Simulation of short-range diffusion experiment in low-wind convective conditions

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Abstract

A previously obtained analytical solution to model the short-range dispersion of pollutants in low winds from surface releases has been used to simulate diffusion tests conducted during winter in weakly convective conditions at the Indian Institute of Technology (IIT) Delhi. The turbulence parameterization based on friction velocity has been tested to simulate diffusion experiment. Such a parameterization in this study is considered justifiable on two counts: (1) prevailing meteorological and dispersion conditions have been generally of weakly unstable type as indicated by values of Monin-Obukhov length and bulk Richardson number, (2) uncertainties associated with the application of convective velocity based similarity parameterization to simulation of diffusion experiment at IIT Delhi, resulting in significant underprediction in most of the cases (Atmos. Environ. 30 (1996a) 1137). With this parameterization, the model simulations have improved considerably and compare reasonably well with the observations. Further, the results from a simple Gaussian model have been included for comparison. This study is in continuation of the work done earlier to simulate near-source dispersion in weak winds.

Keywords: Mathematical model; Low wind dispersion; Friction velocity; Model simulation

1. Introduction

Low wind dispersion studies, though very few have a significant bearing on air pollution problems, particularly small scale, when the dispersion is restricted to a limited area. They assume practical importance in view of the frequent occurrence of low-wind conditions associated with high pollution potential hazards. Attempts have been made recently to address the problem of weak wind dispersion (Oettl et al., 2001; Sharan et al., 1996a,b; Sharan and Yadav, 1998; Arya, 1995; Yadav, 1995). Even the turbulence structure is not fully described for weak winds. Efforts have been made recently in this direction also (Agarwal et al., 1995; Yadav et al., 1996; Gopalakrishnan et al., 1998; Oettl et al., 2001). Some of the commonly used approaches for air pollution dispersion modelling are based on gradient-transfer theory with the assumption of constant eddy diffusivity. This assumption is questionable for describing near-source dispersion and may give erroneous results (Taylor, 1921; Batchelor, 1949; Csanady, 1973; Berkowicz and Prahl, 1979).

In the early stages of plume dispersion from a continuous point source, the statistical theory of diffusion suggests that eddy diffusion coefficients \( (K) \) may be taken as linear functions of downwind distance. Such parameterization is considered by Sharan et al. (1996a) and Sharan and Yadav (1998) to investigate the problem of modelling dispersion in weak wind conditions. The former study dealt with convective conditions whereas the latter with stable conditions. This parameterization accounts for stability through the parameters, which essentially represent turbulent intensities. Further, in the absence of measurements of turbulent...
intensities, turbulence can be parameterized in terms of friction velocity in stable conditions and convective velocity in unstable conditions.

Results obtained by Sharan et al. (1996a) for unstable conditions with convective velocity based similarity parameterization showed consistent underpredictions. An underpredicting trend was also evident for the constant diffusivities model (Sharan et al., 1996b) and Arya’s (1995) model. Since then efforts have been continuing in this direction to find a more appropriate framework that can provide better simulations. One such attempt is to reinvestigate the parameterization of turbulence used in the model. In the present study, we have tried to simulate diffusion tests in convective conditions with an alternative turbulence parameterization in terms of friction velocity, because of the uncertainties associated with the use of convective velocity based similarity parameterization in the previous study (Sharan et al. 1996a). The salient features of the model used for the simulation have been briefly described below for the sake of completeness.

### 2. Model formulation

In the absence of removal (physical or chemical) mechanisms and orienting x-axis in the direction of mean wind flow (U), the concentration c of a pollutant in steady-state conditions is governed by the advection-diffusion equation

\[
\frac{\partial c}{\partial x} = \frac{\partial}{\partial x} \left( K_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c}{\partial z} \right) + S, \tag{1}
\]

where S is the source term and \(K_x, K_y, K_z\) are the eddy diffusion coefficients in \(x, y\) and \(z\) directions, respectively. For non-zero wind speed, the apparent diffusivities \(K\) are specified as linear functions of downwind distance based on Taylor’s (1921) statistical theory of diffusion for small travel times, as follows:

\[
K_x = a U x; \quad K_y = b U y; \quad K_z = g U z
\]

where \(a, b\) and \(g\) represent turbulence parameters varying with the stability of the atmosphere and \(x\) is the downwind distance from the source. To facilitate an analytical solution, a simplifying assumption of keeping \(U\) and \(K\)'s independent of height has been made. In general, it is desirable to consider vertical dependence of \(U\) and \(K\)'s. However, for describing the near-source diffusion in weak winds, analytical solutions of the diffusion equation should be obtained for linearly varying eddy diffusivities with distance from the source (Arya, 1995).

With the above parameterization and accounting for the source term \(S\) through one of the boundaries, Eq. (1) with appropriate boundary conditions can be solved using method of integral transforms to give (Sharan et al., 1996a)

\[
c = \frac{1}{U \pi \sqrt{b y}} \left[ 1 + a \left( \frac{a^2 y^2 + z^2}{x^2} \right)^{-\gamma} \right]. \tag{3}
\]

A simple particular case of this solution called slender plume approximation (crosswind spread of the plume is small compared to the downwind distance travelled) can be obtained by taking limit as \(a \to 0\) in the Eq. (3)

\[
c = \frac{g}{\pi x \sqrt{b U x y}} \exp \left[ \frac{U}{t} \left( \frac{y^2}{2 b U x} \right) \right]. \tag{4}
\]

This equation is analogous to the Gaussian plume solution when \(b\) and \(g\) are written in terms of the dispersion parameters \(s_y\) and \(s_z\), respectively.

### 3. Parameterization

Application of solutions (3) and (4) requires the turbulence parameters \(a, b\) and \(g\) to be specified. Following Taylor’s statistical theory of diffusion, these parameters are identified as intensities of turbulence (Arya, 1995). Empirical relations based on similarity theory can be used for estimating them when measurements of turbulence intensities are not available. In general, the turbulence could be parameterized in terms of friction velocity as well as convective velocity. However, to simplify matters, just as idealized simulations of purely convective or purely stable, it is suggested to restrict to one appropriate velocity scale for parameterization as illustrated below.

Turbulence in stable conditions is manifested in the surface friction velocity (un) and hence plume dispersion in the stable surface layer may be described using the following empirical relations (Sharan and Yadav, 1998):

\[
\alpha = 6.25 \left( \frac{\nu}{U} \right)^2, \quad \beta = 3.61 \left( \frac{\nu}{U} \right)^2, \quad \gamma = 1.69 \left( \frac{\nu}{U} \right)^2. \tag{5}
\]

In unstable conditions, the empirical relations for turbulence parameters based on convective scaling can be written as (Arya, 1999)

\[
\alpha = 0.31 \left( \frac{\nu}{U} \right)^2, \quad \gamma = 0.16 \left( \frac{\nu}{U} \right)^2, \quad \beta = 0.31 \left( \frac{\nu}{U} \right)^2. \tag{6}
\]

where \(wn\) is convective velocity scale.

As reported earlier by Sharan et al. (1996a), these parameterizations (5-6) may not be strictly valid in weak wind conditions. However, it is suggested that they may serve as an alternative in the absence of measurements of turbulence intensities. In one such attempt, the parameterization (6) for convective conditions has yielded significant underestimation of observed concentrations in the earlier study (Sharan et al., 1996a) in which \(wn\) was estimated in terms of mixing length \((z_t)\) and heat flux.
as follows:

\[ \omega^* = \left( \frac{g}{v^2} \frac{\partial \langle \omega' \theta' \rangle}{\partial z_i} \right)^{1/3}, \]  

(7)

where \( g \) is acceleration due to gravity and \( \bar{\theta} \) is (spatial) mean potential temperature between the two levels used in computing surface parameters.

In that study, the reasons attributed for underprediction included likely non-applicability of empirical constants in parameterization (6) to weak wind dispersion, and uncertainty in the estimation of \( \omega^* \). However, the basic question of applicability of \( \bar{\omega}^* \) parameterization to such atmospheric conditions under consideration in this study still remains to be examined. As a result, it was considered desirable to test an alternative parameterization in terms of friction velocity for simulating IIT Delhi diffusion experiment described briefly below.

A diffusion experiment was conducted at IIT Delhi in low-wind conditions during February 1991. The tracer, SF6, was released at a rate \( q = 50 \text{mlmin}^{-1} \). The sampling period for each run was 30min. Wind and temperature measurements were obtained at four levels (2, 4, 15 and 30 m) from 30 m micrometeorological tower. Details of the experiment including the atmospheric stability are given in Singh et al. (1991) and Sharan et al. (1996b). The surface parameters such as friction velocity, Monin-Obukhov length (L) and bulk Richardson number \((Rhi)\) are computed using Monin-Obukhov similarity theory. Roughness length \( Z_0 \) for the experiment site was estimated to be 0.78 m in an earlier study (Raman et al., 1990). The parameters \( \omega^* \), \( \bar{\theta} \), and \( L \) have been estimated using an iterative procedure (Stull, 1988) taking 0.78 and 15 m as the two vertical levels. The temperature profile is extrapolated to obtain temperature at 0.78 m. The values of these parameters including wind speed are given in Table 1. In all, 14 test runs were conducted. Out of these, 5 (Runs 1, 4, 5, 9 and 10) correspond to stable conditions whereas 2 (Runs 3 and 14) are in neutral conditions. A close examination of the pertinent parameters (Table 1) indicates that the atmospheric conditions were, in general, of weakly unstable type during the period of the experiment.

We note that values of \( \omega^* \) and \( \bar{U} \) are sufficiently large in the context of this experiment to exclude the possibility of a free convection case. Consequently, turbulence can be explained in terms of friction velocity measurements available on-site. In fact, the ratios of standard deviation of velocity components to friction velocity available for the same site in the following year during the corresponding period can be used assuming that the atmospheric conditions have remained more or less the same with the turbulence levels in a narrow range. Though this is an alternative arrangement in the absence of concurrent measurements, this approach minimizes the uncertainties pointed out in the earlier study by using the on-site observations. One can rewrite the turbulence parameters \( a, b \) and \( g \) as follows:

\[ \alpha_i = \left( \frac{\sigma_i}{\bar{U}} \right)^2 = \left( \frac{\sigma_i}{\omega^*} \right)^2 \left( \frac{\omega^*}{\bar{U}} \right)^2, \quad i = 1, 2, 3 \]  

(8)

in which \( a_1 = a, a_2 = b, a_3 = g \) and \( \mathcal{S} = 2, 3 \) correspond to \( s_u, s_v, s_w \), respectively.

For model simulations in this study, the values of the ratios \( s_u = \omega^*, s_v = \omega^* \) and \( s_w = \omega^* \) appearing in relations (8) are taken to be 2.07, 2.0 and 1.3, respectively, from Agarwal et al. (1995). Layer-averaged mean wind has been used while simulating the concentration distribution at the sampling height \( z = 0.5 \text{m} \).

### 4. Results and discussion

Concentrations have been computed from Eqs. (3) and (4) using \( \omega^* \) parameterization given in Eq. (8). Peak concentrations computed on sampling arcs from the present model using \( \omega^* \) and \( \bar{\omega}^* \) parameterizations are presented in Tables 2 and 3 at a downwind distance of 50 and 100 m, respectively, from the source. Corresponding results based on slender plume approximation (4) with UN parameterization are included for comparison in these tables. It may be seen from the tables that

<table>
<thead>
<tr>
<th>Run no.</th>
<th>Sampling time (h)</th>
<th>Date (mm-dd-yy)</th>
<th>( \langle j(\text{ms}^{-1}) \rangle ) (at 15m)</th>
<th>( \omega^* ) (ins(^{-1}))</th>
<th>( \bar{\theta} ) (K)</th>
<th>( L(m) )</th>
<th>( Rhi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1200-1230</td>
<td>02-13-91</td>
<td>2.21</td>
<td>0.34</td>
<td>-0.30</td>
<td>-32.78</td>
<td>-0.13</td>
</tr>
<tr>
<td>2</td>
<td>1530-1600</td>
<td>02-13-91</td>
<td>1.09</td>
<td>0.21</td>
<td>-0.43</td>
<td>-8.70</td>
<td>-0.51</td>
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<tr>
<td>6</td>
<td>1000-1030</td>
<td>02-19-91</td>
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<td>0.34</td>
<td>-0.29</td>
<td>-33.25</td>
<td>-0.12</td>
</tr>
<tr>
<td>7</td>
<td>1245-1315</td>
<td>02-19-91</td>
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<td>0.37</td>
<td>-0.35</td>
<td>-33.54</td>
<td>-0.12</td>
</tr>
<tr>
<td>8</td>
<td>1645-1715</td>
<td>02-19-91</td>
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<tr>
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<td>02-21-91</td>
<td>1.49</td>
<td>0.25</td>
<td>-0.26</td>
<td>-19.53</td>
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<tr>
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<td>1530-1600</td>
<td>02-21-91</td>
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<td>0.21</td>
<td>-0.47</td>
<td>-8.11</td>
<td>-0.55</td>
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Table 2
Peak values of tracer concentration in parts per trillion (ppt) observed and predicted at 50 m downwind of the source

<table>
<thead>
<tr>
<th>Run no.</th>
<th>Observed</th>
<th>Present model with un</th>
<th>Slender plume model with un</th>
<th>Gaussian model</th>
<th>Present model with wn</th>
<th>Slender plume model with wn</th>
<th>Gaussian model</th>
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<td>193</td>
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<td>1025</td>
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<td>668</td>
<td>170</td>
<td>732</td>
<td>1012</td>
<td>616</td>
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<tr>
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<td>198</td>
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<td>574</td>
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<tr>
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<td>574</td>
<td>241</td>
<td>578</td>
<td>752</td>
<td>487</td>
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<tr>
<td>13</td>
<td>1060</td>
<td>783</td>
<td>180</td>
<td>799</td>
<td>1447</td>
<td>487</td>
<td>574</td>
</tr>
</tbody>
</table>

Table 3
Peak values of tracer concentration in parts per trillion (ppt) observed and predicted at 100 m downwind of the source

<table>
<thead>
<tr>
<th>Run no.</th>
<th>Observed</th>
<th>Present model with un*</th>
<th>Slender plume model with un*</th>
<th>Gaussian model</th>
</tr>
</thead>
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<tr>
<td>1</td>
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<td>137</td>
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<td>139</td>
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<tr>
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<td>63</td>
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<td>222</td>
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<td>145</td>
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<tr>
<td>13</td>
<td>215</td>
<td>196</td>
<td>45</td>
<td>200</td>
</tr>
</tbody>
</table>

the peak values computed from the present model with UN parameterization are reasonably close to the observations on both the arcs. In fact, the peak concentrations are predicted within a factor of two in most of the runs. In Run 7, the observed concentration at 50 m is suspect because it is lower than that at 100 m arc. This is contrary to the remaining test runs of surface-release diffusion experiment.

The results indicate that the simulated peaks from the present model and the slender plume model with un parameterizations are comparable. In fact, the peak or maximum concentration is predicted along the mean wind. Referring to Eqs. (3) and (4), the expressions for peak concentrations from a ground level source are identical at \( y = 0, z = 0 \). This implies that downwind diffusion does not affect ground-level centreline concentrations, while its contribution shows up away from the centreline and/or above the ground. The difference in the peaks predicted from these two models in Tables 2 and 3 is due to: (1) the mismatch in the direction of the mean wind and the sampled peak, (2) sampling height \( z \) is 0.5m rather than zero. The present model results provide a significant improvement with un parameterization relative to wn parameterization.

It may be observed that the results from a simple Gaussian model in Tables 2 and 3 are as good as or even better than the present model. Nevertheless, it does not conflict with the objective of this study.

Recently, Q-Q (Quantile-Quantile) plots, comparing concentration distributions of predicted and observed values, are used for evaluating the performance of air quality models in regulatory applications (Olesen, 1995; Venkataram, 1999). Fig. 1 gives Q-Q plot for the overall results (both on and off centreline) from the model using the UN and WN parameterizations and the Gaussian model (not same as the slender plume model). The figure shows that the results from the Gaussian model and the present model with un parameterization compare well with the observations and most cases lie within a factor of two lines. On the other hand, the wn parameterization underpredicts the quantiles by more than a factor of two for almost all the concentrations > 30 ppt. Thus, it is clear that the overall results from the model using w* parameterization have improved in comparison to wn parameterization (Fig. 1). This is also evident from the scatter plot (Fig. 2) as well as the values of certain commonly used statistical measures such as fractional bias and normalized mean square error (NMSE) (Yadav and Sharan, 1996). Computed values of FB come out to be 0.73, 1.18 and 0.51 for un, wn and Gaussian cases, respectively. Corresponding values of NMSE are 2.68,
100 - 0.1

10000

Fig. 2. Scatter diagram of the ratio of predicted to observed concentration versus the observed concentration. (—) indicate a factor of two, and (—-) a factor of four.

8.47 and 2.06. However, due to limited data points in this study, it is not possible to comment here, in general, on the importance and applicability of un scaling versus wn scaling for convective conditions. Thus, it is desirable to have further studies in this direction.

5. Conclusions

In this study, an analytical model for dispersion of pollutants in low-wind conditions has been considered to explain the diffusion data, in weakly convective conditions, collected at IIT Delhi. Turbulence has been accounted for in the model through parameters appearing in the expressions for eddy diffusivities for near-source dispersion. Application of the model in an earlier study, with similarity parameterization based on convective velocity, to explain near-source dispersion from a surface release in weakly convective conditions resulted in significant underprediction of the observed concentrations. Therefore, it was suggestive to re-examine the turbulence in an attempt to overcome certain limitations of the earlier study. As a consequence, an alternative parameterization in terms of friction velocity has been considered more appropriate to use in the present study in view of the near-surface dispersion conditions. The model results for peak as well as overall concentrations from UN parameterization are found to be better than those with wn parameterization and compare reasonably well with the observed concentrations. Overall, the model could do well in explaining the near-source dispersion of a tracer from a surface release in weakly convective conditions. It is worthwhile mentioning here that, in this study a simple model (slender plume approach/Gaussian plume model) performs as good as or even better than the present model, particularly in case of centreline (peak) concentrations.

The approach adopted in this study is in contrast to the widely accepted convective diffusion theory validated by laboratory and field studies (Willis and Deardorff, 1976; Briggs, 1993). The authors would like to remark that the present study is not intended to provide a criterion for applicability of un or wn scaling, it is simply an attempt to explain short-range diffusion tests from near-surface release at IIT Delhi. However, with the availability of extensive data, it would be highly desirable to evolve a suitable criterion for applicability of UN as well as wn scaling in convective conditions.

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References


