PBL, especially when sufficient meteorological information is not available. These models can be used to describe explicitly the dynamic, thermodynamic and the turbulent structure of the PBL for different atmospheric stabilities in weak and strong wind conditions.

A simple K-closure, primitive equation meteorological model (i.e. Pielke model) was used to produce dynamically consistent flow and turbulent fields in complex terrain to represent the atmospheric conditions in the vicinity and down stream from the release site. This model has been applied to a wide range of mesoscale flows (Pielke, 1984) including land–sea breezes, mountain – valley circulations and forced air flows over rough terrain. Using the predicted mean meteorological fields along with the turbulent parameters, tracer particles are then released from the source using a Lagrangian particle dispersion (LPD) model.

A few studies were undertaken to simulate episodic dispersion using the coupled models, such as, the simulation carried out to evaluate worst case scenarios for the impact of four conventional power plants along the South Florida coast on the Everglades National park and Big Cypress Preserve in South Florida and the two-dimensional simulation of the first 48 h of Chernobyl accident (Pielke, 1984). In contrast to the Chernobyl and South Florida cases, the impact of accidental release of MIC at Bhopal occurred over a much smaller spatial scale. Further, the domain of our interest could be considered more or less homogeneous (Figs 1 and 2). As a first approximation, the one-dimensional version of the meteorological model was used to study the thermodynamic structure, the wind structure and the turbulent structure during the episode and the pseudo-three-dimensional LPD model was used to study the episodic dispersion of MIC.

2. THE NUMERICAL MODELS

2.1. Boundary layer model

A meteorological boundary layer model using a simple K-closure is used to simulate the Bhopal gas...
leak. The model is a one-dimensional version of a hydrostatic mesoscale meteorological model developed by Pielke (1974). The governing equations of the model are given by

$$\frac{\partial U}{\partial t} = fV - fV_s + \frac{\partial}{\partial Z} \left[ K_m \frac{\partial U}{\partial Z} \right]$$  
(1)

$$\frac{\partial U}{\partial t} = -fU + fU_s + \frac{\partial}{\partial Z} \left[ K_m \frac{\partial V}{\partial Z} \right]$$  
(2)

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial Z} \left[ K_H \frac{\partial \theta}{\partial Z} \right] + F_o$$  
(3)

$$\frac{\partial q}{\partial t} = \frac{\partial}{\partial Z} \left[ K_m \frac{\partial q}{\partial Z} \right]$$  
(4)

where $U$ and $V$ are the east-west and north-south components of velocity, respectively, $U_s$ and $V_s$ are the components of the geostrophic winds, $f$ is the coriolis parameter, $\theta$ is the potential temperature, $q$ is the specific humidity, $K_H$ and $K_m$ are the turbulent exchange coefficient of heat and momentum along the vertical direction and $F_o$ is the heat source term due to radiative and surface forcings.

Equations (1)–(4) are subject to the following boundary and initial conditions.

2.1.1. Boundary conditions. (i) No slip condition was assumed for the components of velocity at the ground, i.e.

$$\text{at } Z = 0, \quad U = V = 0.$$  
(5a)

(ii) The temperature at the ground surface is assumed to be a function of time, i.e.

$$\text{at } Z = 0, \quad \theta = \theta_0(t)$$  
(5b)

where $\theta_0$ was determined through the surface energy balance (Mahrer and Pielke, 1977).

(iii) The surface specific humidity was determined from a prescribed soil moisture content which was held constant during the simulation, i.e.

$$\text{at } Z = 0, \quad q = \text{constant}.$$  
(5c)

(iv) At the upper boundary, the velocity components are prescribed, i.e.

$$\begin{align*}
U &= U_s + \frac{\partial U_s}{\partial Z} (Z - Z_i) = \text{constant} \\
V &= V_s + \frac{\partial V_s}{\partial Z} (Z - Z_i) = \text{constant}
\end{align*}$$  
(5d)

where $U_s$ and $V_s$ are the geostrophic winds on top of the convective boundary layer, $Z_{top}$ is the top of the model and $Z_i$ is the height of PBL. The second term on the right-hand side of equation (5d) represents the shear on the geostrophic wind. A zero value implies a barotropic boundary layer and a non-zero value denotes a baroclinic boundary layer.

(v) At the top of the model, the values of potential temperature and the specific humidity are prescribed from meteorological observations, i.e.

$$\text{at } Z = Z_{top}, \quad \begin{cases} 
\theta = \theta_f \\
q = q_f
\end{cases}$$  
(5e)

We wish to mention that the model top, $Z_{top}$, is kept sufficiently higher than the height of the boundary layer, so that the rigid top does not influence our regime of interest.

2.1.2. Initial conditions. Initially, the profiles of temperature and specific humidity are prescribed along with the geostrophic wind from Radiosonde observations. Equations (1)–(4) form a closed set provided $K_m$, $K_H$ and $F_o$ are known. The determination of these terms are discussed in the following subsections:

2.1.3. Turbulent parametrization. The PBL is composed of two layers, namely the surface layer near the ground and Ekman layer above it. In the surface layer, the turbulent exchange coefficients are calculated based on similarity approach proposed by Businger et al. (1971). In the Ekman layer, under convective conditions to O'Brien (1970) profile is employed and accordingly the eddy diffusivities are parametrized in the PBL as

$$K_z(Z) =
\begin{cases} 
(Z/h) K_{zh} & Z \leq h \\
K_{zl} Z_i^2 + (Z_i - Z)^2/(Z_i - h)^2 \{K_{zh} - K_{zl}\} & Z_i > Z > h
\end{cases}$$  
(6a)

where $h$ is the height of the surface layer and $K_{zh}$ is the value of $K_z$ at height “a”.

The profile requires the information about the height of the boundary layer, the height of the surface layer and the eddy exchange coefficients at the top of the boundary layer. The height of the boundary layer as suggested by Deardorff (1974), for the assumed horizontally homogeneous terrain reduces to

$$\frac{\partial Z_i}{\partial t} = \frac{1.8 W^* + 1.1 U_s^2 - 3.3 U_s^2 f Z_i}{\left( Z_i^2 \frac{\partial Z_i}{\partial t} + 9 W^*_2 + 7.2 U_s^2 \right)}$$  
(6b)

where

$$W^* = \begin{cases} 
\{(-g/\theta_m) U_s \theta_s Z_i\}^{1/3} & \text{for } \theta_s < 0 \\
0 & \text{for } \theta_s > 0.
\end{cases}$$

$\theta_m$ is the mean value of potential temperature above surface layer, $U_s$ and $\theta_s$ are the friction velocity and friction temperature which are determined from the similarity theory (Mahrer and Pielke, 1977).
The height of the surface layer is assumed to be 4% of PBL (Mahrer and Pielke, 1977). A small nonzero value (1.0 cm$^2$s$^{-1}$) for the exchange coefficient is assumed on top of the PBL. While the growing convective boundary layer (CBL) is prescribed by O’Brien profile, exchange coefficients in the stable boundary layer (SBL) are prescribed by closure depending on the local gradient Richardson number, $R_i$ (McNider et al., 1988) and are given by

$$K_z(Z) = \begin{cases} 1.1(R_i - R_i^c) I^2 S/R_i & \frac{\partial \theta}{\partial Z} > 0 \\ (1 - 18R_i)^{-1/2} I^2 S, & \frac{\partial \theta}{\partial Z} \leq 0 \end{cases}$$

(6c)

where $R_i^c$ is the critical Richardson number, $I$ is the mixing length and $S$ is the local shear.

The above parametrizations were tested under different case studies ranging from convective to stable conditions (McNider and Pielke, 1981).

2.1.4. Radiative and Surface Forcings, $F_r$. The contribution of radiation fluxes in the boundary layer cannot be neglected. In fact, in the nocturnal boundary layer, when the turbulence level is generally low, the radiation fluxes due to long wave contribute significantly to the local heat budget. In the absence of phase change of water vapor, other than the turbulent mixing, the contribution of radiative flux divergence in the boundary layer or the surface cooling/heating or a combination of both attains significance. While radiative flux divergence at any level in the atmosphere is computed using the work of Jacobs et al. (1974), the surface temperature is computed by surface energy balance method (Mahrer and Pielke, 1977).

Equations (1)-(4) with boundary and initial conditions were solved numerically.

2.2. Lagrangian particle model

The LPD model was used to determine the trajectory of non-buoyant tracer particles. The particles are known as the marker particles each representing a fraction of the mass of the gaseous pollutant released. The pollutants released from a source are advected in a Lagrangian manner. The position of a marker particle at time $t + \Delta t$ is given by

$$X(t + \Delta t) = X(t) + [U(t) + U'(t)]\Delta t$$

(7)

$$Y(t + \Delta t) = Y(t) + [V(t) + V'(t)]\Delta t$$

(8)

$$Z(t + \Delta t) = Z(t) + [W(t) + W'(t)]\Delta t$$

(9)

where $U$, $V$, $W$ are the velocity components available from the one-dimensional model described in the previous section. $U'$, $V'$, $W'$ are the turbulent velocity components evaluated statistically using the boundary layer formulation. These turbulent velocity fluctuations are related to the fluctuations at the previous time step (Smith, 1968):

$$U'(t + \Delta t) = R_U(\Delta t) U'(t) + U'^*$$

(10)

$$V'(t + \Delta t) = R_V(\Delta t) V'(t) + V'^*$$

(11)

$$W'(t + \Delta t) = R_W(\Delta t) W'(t) + W'^*$$

(12)

where $R(\Delta t)$ is the autocorrelation coefficient and $U'^*$, $V'^*$, $W'^*$ are random component of fluctuations assumed to be independent of $U'$, $V'$, $W'$.

An exponential fit was suggested by Hanna (1978) for the autocorrelation coefficient in the following form:

$$R_U(\Delta t) = \exp(-\Delta t/T_U)$$

(13)

$$R_V(\Delta t) = \exp(-\Delta t/T_{UV})$$

(14)

$$R_W(\Delta t) = \exp(-\Delta t/T_{UW})$$

(15)

in which $T_L$ is the Lagrangian time scale. The random component of fluctuations, i.e. $U'^*$, $V'^*$ and $W'^*$ can be expressed as follows:

$$U'^* = \sigma_u \Gamma_i [1 - R^c_\theta(\Delta t)]^{1/2}$$

(16)

$$V'^* = \sigma_v \Gamma_i [1 - R^c_{uv}(\Delta t)]^{1/2}$$

(17)

$$W'^* = \sigma_w \Gamma_i [1 - R^c_{uw}(\Delta t)]^{1/2}$$

(18)

where $\Gamma_i$ is the random normal variate with mean zero and standard deviation one. $\sigma_u$, $\sigma_v$, $\sigma_w$ are the standard deviation of turbulent velocity fluctuations.

2.2.1. Determination of $\sigma_u$, $\sigma_v$, $\sigma_w$ and $T_L$. From equations (10)-(18), it is clear that the quantities $\sigma_u$, $\sigma_v$, $\sigma_w$ and $T_L$ are to be known a priori in order to have a complete set of equations. Under convective condition, $\sigma_w$ is determined from the expression

$$\sigma_w = K_w/\lambda_{mw}$$

(19)

where $K_w$ is obtained from the boundary layer model and $\lambda$ is a function of stability (McNider et al., 1988). $\lambda_{mw}$ is the wavelength associated with the peak in vertical velocity spectra and signifies the size of the largest eddy in the vertical. $\sigma_u$ and $\sigma_v$ can be obtained from the following relationships proposed by Panofsky et al. (1977):

$$\sigma_u = \sigma_v = U_u (12 + 0.5Z/L)^{1/3} \quad Z/L < 0$$

(20)

where $L$ is the Monin–Obukhov length.

For the stable boundary layer, $\sigma_w$ is not obtained from the vertical exchange coefficient, rather an expression is used based on second-order closure work of Blackadar (1979). This expression is given by

$$\sigma_w = 1.21 S \left[ \frac{R_i - R_i^c}{R_i} \right]^{0.58}$$

(21)

$\sigma_u$ and $\sigma_v$ were computed using the relationship suggested by Panofsky et al. (1977) in stable boundary layer:

$$\sigma_u = \sigma_v = 2.34 U_u$$

(22)

The Lagrangian time scale for each component is determined from

$$T_{L_u} = 0.2 \beta \lambda_{uw}/\bar{U}$$

(23)

$$T_{L_v} = 0.2 \beta \lambda_{mv}/\bar{U}$$

(24)
\[ T_{w} = 0.2 \beta \lambda_{mW}/\bar{U} \]  
(25)

where \( \bar{U} = (U^2 + V^2)^{0.5} \) and \( \beta \) is the ratio of Lagrangian to Eulerian time scale which is given by \( \beta = 0.6 \bar{U}/\sigma_w \) such that \( \beta < 10 \).

The maximum wavelength associated with the three components of velocity (\( \lambda_{mU}, \lambda_{mv}, \lambda_{mW} \)) are given by the following relationships (McNider et al., 1988).

In the CBL:
\[ \lambda_{mW} = \begin{cases} Z/(0.55 - 0.38|Z/L|), & 0 < Z < L_i \\ 1.8 Z,[1 - \exp(-4Z/Z_i) - 0.0003 \exp(8Z/Z_i)], & 0.1Z_i < Z < Z_i \end{cases} \]  
(26)

In the SBL:
\[ \lambda_{mW} = Z/((0.55 + 0.8Z)/L_i) \]
\[ \lambda_{mv} = 0.7(Z/Z_i)^{0.5} \]
\[ \lambda_{mV} = \lambda_{mW}. \]  
(27)

3. NUMERICAL EXPERIMENTS AND RESULTS

The meteorological model was used to study the thermodynamic structure, the wind structure and the turbulent structure in the PBL during the episode. Further, it was coupled with the LPD to study the dispersion of MIC during the night of release. We started the simulation on the 2 December 1984 at sunrise and simulated the model for 24 h to study the diurnal variations of the field variables in the PBL. The values of the input parameters are specified in Table 2. The Radiosonde observations received from the India Meteorological Department were used to initialize the meteorological model.

3.1. Thermodynamic structure

The diurnal evolution of potential temperature in the PBL is shown in Figs 3 and 4. During the day, surface heating leads to superadiabatic lapse rate near the ground resulting in a well-mixed CBL. The mixing layer is topped by subsidence inversion. At sunset, long wave radiative cooling results in the formation of a stable boundary layer at the surface. The radiative inversion height is the height above the surface at which the potential temperature gradient becomes smaller than \( 3.5 \times 10^{-3} \) K m\(^{-1} \) (Andre and Mahart, 1982) and is indicated by \( h_i \) in Fig. 4. The evolution of radiation inversion in the SBL is discussed below. The layer above this SBL is the residual layer where potential temperature remains almost neutral, like in a mixed layer, except that, the potential temperature in this layer starts decreasing slowly with time due to radiation divergence. The residual layer is capped by the subsidence inversion.

3.2. Wind fields

Figures 5 and 6 represent the diurnal evolution of the mean wind fields. During the day, the wind profiles are nearly constant with height in the mixed layer.

![Fig. 3. Potential temperature profiles in the CBL on 2 December 1984.](image-url)
due to turbulent mixing. The strong gradient near the surface is because of the surface friction. The winds are subgeostrophic all through the day (Fig. 5). At sunset a new shallow frictional boundary layer grows with strong shear at the surface. However, its growth is restricted by the imposed geostrophic wind. Above the frictional layer, acceleration in velocity is observed as the wind field adjusts to a new balance with the existing pressure gradient (Blackader, 1957). This leads to the development of supergeostrophic component located roughly about 50 m (Fig. 6). Unlike the previous case study by McNider and Pielke (1981), in which the wind maxima is pronounced so as to be characterized as a low level jet, we find that the wind maxima is not so well defined at a particular level. Besides, the maxima is observed close to the surface. The essential difference is probably due to geostrophic wind on top of the PBL. In the former study, the geostrophic wind on top of the PBL was 10 m s$^{-1}$, whereas in the present case it is 3 m s$^{-1}$ which corresponds to a weak wind situation. The wind profile under such conditions is consistent with those obtained by Estournel and Guedalia (1987).

3.3. Turbulent structure of the NBL

Figure 7 shows the variation of Richardson number with height, and Fig. 8 indicates the growth of radiation inversion with time. The structure of SBL and its evolution is governed by two components (i) turbulence generated by wind shear in the layers close to the surface and (ii) the radiative cooling. Turbulence produced by wind shear causes mixing of heat, momentum, moisture and pollutants, while radiative cooling leads to the growth of radiation inversion. The contribution of each varies with the geostrophic wind, the surface roughness and the ground cooling rate (Estournel and Guedalia, 1987). Delage (1974) pointed out that by increasing surface roughness by tenfold, the change in the height of radiative inversion

Fig. 4. Potential temperature profiles in the NBL on 2–3 December 1984. In the figure the radiation inversion height is represented by $h_i$.

Fig. 5. Velocity components in the CBL on 2 December 1984.

Fig. 6. Velocity components in the NBL on 2–3 December 1984.
is marginal. In the present study, the contribution of radiative cooling seems to be important. This causes a strong vertical temperature gradient that acts to stabilize the atmosphere and hence suppresses turbulence. The strong stability is clearly seen from the potential temperature profile (Fig. 4) and the shallow friction layer is clear from the wind profile (Fig. 6). Although this frictional layer is about 50 m thick, the turbulent layer is restricted to a fraction of the frictional layer as indicated in Fig. 7. This is due to the strong stability that inhibits turbulence in the SBL. The height of the turbulent layer is practically the same throughout the night, whereas the height of inversion layer increases (Fig. 8). This results in difference between the depth of inversion and mixing. It seems that the difference between the two layers is a consequence of the prevailing weak winds and strong stability. This is consistent with the arguments proposed by Estournel and Guedalia (1985). The difference between the inversion height and height of turbulent mixing is large because the Andre and Mahrt (1982) convention was used to compute the height of the inversion. The height of the inversion layer is about 250 m (Fig. 8) at the time of the episode. This grows slowly and reaches a value of 300 m at 0530 IST.

Thus, the simple K-closure model is able to simulate physically consistent diurnal variations in the boundary layer. Moreover, the model is able to explain the turbulent structure of the NBL under strong stability and weak winds, consistent with the available information under such situations.

3.4. Pre- and post-accident simulations

In Table 3 we have summarized the details about the available meteorological observations during the period 05.30 IST on 2 December 1984 and 17.30 IST on 3 December 1984. Since meteorological observations were not made available during the episode and the following morning, we have compared the model predictions whenever the observations were available. Since observations were available in the evenings of 2 and 3 December 1984, we have simulated the model continuously for 36 h from the morning of 2 December 1984. Figures 9a and b compare the observations and the predictions of the mean potential temperature fields on the two evenings. There is a reasonably close agreement in both the cases. The predicted and observed winds exhibit similar trends (Figs 10a and b). However, the results are less satisfactory than the thermodynamic structure. Note that while observations are instantaneous values obtained from Radiosonde, the simulated results are ensemble averages. On the other hand, potential temperature profiles are relatively stationary under a given synoptic condition and hence the simulated potential temperatures are found to give a closer match with observations.

3.5. LPD model simulation

Using the meteorological fields and the turbulent parameters from the boundary layer model as the

<table>
<thead>
<tr>
<th>Observations</th>
<th>Time</th>
<th>Date</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>05.30 IST</td>
<td>2 December 1984</td>
<td>Available</td>
</tr>
<tr>
<td>(2)</td>
<td>17.30 IST</td>
<td>2 December 1984</td>
<td>Available</td>
</tr>
<tr>
<td>(3)</td>
<td>05.30 IST</td>
<td>3 December 1984</td>
<td>Not available</td>
</tr>
<tr>
<td>(4)</td>
<td>17.30 IST</td>
<td>3 December 1984</td>
<td>Available</td>
</tr>
</tbody>
</table>

IST: Indian standard time

Table 3. List of meteorological (wind, temperature and humidity at standard pressure levels) information
Fig. 9. (a) Comparison of potential temperature profiles on 2 December 1984 at 17.30 IST. (b) Comparison of potential temperature profile on 3 December 1984 at 17.30 IST.

Fig. 10. (a) Comparison of the components of velocity on 2 December 1984 at 17.30 IST. (b) Comparison of the components of velocity on 3 December 1984 at 17.30 IST.

input, the LPD model was used to study the dispersion of MIC. One marker particle was released every 4 s for a period of 90 min from 0030 IST. The Holland (1953) plume rise formulation was used to compute the plume rise (Singh and Ghosh, 1985) and the effective stack height was found to be 39.6 m. Although the release of the particles was stopped after 90 min, the simulation was continued until no particles were present in the domain. The dispersion scenario along the \(X-Y\) plane is shown in Figs 11a–d. The positions of
the plume are plotted at different instant of time. Modelled particle positions are in the predominant direction in which the worst effects of the accident were felt (Fig. 1). However, there were a few other zones, mostly south of the stack (Fig. 1) which were also affected mildly (Table 1). This may be due to modification of flow induced by complex terrain which has not been accounted in the present study.

The model predicts very little spread along the vertical and thus a very thin plume emanating from the stack is found to travel a very long distance with very little mixing (Figs 12a–d). Despite the fact that concentration measurements were not made, we made an attempt to correlate qualitatively the modelled predictions with the fatality statistics. The fatality statistics in Fig. 1 (and Table 1) reveal that the worst affected area was about half a kilometer downwind of the stack. It is reasonable to expect such a plume in weak wind and highly stable conditions, as under these conditions the plume grows more readily along the horizontal than along the vertical.

3.6. Influence of input parameters

The model input parameters are listed in Table 2. Some of these parameters have been assigned from the observations. The geostrophic wind, surface roughness and the soil roughness are known to influence the structure of the SBL considerably. However, there is an uncertainty in prescribing the values of these parameters. The geostrophic wind was assigned from observations at 800 mb. Because other observations were not available we had to rely upon a single point instantaneous observations from the sounding. Figures 13a, b and 14a reveal that the mean thermodynamic structure, mean wind structure and the turbulent structure remain practically unaffected by doubling of the geostrophic wind from 3 to 6 m s$^{-1}$. However, there are minor differences in the growth of
radiation inversion in either case. While the height of radiation inversion increases throughout the night when the geostrophic wind is 3 m s\(^{-1}\) (Fig. 14b), the growth rate becomes slower after 00.30 IST when the geostrophic wind is 6 m s\(^{-1}\). This behaviour is consistent with the study proposed by Estournel and Guedalia (1987) in weak wind conditions. Since the height of the inversion layer is much more than the stack height and the mixing is restricted to a shallow layer, it is expected that the characteristic nature of the trajectories would not have altered due to the small variations in geostrophic wind. Further, the evening sounding of 2 December 1984 suggests that the winds do not exceed even 5 m s\(^{-1}\) up to 550 mb.

In the present model, we have specified the soil conductivity, specific heat capacity and thermal diffusivity corresponding to clay soil (Pielke, 1984). We wish to mention that the clay soil was considered to be representative of Bhopal and its surroundings. However, the soil parameters corresponding to concrete may also be used to represent the surface characteristics of the portion that includes the city. We have observed that concrete surfaces produce about the same level of turbulence. Further, the influence of soil parameters on the flow pattern could not be analysed from this model and needs to be studied using a three-dimensional model. Finally, it is observed that by increasing the surface roughness by tenfold the structure of SBL was not altered. We studied instantaneous position of the plume in the light of sensitivity analysis and we found that its behaviour did not alter appreciably.
4. DISCUSSION

The numerical simulation of the episode provides insight into the prevailing structure of the SBL. The turbulent mixing is restricted to a shallow layer near the ground in weak wind and stable conditions and a thin plume emanating from the stack travels for a long distance before reaching the ground. It is difficult to compare the results of the model when no measurements of air concentrations were made. However, the reports suggest that the effect of the gas was realized even at a relatively smaller distance from the stack (Fig. 1 and Table 1). Further the one-dimensional meteorological model does not produce any significant change in the wind direction during the episode so as to produce a larger horizontal mixing to match the extent of the affected areas. Now, we analyze it further in the light of the assumptions of the model and suggest a few mechanisms that could explain the enhanced mixing in vertical and the horizontal directions.

The model assumes horizontal homogeneity. This may be reasonable in view of the location of the Union Carbide and the worst affected zones (Fig. 2).
However, there are two large lakes in the Southwest and South of the stack, respectively. These lakes are about 4 km from the stack and are indicated in the topographical map of Bhopal (Fig. 2). Moreover, there are a few hillocks mostly located to the Southwest of the stack. Although the lakes and the hillocks are far away from the stack, the role of topographically induced circulation needs to be examined using a mesoscale model.

Secondly, the role of urban heat island could not be examined in the present case study because of the assumption of horizontal homogeneity. A section of Bhopal is covered by the city area (Fig. 2) and it would be necessary to consider the effect of asphalt and concrete that are characteristic features of the city. It is known that asphalt and concrete have the capacity to convert and store the incoming radiation as sensible heat better than the surrounding rural area. At night when the incoming radiation is cut off, even while a substantial stable boundary layer has developed over the rural area, the urban zone may still be weakly convective, lending to larger vertical mixing. A critical re-examination of the heat island effect in the light of the episode would be necessary to explain the enhanced mixing.

A third factor that could have influenced vertical mixing along with the horizontal flow pattern is the aerodynamic roughness. The effect of changes in the surface roughness, when air is flowing from one type of surface to the other, results in the formation of internal boundary layer (Arya, 1988). However, its influence on the flow pattern can only be studied using a three-dimensional model.

The LPD model assumes that the plume is neutrally buoyant. Since MIC was emitted with a high velocity and temperature compared to the ambient air, it is expected to rise initially. The plume rise was found to be 6.6 m (Singh and Ghosh, 1987) and it was accounted in the model in terms of effective stack height. However, MIC is twice as heavy as air. Singh and Ghosh (1987) have analyzed this aspect in details and have pointed out that it could be considered as a passive plume in view of a substantial entrainment, initial dilution, mixing and heat generation. Since the extent of these physical processes are not fully understood, the plume under question may also be examined as a borderline case (one with density effects and one which is a passive plume) in future to provide a further insight into the dispersion pattern of MIC. It is probable that the vertical spreading is dominated by two factors, the first factor is the usual spreading due to passive diffusion, and second factor corresponds to spreading due to gravitational settling effects.

Finally, it was noticed that a large amount of heat was generated during the release of MIC. It is known that MIC reacts with moisture rapidly. In addition, MIC could have undergone a series of chemical reactions. Singh and Ghosh (1987), in an earlier study, have considered the chemical removal by assuming a first-order chemical reaction and dry deposition. The LPD model in our present study does not take into consideration the chemical removal and dry deposition. It is also known that the urban area in Bhopal has large content of suspended particulate matter (SPM). It could be possible that the vapors might have condensed on the SPM nuclei and settled down at the surface.

5. CONCLUSIONS

Coupled meteorological and particle models were used to simulate numerically the Bhopal gas leak. The simulation seems to describe the salient features of the nocturnal boundary layer that existed during the accident. The meteorological simulations are found to be numerically and physically consistent. The LPD model directs a narrow plume downwind near the centerline of the observed affected zones. However, it appears that the model fails to produce sufficient mixing in the vertical to bring the material to the ground, and it may not reproduce horizontal pattern as well. Further, the LPD simulation is not able to explain the high ground level concentration within the first kilometer from the stack. As pointed out in the earlier section, we propose to study the various aspects of the episode by considering (i) geographic effects on the flow modification, (ii) heat island effects and surface inhomogeneities, (iii) MIC as a partially heavy gas and (iv) the role of chemical reactions.

The turbulent structure obtained for a weak wind and strong stability conditions is found to be consistent with the available studies (Delege, 1974; Estournal and Guedalia, 1987; Kurzeja et al., 1991). However, the lack of data is a limitation in understanding the turbulent structure in weak/low winds and strongly stable conditions.

Acknowledgements—Authors are grateful to the India Meteorological Department for providing the necessary data. We also thank the reviewers for their useful comments on improving the original version of this manuscript.

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