INFLUENCE OF DIURNAL AND INERTIAL BOUNDARY-LAYER OSCILLATIONS ON LONG-RANGE DISPERSION

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Abstract—Coupled meteorological and Lagrangian particle models are used to examine horizontal dispersion over one to two diurnal cycles. Seven numerical experiments were run in which different portions of the atmospheric energy spectrum were included or excluded in the simulation of releases of a non-buoyant pollutant from an elevated point source. The results of the experiments indicate that vertical shear in the horizontal wind produced by diurnal and/or inertial oscillations in conjunction with or followed by vertical PBL mixing are capable of maintaining plume growth rates which are nearly linear with diffusion times up to 48 h. The model results agree reasonably well with long-range dispersion observations of an isolated smelter plume made in Australia. Periods of accelerating diffusion found in the simulations have also been indicated in observations. These accelerating diffusion periods in the simulations are due to time-dependent shear in the planetary boundary layer at night. Shear due to synoptic-scale horizontal temperature gradients was also found to have a significant impact on the modeled plume growth rates.

Key word index: Boundary-layer model, Lagrangian particle model, long-range dispersion, wind shear, accelerating diffusion, inertial oscillation, plume growth rates, mesoscale dispersion, geostrophic shear.

I. INTRODUCTION

Although the estimation of atmospheric diffusion at large downwind distances from a source has been of interest for years (e.g. Richardson, 1926; Richardson and Proctor, 1925), relatively new environmental problems such as acid rain and the 1986 Chernobyl disaster emphasize the relevance of this topic. Recent observations of long-range plume dispersion (Carras and Williams, 1981) and a synthesis with other available observations (Gifford, 1985) indicate that boundary-layer plumes continue to spread in the horizontal at large downwind distances at a rate much faster than can be explained by classical theory using an atmospheric energy spectrum with a mesoscale gap. The observations have lead to some discussion (Gifford, 1983a; Smith, 1983) on what physical mechanisms are responsible for this sustained growth.

Figure 1 shows a composite of plume observations developed by Gifford (1985) indicating a lateral growth rate more or less linearly proportional to time out to two or three days. Gifford proposes that this growth is sustained after several hours by substantial energy present in the mesoscale (atmospheric motions with periods from 1 to 48 h). Traditional views of the atmospheric energy spectrum, based primarily on the work of Van der Hoven (1957), have included a spectral gap in this region, i.e. little atmospheric energy between planetary-boundary-layer-scale tur-

bulence and synoptic-scale weather systems. With such a gap, horizontal growth rates which are linearly proportional to time can be maintained out to at most one hour. Gifford (1982) points to more recent observations of the atmospheric energy spectrum such as those of Gage (1979), which do not exhibit a spectral gap, as evidence of the presence of mesoscale energy.
able to support these sustained growth rates. Pasquill and Smith (1983), on the other hand, suggest vertical shear of the horizontal wind in the planetary boundary layer (PBL) to be the mechanism responsible for maintaining the plume growth rates. Gifford does not discount shear but believes there should be more precision in describing the mechanisms producing the shear.

In this paper, an attempt is made to resolve this issue by numerically simulating long-range plume dispersion using a coupled boundary-layer model and a Lagrangian particle model. The use of the numerical models allows the inclusion or exclusion of various portions of the atmospheric energy spectrum and both PBL shear and synoptic shear in different combinations. The results of the numerical simulations show more clearly than can discrete observations how complex boundary-layer dispersion can become over one to two diurnal cycles even for very idealized experiments. The complexity is introduced by the presence of several mesoscale time scales, the coupling between vertical wind shear and small-scale turbulence, and the influence of synoptic-scale horizontal temperature gradients.

The impetus for the present paper is clearly summarized by the following quote from Gifford (1983b): "Many, virtually all details of mechanisms (governing long-range diffusion) remain to be clarified, particularly the role of PBL wind-direction shear in the diffusion process. This must involve the diurnal cycle of PBL stability changes, as Pasquill (1974) has pointed out." In this study we explicitly consider PBL shear throughout the diurnal cycle and other factors such as inertial effects and geostrophic shear.

As clarification of terminology used in this paper in subsequent sections, we will use the term 'dispersion' to include both turbulent diffusion and differential advection. Differential advection due to shear can arise both from diurnal effects and from large-scale temperature gradients which impose a thermal wind.

2. METHODS AND OBSERVATIONS

2.1. Mt. Isa observations

Carras and Williams (1981) reported on a unique set of observations of plume dispersion from a sulfide smelter at Mt. Isa in Queensland, Australia. The plume observations were made against the relatively unpolluted background of the Southern Hemisphere; this together with persistent easterly flows allowed the plume to be tracked for over 1000 km downwind. Figure 2 shows the location of the Mt. Isa smelter. The plume was tracked to the west over nearly uniform flat terrain on a number of occasions during the Southern Hemisphere winter (i.e. June, July, August) of 1977 and 1979. The measurements of plume widths were made at heights of between 30 and 60 m by aircraft or at the surface by four-wheel-drive vehicle. Traverses were made in a direction approximately perpendicular to the wind direction and three different detection techniques were used simultaneously in order to locate the plume accurately. Sampling time varied from a few minutes to 1.5 h for the widest plumes. Table 1 gives the plume width data of Carras and Williams (1981). Note that some of the plumes had experienced nearly two full diurnal cycles at the time of observation. These observations and earlier Mt. Isa plume observations reported by Bigg et al. (1978) are used to evaluate the results of the numerical dispersion experiments described herein.

Fig. 2. Background map showing location of Mt. Isa smelter. Easterly winds carried plume to the west over generally uniform terrain. (Adapted from Carras and Williams, 1981).
Table 1. Plume widths and ages reported by Carras and Williams (1981)

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<th>Date</th>
<th>Time of measurement (Australian EST)</th>
<th>Downwind distance (km)</th>
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Table 2. Summary of turbulent parameterization. $\bar{w}\theta_0$ refers to the sign of the surface heat flux; $K_{\text{sl}}$ and $K_{\text{sl}} = 1 \text{ cm}^2 \text{s}^{-1}$ are the exchange coefficients at the top of the surface layer and boundary layer, respectively.

$$K_{\text{sl}} = \begin{cases} K_{\text{sl}} + [(z_h - z) / (z_h - h)]^2 \{ K_{\text{sl}} - K_{\text{sl}} \} \\
+ (z - h) \int \left[ \frac{\partial}{\partial z^*} K_{\text{sl}} + 2(K_{\text{sl}} - K_{\text{sl}}) \right] \\
(z_h - h) \int, z > z > h \end{cases}$$

$$K_{\text{sl}} = 1.1 (R_i - R) \frac{p}{R_i} \frac{\theta}{\theta^*} > 0$$

$$K_{\text{sl}} = (1 - R) \frac{p}{R} \frac{\theta}{\theta^*} < 0$$
2.2. Boundary-layer model

A one-dimensional, numerical meteorological model with a high resolution boundary layer was used to simulate the diurnal evolution of the planetary boundary layer, including profiles of the mean wind and turbulence statistics. The model, a one-dimensional version of a hydrostatic mesoscale meteorological model originally developed by Pielke (1974), is described in its present form by McNider and Pielke (1981). The one-dimensional model equations are as follows:

\[
\frac{du}{dt} = \frac{f_0 - f V_u}{\rho} + \frac{\partial}{\partial z} \left( K_m \frac{\partial u}{\partial z} \right) \tag{1}
\]

\[
\frac{dv}{dt} = -f u + f U_u + \frac{\partial}{\partial z} \left( K_m \frac{\partial v}{\partial z} \right) \tag{2}
\]

\[
\frac{d\theta}{dt} = \frac{\partial}{\partial z} \left( K_H \frac{\partial \theta}{\partial z} \right) + R_s + R_L \tag{3}
\]

\[
\frac{dq}{dt} = \frac{\partial}{\partial z} \left( K_m \frac{\partial q}{\partial z} \right), \tag{4}
\]

where \(u\) and \(v\) are the east–west and north–south velocity components, \(\theta\) is potential temperature, \(q\) is specific humidity and \(K_H\) and \(K_m\) are the vertical turbulent exchange coefficients for heat and momentum, respectively. Also, \(f\) is the Coriolis parameter, \(U_u\) and \(V_u\) are the steady east–west and north–south geostrophic wind components, and \(R_L\) and \(R_s\) are long-wave and short-wave heating functions.

The last term on the right-hand side of (1) and (2) is used to represent the influence of motion on a scale which is too small to be explicitly resolved by the meteorological model. The dependent variables \(u, v\) and \(w\) can be written as \(u = u_0 + u', v = v_0 + v', w = w_0 + w'\) where the subscript ‘zero’ refers to the scale in which the wind is essentially in gradient balance (i.e. the synoptic scale). The prime superscript corresponds to a hydrostatic departure from the synoptic scale which may not be in gradient balance but which can be resolved by the meteorological model.

Surface fluxes of heat and momentum are based upon surface similarity theory using the non-dimensional profiles given by Businger et al. (1971). The turbulent exchange coefficients are specified in the convective boundary layer by means of a cubic interpolating polynomial (O'Brien, 1970) and a prognostic equation for PBL height (Deardorff, 1974a), and in the stable boundary layer by an algebraic closure form dependent upon the local gradient Richardson number as suggested by Blackadar (1979). See Table 2 for a summary of the vertical diffusion coefficient formulation. Horizontal diffusion is neglected in the present one-dimensional version of the model.

The boundary-layer parameterization in the meteorological model has been tested against various boundary-layer data sets, including those from Wan-gara, Australia (Clarke et al., 1971), the Great Plains of the U.S. and Koorin, Australia (Clarke and Brook, 1979). For details concerning the first two of these tests and a more complete model description, see McNider and Pielke (1981). Information concerning the Koorin comparison may be found in Garratt and Physick (1985).

2.3. Lagrangian particle model

The Lagrangian particle model is based upon conditioned particle concepts (Smith, 1968) in which the Lagrangian turbulent velocity fluctuation of a non-buoyant tracer particle is linearly related to the turbulent fluctuation at the previous time step, i.e.

\[
u''(t + \Delta t) = \nu''(t) R_s(\Delta t) + \nu''(t), \quad x = 1, 2, 3 \tag{5}
\]

where \(\nu''\) and \(R_s\) are the subgrid-scale velocity component and autocorrelation coefficient, respectively, in the \(x, y, z\) directions, and \(\nu''(t)\) is a random turbulent component which is assumed to be independent of \(\nu''(t)\). The random component is taken to be Gaussian with zero mean and a standard deviation

\[
sigma'' = \sigma''(1 - R_s^2(\Delta t))^{1/2}. \tag{6}
\]

where \(\sigma''\) is the local Eulerian turbulent velocity standard deviation. The autocorrelation coefficient is exponential (Gifford, 1982), i.e. \(R_s(\Delta t) = \exp(-\Delta t/T_L)\) where \(T_L\) is the Lagrangian integral time scale of the sub-grid scale turbulence.

Equation (5) is the finite difference analog to the Langevin stochastic differential equation (Gifford, 1982). Using field measurements, Hanna (1979) verified to a good degree of confidence the validity of the linearity assumption and independence of the random component in (5) and performed simple dispersion experiments using this equation. Reid (1979) considered dispersion in a neutral surface layer using the conditioned particle scheme while Lamb (1978) and McNider et al. (1980) examined dispersion in a convective PBL. More recent applications of this type of model include Legg and Raupach (1982), Ley (1982), Thomson (1984) and de Baas et al. (1986).

In the present investigation we employ the conditioned particle scheme to examine particle dispersion in the boundary layer and use the meteorological model described in section 2.2 to deduce the turbulent quantities \(\sigma''\) and \(T_L\) needed to close the conditioned particle scheme, as well as to simulate the diurnal behavior of the wind field. Particle positions are then computed in a Lagrangian manner from the equations

\[
x(t + \Delta t) = x(t) + [u(t) + \nu''(t)] \Delta t,
\]

\[
y(t + \Delta t) = y(t) + [v(t) + \nu''(t)] \Delta t,
\]

\[
z(t + \Delta t) = z(t) + [w(t) + \nu''(t)] \Delta t, \tag{7}
\]

where \(u, v\) and \(w\) are meteorological model resolved velocity components and \(\nu''\). \(\nu''\) and \(\nu''\) are the corresponding subgrid-scale turbulent components as given by (5). Since the grid-scale velocity components
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are only defined on the meteorological model grid mesh, a volume-weighting interpolation scheme described by Teuscher and Hauser (1974) is used to estimate the boundary-layer velocity at the particle position. Also, for computational efficiency in relating boundary-layer grid parameters to the particle positions, the particle positions are defined in terms of fractions of cardinal grid points rather than absolute coordinates.

The \( u \) and \( v \) particle velocities below the first meteorological model grid point are computed from similarity theory using the profile functions employed in the meteorological model. Particles are assumed to reflect perfectly from the ground surface.

2.3a. Turbulence statistics from the meteorological model. Since the Lagrangian particle model is ultimately to be used in conjunction with the flow fields predicted by the meteorological model, the turbulent statistics \( \sigma' \) and \( T_\lambda \) needed to apply the conditioned particle scheme must be deduced so as to be consistent with the dynamically evolving boundary-layer flow. This is accomplished for the vertical component \( \sigma'_w \) by inverting a relationship suggested by Hanna (1968) so that

\[
\sigma'_w = \frac{K_m}{A \lambda_{m,w}}, \tag{8}
\]

where \( K_m \) is the vertical momentum exchange coefficient, \( \lambda_{m,w} \) is the wavelength of the peak in the vertical velocity spectrum and \( A \) is a proportionality factor. \( K_m \) is predicted by the meteorological model; however, the functional form for the length scale \( \lambda_{m,w} \) must be determined from observations. Fortunately, recent technical advances and field experiments have provided fairly good estimates of \( \lambda_{m,w} \) throughout the boundary layer.

For the unstable PBL, estimates of \( \lambda_{m,w} \) are given by Kaimal et al. (1976) as a function of \( z_i \) (the PBL height), and \( z/L \); i.e.

\[
\lambda_{m,w} = \begin{cases} 
0 & 0 < z < 0.1z_i \\
5.9z_i & 0.1z_i < z < 0.41z_i \\
1.8z_i \left[ 1 - \exp(-4z/z_i) \right] & 0.41z_i < z < 0.81z_i \\
-0.0003 \exp(8z/z_i) & 0.81z_i < z < z_i
\end{cases} \tag{9}
\]

The last expression for the unstable case contains a modification suggested by Caughey and Palmer (1979) reflecting additional observations near the top of the boundary layer which show a contraction in \( \lambda_{m,w} \) near \( z_i \). Note that \( z_i \) and \( L \) (the Monin-Obukhov length) are diagnosed in the meteorological model so that there is internal consistency in the expression relating the length scale \( \lambda_{m,w} \) and the eddy exchange coefficient \( K_m \).

In the initial tests using (8) and the most recent estimates of \( A = 0.17 \), it was found that the near-surface ratio \( \sigma'_w/u_* \) did not converge to the expected value of approximately 1.3 even though the modeled surface layer obeyed similarity laws. Further pursuit of this contradiction using well known expressions for similarity forms of \( K_m \) in the surface layer and formulations of \( \sigma'_w \) and \( \lambda_{m,w} \) in the surface layer indicated that \( A \) is not constant, but rather is a function of stability. Figure 3 shows estimates of \( A \) as a function of \( z/L \).

Using \( A(z/L) \) as shown in Fig. 3 and \( K_m \) from the meteorological model using (8) produced \( \sigma'_w/u_* \) profiles consistent with observations in the convective surface layer (Fig. 4). In the convective mixed layer, the model produced profiles which were also reasonably consistent with observations (Fig. 5). The \( \sigma'_w \) values drop off more rapidly near \( z_i \) than do the observations due to the shape of the cubic polynomial. A difference which can probably be corrected by different constraints on the interpolation procedure. It is felt that

\[
A = \frac{K_m}{\sigma'_w \lambda_{m,w}}
\]

\[
\text{Fig. 3. Plot of } A = \frac{K_m}{\sigma'_w \lambda_{m,w}} \text{ as a function of } z/L \text{ based on standard surface-layer formulas for } K_m, \sigma'_w \text{ and } \lambda_{m,w}.\]
Fig. 4. Plot of $\sigma_w^*/u_*$ near the surface extracted from the meteorological model at several sampling times compared to the observational best fit by Panofsky et al. (1977). Times are local standard time (LST).

Fig. 5. Plot of $\sigma_w^*/w_*$ extracted from the meteorological model for Wangara Case day 33 compared to observational composites and the numerical study by Deardorff (1974b). The dashed line was extracted from an unpublished study by F. B. Smith.
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The length scales $\lambda_{m,w}$ and $\lambda_{m,r}$ in the convective boundary layer were also taken from the work of Kaimal et al. (1976):

$$\lambda_{m,w} = \lambda_{m,r} = 1.5z_i.$$  \hspace{1cm} (14)

Standard methods (Pasquill, 1974) were used to relate the length scales $\lambda_{m,w}$, $\lambda_{m,x}$, and $\lambda_{m,r}$ to $T_L$ [needed in (5)]. Specifically, the Eulerian integral time scale, $T_E$, was computed by the expressions

$$T_{E,w} = 0.2 \lambda_{m,w}/\bar{u}, \quad T_{E,x} = 0.2 \lambda_{m,x}/\bar{u},$$  \hspace{1cm} (15)

and the Lagrangian integral time scale, $T_L$, by the expressions

$$T_{L,w} = \beta T_{E,w}, \quad T_{L,x} = \beta T_{E,x}, \quad T_{L,r} = \beta T_{E,r},$$  \hspace{1cm} (16)

where the ratio of the Lagrangian to Eulerian time scale, $\beta$, is given by

$$\beta = 0.6 \bar{u}/\sigma_w' \hspace{1cm} (17)$$

limited by

$$\beta \leq 10. \hspace{1cm} (18)$$

As already indicated the autocorrelation function $R_\alpha(\Delta t)$ was taken to be exponential so that

$$R_\alpha(\Delta t) = \exp(-\Delta t/T_{L,w}); \quad R_\xi(\Delta t) = \exp(-\Delta t/T_{L,x}); \quad R_\zeta(\Delta t) = \exp(-\Delta t/T_{L,r}).$$  \hspace{1cm} (19)

This form for the autocorrelation function has been shown by Gifford (1982) to arise from the solution of the Langevin equation.

In general the PBL turbulence statistics deduced from the meteorological model appear to agree well with the available observations. Although (8) was used to relate the meteorological model exchange coefficients to $\sigma_w'$, an alternative which might be more

![Fig. 6. Plot of $\sigma_w'/\bar{u}_w$ from the boundary-layer model in the stable boundary layer compared against the data of Caughey et al. (1979). $H$ is the estimated height of the boundary layer.](image)
successful in convective situations would be to use model-predicted parameters such as $z_1$, L, and $u_s$ in similarity expressions for the boundary layer such as those compiled by Irwin (1979). The present formulation, however, ensures that the turbulent velocities used in the particle model are consistent with the dynamic meteorological model solution.

2.3b. Drift correction in inhomogeneous turbulence. Although the present particle model parameterization was formulated several years ago (McNider et al., 1980), application of the model in vertically inhomogeneous turbulence indicated an unrealistic particle drift toward regions of lower turbulent energy. This problem was encountered in other particle models of similar form at that time (e.g. Lamb, 1978; Wilson et al., 1981). While empirical corrections were attempted (McNider, 1983), the analysis of Legg and Raupach (1982) established a drift correction term of the form

$$w_c = T_{L,w} \frac{\partial \sigma z}{\partial z} \left[ 1 - \exp(-\Delta t/T_{L,w}) \right]. \quad (20)$$

so that

$$z(t + \Delta t) = z(t) + (w(t) + w'(t) + w_c)\Delta t. \quad (21)$$

The addition of this term has been widely adopted for application of (5), although some controversy remains (e.g. Durbin, 1984).

Physically unrealistic particle drifts are of special importance for the long integration times undertaken in the present study. To ensure that unrealistic particle accumulations did not occur, a special experiment was first carried out. In this experiment particles were uniformly distributed in the vertical within a convective boundary layer. Equation 7 was then integrated in time out to 18 h using turbulence statistics from the meteorological model for a single time. Table 3 shows the results of this experiment. Although there is a slight mean drift upward (after 18 h), the drift is small enough that the conclusions from the experiments which are presented next are not significantly affected.

3. NUMERICAL EXPERIMENTS

In order to evaluate the rate of horizontal dispersion for long travel times, a series of numerical experiments were undertaken. These are summarized in Table 4 and discussed below.

3.1. Meteorological simulations

As a baseline case the meteorological model was initialized using the mean July 1979 sounding for the Mt. Isa area (see Fig. 7) with an imposed geostrophic easterly component of 7.5 m s$^{-1}$ constant with height. This case is referred to as the barotropic case since there was no inclusion of a thermal wind on the imposed geostrophic wind profile. The model was integrated in time for 48 h starting at 0800 LST so that two complete diurnal cycles were included. This time period is consistent with the observations of Carras and Williams (1981) (see Table 1). Table 5 gives additional details on experimental design.

Figures 8-9 show the wind and turbulence profiles which developed during the baseline meteorological simulation. A deep convective boundary layer developed during the day with a boundary-layer

<table>
<thead>
<tr>
<th>Elapsed time (h)</th>
<th>Without drift correction</th>
<th>With drift correction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>z</td>
<td>$\sigma_z$</td>
</tr>
<tr>
<td>0</td>
<td>450.0</td>
<td>270.9</td>
</tr>
<tr>
<td>3</td>
<td>489.3</td>
<td>270.9</td>
</tr>
<tr>
<td>6</td>
<td>533.9</td>
<td>259.2</td>
</tr>
<tr>
<td>9</td>
<td>547.5</td>
<td>259.7</td>
</tr>
<tr>
<td>12</td>
<td>569.9</td>
<td>260.9</td>
</tr>
<tr>
<td>15</td>
<td>586.6</td>
<td>262.9</td>
</tr>
<tr>
<td>18</td>
<td>602.9</td>
<td>258.6</td>
</tr>
</tbody>
</table>

Table 3. Particle drift in inhomogeneous turbulence. The symbol $z$ gives average height in meters (m) for 275 particles released into a convective boundary layer with a height of 900 m. The standard deviation of particles in the vertical is given by $\sigma_z$ (m).

Table 4. Summary of numerical dispersion experiments

<table>
<thead>
<tr>
<th>Case</th>
<th>Type</th>
<th>Boundary-layer model case</th>
<th>PBL turbulence</th>
<th>PBL shear</th>
<th>Coriolis force</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>Plume</td>
<td>Barotropic</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
</tr>
<tr>
<td>5</td>
<td>Plume</td>
<td>Barotropic</td>
<td>yes</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>6</td>
<td>Plume</td>
<td>Barotropic</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>7</td>
<td>Plume</td>
<td>Baroclinic</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>8</td>
<td>Plume</td>
<td>Baroclinic</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>9</td>
<td>Plume</td>
<td>Baroclinic</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
</tbody>
</table>
Influence of boundary-layer oscillations on long-range dispersion

Fig. 7. Mean July 1979 sounding plotted on a skew-$T$ diagram for Mt. Isa. Note the strong shear with height, turning from surface easterlies to upper-level westerlies. Solid line is temperature. Dashed line ($T_D$) is dew point. Other dashed line is a pseudo-adiabat.

Table 5. Meteorological model parameters for Mt. Isa simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude</td>
<td>20°S</td>
</tr>
<tr>
<td>Surface roughness ($z_0$)</td>
<td>8 cm</td>
</tr>
<tr>
<td>Albedo</td>
<td>0.25</td>
</tr>
<tr>
<td>Geostrophic wind speed</td>
<td>7.5 m s$^{-1}$</td>
</tr>
<tr>
<td>Geostrophic wind direction</td>
<td>90° (easterly)</td>
</tr>
<tr>
<td>Geostrophic shear (baroclinic case only)</td>
<td>0.0054 s$^{-1}$</td>
</tr>
<tr>
<td>Soil thermal diffusivity</td>
<td>0.003 cm$^2$s$^{-1}$</td>
</tr>
<tr>
<td>Soil density</td>
<td>1.5 g cm$^{-3}$</td>
</tr>
<tr>
<td>Soil heat capacity</td>
<td>0.3 cal g$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>Soil wetness</td>
<td>0.05</td>
</tr>
<tr>
<td>Number of vertical levels</td>
<td>22 (at 3.5, 15, 35, 60, 100, 150, 250, 500, 750, 1000, 1250, 1500, 1750, 2000, 2250, 2500, 3000, 3500, 4000, 4500, 5000, 6000 m)</td>
</tr>
<tr>
<td>Time step</td>
<td>30 s</td>
</tr>
</tbody>
</table>

Fig. 8. Mean wind speed profiles from the meteorological model for the barotropic case at two times. $V_g$ and $U_g$ denote imposed geostrophic winds.

height > 1.5 km. At night as the surface cooled, a shallow nocturnal boundary layer developed with a depth < 300 m. The mean flow in the upper part of the old convective boundary layer exhibited a marked acceleration, and even at these latitudes a substantial inertial oscillation developed (Fig. 8). Note the sharp reduction in the vertical turbulent component from day to night (Fig. 9).

A second boundary-layer experiment was run with the same initial and boundary conditions as used for the barotropic case above except that westerly shear was included in the background geostrophic flow. This case was suggested by the substantial vertical shear which was evident in the mean July 1979 sounding (Fig. 7). It will be referred to as the baroclinic case since it includes vertical variation in the geostrophic wind due to horizontal synoptic-scale temperature gradient. Figure 10 shows the mean wind profiles for this case and the large boundary-layer shear which develops, especially at night. This nocturnal shear, coupled with the near neutral conditions in
the old convective boundary layer, maintains a significant amount of turbulence as indicated in Fig. 11.

These two meteorological simulations were used to provide mean wind and turbulence input to the dispersion experiments which follow. It should be emphasized that these two meteorological model simulations were entirely one-dimensional, i.e. variations were included only in the vertical so that horizontal fields were homogeneous. The importance of using the meteorological model is that vertical mixing influenced by both the PBL and geostrophic shear is incorporated in a dynamically consistent manner.

3.2. Numerical dispersion experiments

Using the turbulence and wind profile information derived from the meteorological model, a series of dispersion experiments were carried out with the Lagrangian particle model to examine the rate of lateral plume spread as a function of various physical processes. Table 4 gives a summary of these experiments.

Computationally, these experiments were made by using wind and turbulence profiles from the one-dimensional meteorological model at 600-s intervals. A pseudo-three-dimensional domain was then created by assigning these components to a three-dimensional grid. Homogeneity in horizontal space was maintained by using the same meteorological profiles at all horizontal grid points. All of the releases for the numerical simulations were started at 1115 LST so that the PBL was initially convective and well mixed. A release height of 300 m was assigned in all of the dispersion experiments.
The series of experiments can be thought of in one sense as including or excluding various parts of the atmospheric energy spectrum. The meteorological model, in conjunction with the turbulence parameterized in the Lagrangian particle model, incorporates three components of the atmospheric motion frequency spectrum:

1. A diurnal component (period 24 h) due to the daily heating and cooling of the boundary layer. This component affects the induced turbulence in the PBL as well as the mean wind profile.

2. An inertial component (period 35 h at 20° south latitude) due to the Coriolis term and frictional decoupling. This component leads to shear when the mean wind in the upper part of the decaying daytime convective layer accelerates and turns counterclockwise (in the southern hemisphere) as the surface layer stabilizes during the night.

3. PBL-scale turbulence (period 0.05 hours-0.3 hours). This component is driven by both buoyancy and mechanical shear and varies in intensity and structure throughout the diurnal cycle.

The first two components are resolved explicitly by the meteorological model; the third is parameterized in the Lagrangian particle model in terms of quantities predicted by the meteorological model.

In addition to these explicit components, synoptic-scale effects were included in the baroclinic case via the thermal shear. It should be emphasized that the diurnal and Coriolis components of the spectrum are included only in terms of a spatially uniform frequency. There are no spatial scales associated with these frequency components, i.e., motions due to these components are coherent or homogeneous over the entire horizontal domain. Thus, in terms of a wavelength spectrum there is only a contribution of energy at PBL scales. Nevertheless, time oscillations in PBL winds and turbulence can affect long-range pollutant dispersion significantly as will now be shown.

It should be noted that these experiments were intended to be idealistic in that the full atmospheric spectrum was not included so as to isolate the effects of PBL-scale turbulence and PBL shear on dispersion. In the actual atmosphere many scales of motion may be operating to affect dispersion rates. In fact, recent data such as those reported by Gage (1979) show substantial energy in the mesoscale region.

3.2a. Case I. The first case tested was a short-term release which included both PBL-scale turbulence and PBL shear. Case 1, therefore, represents a case in which dispersion is due to turbulent diffusion alone; differential advection is not a factor. The barotropic meteorological model simulation was used to provide the turbulent parameters (i.e., $K_w$, $L$, $R_i$, $u^*$, $z_i$) while the mean wind profile was assumed to be uniform with height. To explain the term "short-term release", an ensemble of particles was released instantaneously in the particle model from a point. This would be considered a puff release except that (1) turbulent components of the particle velocities were initialized independently, i.e., a range of particle velocities was imposed randomly with a standard deviation which is proportional to the local turbulence intensity; and (2) the calculation of the subgrid-scale turbulent velocities at later times is done independently even for particles at the same location. Formally, for the initial release,

$$u_i^*(0) = \sigma_i^*, \Gamma_i,$$

where $u_i^*(0)$ is the initial turbulent velocity for the $i$th particle and $\Gamma_i$ is the $i$th realization of a random normal variate with zero mean and standard deviation of 1.0. The turbulent velocity standard deviations $\sigma_i^*$ were determined from the boundary-layer parameterization as a function of vertical position at the time of release. The inclusion of a range of initial velocities gives in effect an averaging time for the particle spread statistics on the order of 30 min to one hour. We will thus use the term 'pseudo-puff' to refer to this type of release.

Figure 12 shows the horizontal spread of the pseudo-puff for this case compared against the Mt. Isa plume observations of Bigg et al. (1978) and Carras and Williams (1981). Model pseudo-puff widths were determined by computing standard deviations of particle cross-wind positions including particles at all downwind distances. The standard deviations were multiplied by 4.28 to obtain the final pseudo-puff widths plotted. This corresponds to truncating a Gaussian distribution on both wings at the points where the probability density function is ten per cent of its centerline value.

As can be seen from Fig. 12, if only the PBL-scale turbulence is included, plume growth rates are greatly underestimated. This is consistent with the discussion in the Introduction that PBL turbulence alone cannot maintain the long-range plume growth rates which have been observed.

3.2b. Case 2. The next case tested was a short-term release which included both PBL-scale turbulence and PBL shear. Dispersion, therefore, is a result of both turbulent diffusion and differential advection. Figure 13 shows model-predicted pseudo-puff widths vs the composite Mt. Isa plume observations. The predictions show substantially enhanced growth as compared to Fig. 12 in which PBL shear was neglected. Note that the plume widths are vertically integrated so that a plume depicted as a certain width may actually be distorted or stretched by the shear. Subsequent or concomitant vertical mixing would be required to fulfill the depiction of diffusion indicated by the statistics.

There is also an interesting time dependence exhibited by the growth rates. During convective conditions in which momentum is well mixed (little shear), the growth rates approximate those in Fig. 12. At night, however, an initial slowing of the growth rate is followed by a period of dramatic horizontal growth.
Fig. 12. Horizontal spread for a short-term release (pseudo-puff) into barotropic flow. Vertical shear of the horizontal wind was not included so dispersion is totally due to PBL-scale turbulence. Local time applies to meteorological simulation results.

Gifford (1982) also discussed this accelerating dispersion and suggested that it might be due to substantial energy in the mesoscale region beyond PBL-scale turbulence. In the present case, this accelerating dispersion is due to the development of directional shear with height as the upper part of the old convective boundary layer decouples from the lower layer and accelerates, first toward lower pressure and then toward high pressure as the inertial oscillation progresses.

It should be noted that the accelerating growth here cannot be due to horizontal motions having scales larger than PBL turbulent scales since we do not include such components in our wavelength spectrum. (The only parts of the wavelength spectrum which are active are the PBL components.) The accelerating dispersion shown is directly related to PBL shear enhanced by having the diurnal and inertial components in the frequency spectrum.

Gifford (1987) has shown that autocorrelations of the form used in (19) only match observed diffusion rates if $T_L$ is of order $10^4$ s. The subgrid-scale $T_L$ directly arising from the PBL parameterizations in the present study is only $10^3$ s. In the present simulations, the actual Lagrangian time scales of the particles are, however, influenced by the mean shear and inertial oscillations so that the effective $T_L$ is much larger than $10^3$ s.

3.2c. Case 3. The final case for a short-term release is similar to Case 2 in that both PBL-scale turbulence and PBL shear are included. The difference is that the meteorological simulation includes the imposition of geostrophic shear (i.e. baroclinic case). As mentioned earlier, the Mt. Isa mean July 1979 sounding showed marked shear in the wind profile with strong easterlies near the surface and a strong westerly flow at 500 mb. Inclusion of this geostrophic shear accentuated the intensity of the low-level jet and the oscillations in the mean wind as shown in Fig. 10. Also, at night this shear coupled with near neutral conditions in the upper part of the old convective boundary layer, maintained significant turbulence aloft (Fig. 11).

Figure 14 shows the rate of spread of this pseudo-puff release compared to the Mt. Isa observations. The rate of spread is quite large for this case, especially at night, and is larger than either Cases 1 or 2. This is due to the enhanced PBL shear in response to the imposed geostrophic shear.

The modelled pseudo-puff growth rate also exceeds that of the plume observations; for larger diffusion times, however, this is partly a result of our method for
the computation of $\sigma_y$. Our calculation of pseudo-puff widths at specific diffusion times incorporate particles at all distances. That is, the pseudo-puff widths are based upon the standard deviation of all the particles lateral coordinate positions regardless of their downwind position and vertical level. In the highly sheared simulated environment for Case 3, the particle ensemble becomes very elongated so that particles contributing to the apparent spread are separated in downwind distance by a large amount. This is in contrast to the observations, in which plume widths were measured over a relatively short time so that parcels contributing to the width statistics had a limited downwind distance difference and were at a single level. The particles sampled in the observations may also have had different release times. Figure 15 gives an instantaneous picture of the puffs in Case 2 and Case 3 and show how the pseudo-puffs have been stretched by the speed shear in the along-wind direction. Thus, while the spread statistics presented in Figs 12–14 demonstrate the effect of boundary-layer shear and geostrophic shear on the rate of crosswind spread, the comparisons with the observations should be viewed with caution. The experiments in the next section are designed to avoid this problem by releasing particles and sampling in a manner more consistent with the observations.

3.2d. Cases 4 and 5. In order to alleviate the sampling problem described above, a series of cases were run in which particles were released continuously in time so as to more closely mimic the Mt. Isa plume. Particles were released at the rate of 36 particles per hour so that for the 42-h period of integration, a total of 1506 particles were released.

Case 4 involves a plume simulation which includes only boundary-layer turbulence and excludes shear and inertial effects. Figure 16a shows a plan view of the plume for this case 42 h after start of the release. In Case 5 turbulence is not included so that the particles move only with the mean wind at the release height. While this case is of no interest in terms of lateral dispersion statistics, a plan view of the plume (Fig. 16b) shows meander in the plume driven by the diurnal and inertial oscillation in the mean wind.

3.2e. Cases 6 and 7. The last two cases include both boundary-layer turbulence and boundary-layer shear for the barotropic and baroclinic simulations, respectively. While these releases more closely resemble the Mt. Isa situation (see Figs 16c and 16d), there are still some interpretation problems. Figure 17 shows plume width as a function of distance at a fixed time (42 h after the start of release of the particles). The results here were initially surprising in that the middle of the plume was wider than the furthest downwind part of

Fig. 13. Same as Fig. 12 except PBL shear is included.
the plume. This is not due to a contraction in the plume (which is physically impossible for the set of equations employed) but rather is a result of part of the plume lagging behind near the ground while the upper part is accelerated ahead.

As can be seen in Fig. 17, most of the plume widths are in reasonable agreement with observations. Neglecting geostrophic shear but including PBL shear (the barotropic case) produces widths slightly less than those observed. On the other hand, including geostrophic shear produces widths which exceed the observations. It should be noted that our geostrophic shear may be overstated in the boundary layer since we interpolated downward from 850 mb using the same gradient which existed between 700 mb and 850 mb. We have no information of the true geostrophic wind below 850 mb.

One other relevant factor with regard to Fig. 17 is the method employed to calculate the model $\sigma_i$ for the continuous releases. Unlike the first three cases, plume $\sigma_i$s were calculated for 50-km-wide (in the downwind $x$-direction) plume segments. All particles in a segment were considered, no matter what their release time or vertical position. Note that sampling at a single elevation as was done for the Mt. Isa observations may not catch all of the plume, especially at night.

Carras and Williams (1981) also attributed the observed plume widths at large downwind distances to shear. Using rawinsonde winds for computing sample trajectories at different heights, they were able to reasonably duplicate the observed widths. The present study clarifies the importance of the diurnal and inertial oscillation of the boundary layer in producing vertical wind shears. Figure 18 gives a time-height cross-section of simulated horizontal velocity vectors showing the directional oscillation and vertical shears which developed in the barotropic case. As can be seen, the differential oscillation with height produces substantial shear. Figure 18 can be used to explain the accelerating diffusion seen in Fig. 13 between 1800 and 0600 LST. Gifford (1982) attributed this accelerating diffusion to energy at mesoscale wavelengths. The present study suggests that this accelerating diffusion is due to diurnal oscillations in the vertical shear of the horizontal wind. Figure 18 also shows clearly the source of the plume meander at 300 m evident in Fig. 16b.

4. SUMMARY AND CONCLUSIONS

Coupled one-dimensional meteorological and Lagrangian particle models have been used to isolate and examine the role of vertical shear in the horizontal dispersion of pollutants over one or two days. Through a series of controlled numerical experiments
it is found that the vertical shear of the horizontal wind induced by diurnal and inertial forces maintains plume growth rates for large downwind distances that are only slightly less than those observed by Carras and Williams (1981). The inclusion of an externally imposed geostrophic shear into the meteorological model due to a synoptic-scale horizontal temperature gradient produces growth rates that equal or exceed those of the observations.

The numerical experiments also demonstrated periods of accelerating diffusion. Such periods of accelerating diffusion have been observed. The present study suggests that those periods of accelerating diffusion may be produced by a decoupling of the
atmospheric boundary layer and an inertial oscillation. The persistence of an accelerated diffusion region in the composite data of Gifford (1983b) is perhaps due to the same release time for most of the observations. That is, many of the releases may have occurred near midday so that the accelerated diffusion overnight shows up at the same diffusion time. At this point, this is a conjecture and not all the accelerating data may be due to this mechanism (see Barr and Gifford, 1987). Also, it should be clarified that the acceleration only occurs in the vertically integrated plume and such acceleration would only occur in a previously well mixed plume.

In addressing the fundamental question posed by Gifford (1982) on what mechanism maintains the observed plume growth at times greater than the time scale of PBL turbulence, we offer the following conclusions based on the numerical experiments described above. Firstly, it is apparent that vertical shear of the horizontal wind, when coupled with PBL turbulence, can produce average horizontal growth rates which are reasonably consistent with the observed growth rates. Carras and Williams (1981) also concluded that shear was responsible for the sustained growth rates based on trajectory calculations performed with rawinsonde data. The present study shows, however, that the shears are introduced by adding a diurnal and inertial component to the frequency spectrum. The growth rates influenced by shear necessarily require concurrent or later vertical mixing to give true diffusion (i.e. a reduction in concentration). Thus, in addressing the discussion between Gifford and Smith (and Pasquill), we side with Smith and Pasquill in attributing the growth rates to vertical shear coupled with vertical mixing. The observed large spread rates in the upper troposphere or stratosphere in other studies (Barr and Gifford, 1987) would have to be due to other mechanisms.

On the other hand, it must be stated that Gifford never discounted shear as a mechanism, but, if shear were responsible, he wanted the shear related to fundamental atmospheric processes. The present study has shown that the shears largely responsible for the growth rates are produced by diurnal and inertial oscillations of the PBL. Thus, contributions to the atmospheric frequency spectrum in the mesoscale time range (1-48 h) are then largely responsible for the growth rates. Thus Gifford is correct in that mesoscale energy maintains the growth; however, the mesoscale energy does not have to be associated with mesoscale spatial circulations as we feel he had envisioned. This is not to say, however, that mesoscale spatial circulations may not have a large impact in some cases, but for the growth rates observed at Mt. Isa such circulations are not required.

In some of the numerical case studies presented here, geostrophic shear was also considered. While the present study may have overstated the geostrophic shear in the boundary layer, it is obvious that geostrophic shear can have a substantial impact on plume growth rates. In mid-latitudes, geostrophic shear related to the north–south temperature gradient is the rule rather than the exception. Much more work needs to be done on incorporating this physical feature in long-range transport models. It must also be stated that present experiments have not proved that PBL shear
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C. Fig. 18. Time–height cross section of horizontal wind vectors showing the diurnal and inertial oscillations. The vectors are plotted in compass coordinates (i.e. up is north, left is west, etc.) Note that the terrain height used in the simulations was 250 m ASL.

and geostrophic shear explain all of the large growth rates found in the composite observations. Other scales of atmospheric motion are undoubtedly involved in some of the data. Yet, the simple experiments here show the strong impact PBL shear and geostrophic shear can have on dispersion rates, and both PBL shear and geostrophic shear are a prevalent component of our atmosphere.

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