Treatment of Interfaces in Random Walk Dispersion Models

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ABSTRACT

The problem of how to formulate random walk dispersion models in situations where the flow properties vary discontinuously across an interface is considered. It is shown how the dispersion model can be made consistent with the assumptions made about the turbulence. The approach does not lead to a unique model, but it is argued that in many cases the rate of diffusion through the interface is limited not by the detailed physics of the interface but by the rates of diffusion on either side of the interface and, in such situations, results may be insensitive to which of the consistent models is chosen. Some simulations are presented to illustrate these ideas.

1. Introduction

Random walk models are becoming increasingly popular as a tool for modeling atmospheric dispersion, particularly when coupled to numerical weather prediction models, for example, the UK Nuclear Accident Response Model (NAME) (Maryon et al. 1991; Ryall et al. 1997), the Australian Lagrangian Atmospheric Dispersion Model (LADM) (Physick et al. 1992), the Regional Atmospheric Modeling System Lagrangian Particle Dispersion Model (RAMS-LPDM) (Eastman et al. 1995), the Random Particle Transport And Diffusion Model (RAPTAD) (Yamada and Bunker 1988), and the Mesoscale Dispersion Modeling System (MDMS) (Uliasz 1993). In this paper, we consider the problem of how such models should be designed in situations where there are interfaces with discontinuities in turbulence statistics. The archetypical example of such an interface is the capping inversion at the top of a convective boundary layer. In many models the rapid but continuous change in turbulence statistics that occurs may be represented by a discontinuity, and there may be low levels of turbulence above the discontinuity due to gravity waves, etc. In this paper, we show how random walk models can be made mathematically consistent in the presence of an interface. However, we do not derive a unique model—selecting the most appropriate of the consistent models requires, in general, consideration of the physics within the interface. Despite this it seems likely that in many cases the rate of diffusion through the interface is limited not by the detailed physics of the interface but by the rates of diffusion on either side of the interface. In such situations the analysis presented here is all that is needed to derive a satisfactory model.

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2. Analysis

Our aim is to derive a model for situations where the turbulence statistics change discontinuously at an infinitesimally thin interface. We want this model to behave in the same way as a random walk model [of the type considered by, e.g., Thomson (1987)] would at an interface where the turbulence statistics change rapidly but continuously, and so we will assume for the purpose of this investigation that random walk models for situations with continuous changes in turbulence statistics represent ‘‘truth.’’

We start by considering what would happen if the interface was thin but of nonzero thickness with the turbulence statistics changing continuously in space. We will use z and w to denote the height and velocity of a particle, and we will assume that the interface is horizontal at height z_i and stationary with z_{i+} and z_{i-} being the heights

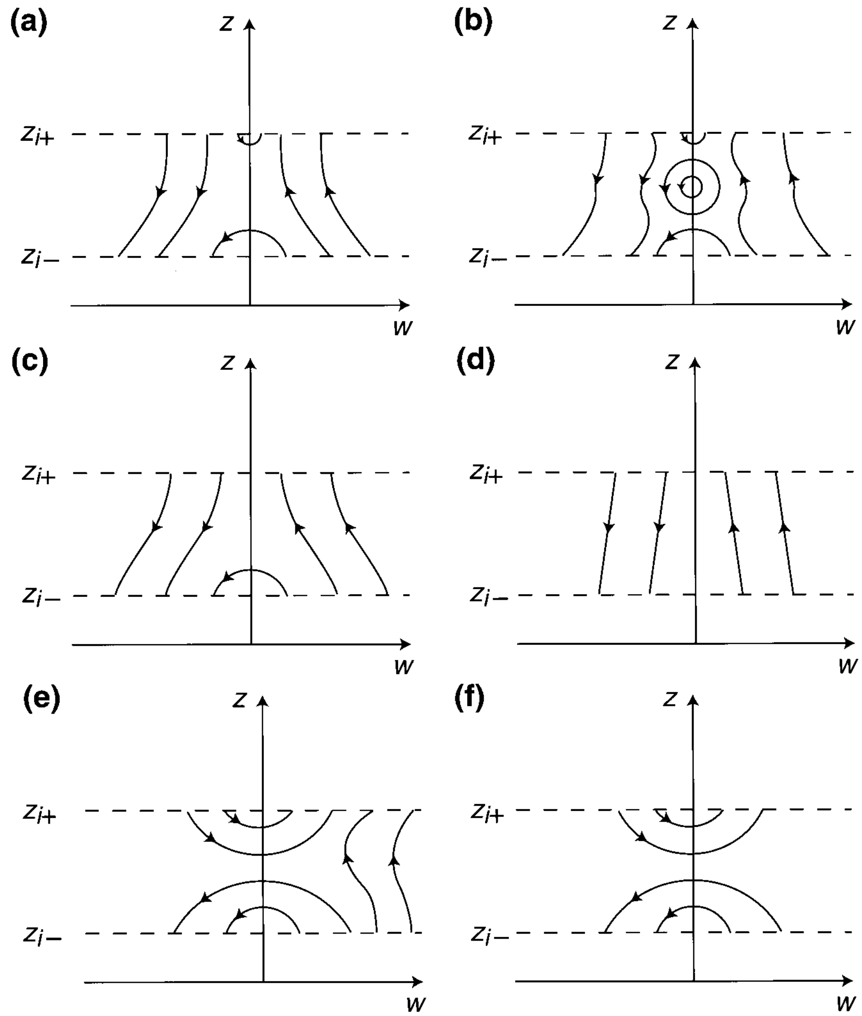

FIG. 1. Illustration of possible flows in (z, w) space.

of the top and bottom of the interface. We will also assume that the turbulence statistics are stationary in time and horizontally homogeneous or, more precisely, change slowly compared to the time a particle spends in the interface region and the horizontal distance traveled by a particle in crossing the interface. This last assumption is not a real restriction because of the assumed thinness of the interface. Finally, we assume that the vertical motion is described by a random walk model in which a particle's state is represented by z and w. This is a real restriction and implies that the vertical motion can be considered in isolation from the horizontal motion. This assumption is considered further below.

Suppose the Lagrangian timescale τ on which particles forget their velocity is much larger than the time particles spend within the interface. This implies that within the interface the particle trajectories in (z, w) space are deterministic and do not cross each other. As a result, the trajectories will generally take the form illustrated in Fig. 1a, although cutoff circulations (Fig. 1b) or no reflection from one or both sides (Figs. 1c and d) and no transmission from one or both sides (Figs. 1e and f) are also possible. The situation in Fig. 1e is only possible if there is a mean vertical velocity through the interface.

Let $p(z, w)$ denote the density of tracer particles in (z, w) space, and let $p_a(z, w)$ denote the density when the particles are well mixed. Consider the flux of particles across a surface of constant z with $w_1 < w < w_2$ for some w_1 and w_2 (see Fig. 2). When the particles are well mixed this is given by

$$\int_{w_1}^{w_2} wp_a(z, w)\, dw.$$

Since integrals such as this occur frequently in the analysis, we will write $F_{w_1}^{w_2}(z)$ for $\int_{w_1}^{w_2} wp_a(z, w)\, dw$. The quantity $F_{-\infty}^{\infty}(z)/\int_{-\infty}^{\infty} p_a(z, w)\, dw$ is the mean vertical velocity and, if this is zero, we have $F_0^{\infty}(z) = -F_{-\infty}^{0}(z)$. More generally, $F_{-\infty}^{\infty}(z)$ is nonzero but can be assumed constant

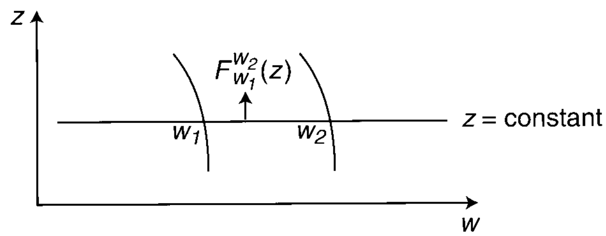

FIG. 2. Illustration of the flux of particles across the surface $z =$ const. with $w_1 < w < w_2$.

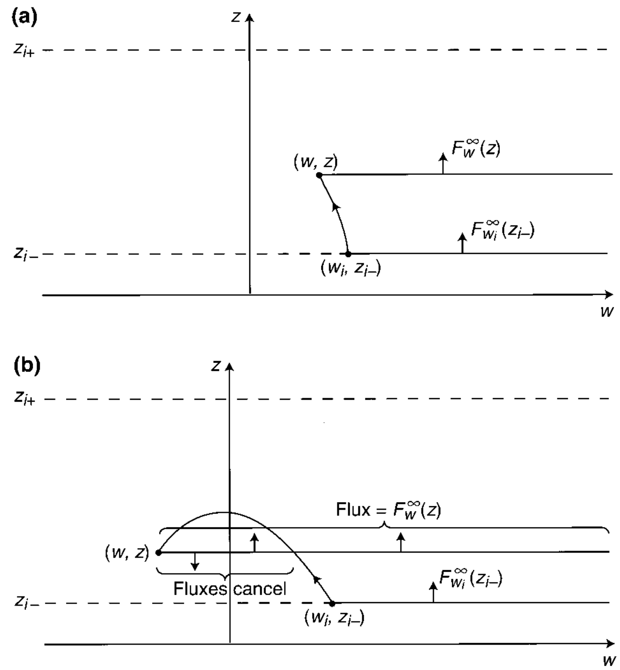

FIG. 3. Illustration of the conservation of flux of particles.

within the interface because of the interface's thinness. The flux between two streamlines in (z, w) space must be conserved and so the streamlines and the motion of the particles are determined once p_a is known. Suppose a particle enters the interface from below with incident velocity w_i. If it ever reaches height z ($z_{i-} \leq z \leq z_{i+}$) and has $w > 0$ (this must be so the first time it reaches z), then its velocity w must be given by $F^{\infty}_{w}(z) = F^{\infty}_{w_i}(z_{i-})$ because of conservation of flux (see Fig. 3a). Similarly, if it ever reaches height z with $w < 0$, then w must again be given by $F^{\infty}_{w}(z) = F^{\infty}_{w_i}(z_{i-})$ although this time we are seeking the solution with $w < 0$ (see Fig. 3b). Hence, we have the following results on the fate of the particle. If $F^{\infty}_{0}(z) < F^{\infty}_{w_i}(z_{i-})$ at any height z in the interface, then the particle will be reflected—that is, the particle will be reflected if w_i is less than the critical value w_c, which is defined by

$$F^{\infty}_{w_c}(z_{i-}) = \min(F^{\infty}_{0}(z)\colon z_{i-} \leq z \leq z_{i+}). \qquad (1)$$

Otherwise, the particle will be transmitted. The reflection and transmission velocities w_r and w_t will be given by

$$F^{\infty}_{w_t}(z_{i+}) = F^{\infty}_{w_i}(z_{i-}), \qquad w_t > 0 \qquad (2)$$

and

$$F^{\infty}_{w_r}(z_{i-}) = F^{\infty}_{w_i}(z_{i-}), \qquad w_r < 0. \qquad (3)$$

Similar results apply to particles entering the interface from above. If we denote the critical velocity for particles entering the interface from above by w'_c, then w'_c is related to w_c by

$$F^{w'_c}_{-\infty}(z_{i+}) + F^{\infty}_{w_c}(z_{i-}) = F^{\infty}_{-\infty}. \qquad (4)$$

We would like to be able to express the above in terms of probabilities for the various possible fates of a particle. To do this we need to consider the difference between the probability distribution of velocities measured at a fixed height z and the probability distribution of the velocity of particles crossing the height z. The density function of the former is proportional to $p_a(z, w)$ and can be thought of as being proportional to the fraction of time that the vertical velocity at a point at height z is close to w. In contrast, the density function of the latter is, for well-mixed particles, proportional to $|w|p_a(z, w)$; the factor $|w|$ reflects the fact that, when the vertical velocity is close to w, the number of particles crossing the surface per unit time will be proportional to $|w|$. For example, suppose that just two values of w occur and that these values occur for equal fractions of the time. Then, more particles will cross the height z when the value of w with the larger magnitude occurs, and so, for particles crossing height z, the two values of w will not be equally probable. As a result of this, the probability density function of the velocity of particles impinging on the interface from below is, in the well-mixed state, proportional to $|w|p_a(z_{i-}, w)$, for $w > 0$. Only particles with $w > w_c$ are transmitted and so the probability of transmission P_t is given by

$$P_t = F^{\infty}_{w_c}(z_{i-})/F^{\infty}_{0}(z_{i-}).$$

If we consider all the particles reaching the interface from above and below for a well-mixed distribution of particles, then the particles impinging on the interface have a velocity pdf proportional to $f_i(w)$, where

$$f_i(w) = \begin{cases} |w|p_a(z_{i-}, w), & \text{if } w > 0, \\ |w|p_a(z_{i+}, w), & \text{if } w < 0, \end{cases}$$

and the particles leaving the interface have a velocity pdf proportional to $f_e(w)$, where

$$f_e(w) = \begin{cases} |w|p_a(z_{i+}, w), & \text{if } w > 0, \\ |w|p_a(z_{i-}, w), & \text{if } w < 0. \end{cases}$$

The above results remain meaningful in the limit $z_{i+} - z_{i-} \to 0$ and so we can apply them in a random walk model that represents the interface as a discontinuity. We will generally know or be able to estimate $p_a(z_{i-}, w)$ and $p_a(z_{i+}, w)$ and, if we also know either w_c or w'_c, it is then possible to determine the fate of a particle from Eqs. (2), (3), and (4) together with the equivalent of Eqs. (2) and (3) for a particle entering the interface from above. We cannot, however, determine w_c (or w'_c) because, according to (1), it depends on the details of what happens within the interface, which will generally be unknown. However, we can determine limits on w_c. Here, w_c has a lower limit determined by $F_0^\infty(z_{i+}) = F_{w_c}^\infty(z_{i-})$ [or zero if $F_0^\infty(z_{i+}) > F_0^\infty(z_{i-})$] and an upper limit determined by $F_{-\infty}^\infty(z_{i-}) = F_{w_c}^\infty(z_{i-})$ [or infinity if $F_{-\infty}^\infty(z_{i-}) \le 0$]. The lower limit on w_c can easily be derived from (1), while the upper limit follows by considering the signs of the terms in (4). The lower limit (if nonzero) corresponds to the value for which w'_c is zero, and the upper limit (if not infinite) corresponds to the value for which w'_c is infinite. These limits on w_c correspond, respectively, to an upper limit on P_t of $F_0^\infty(z_{i+})/F_0^\infty(z_{i-})$ (or unity if this is smaller) and a lower limit of $F_{-\infty}^\infty(z_{i-})/F_0^\infty(z_{i-})$ (or zero if this is bigger). For the case with zero mean velocity, the upper limit on w_c is infinity, and the lower limit on P_t is zero corresponding to total reflection (Fig. 1f).

If $F_0^\infty(z)$ varies monotonically within the interface (e.g., Figs. 1c or 1d), then the problem simplifies. In this case, w_c is equal to its smallest possible value, which is given by

$$F_0^\infty(z_{i+}) = F_{w_c}^\infty(z_{i-}) \quad (5)$$

[or zero if $F_0^\infty(z_{i+}) > F_0^\infty(z_{i-})$], and the fraction of particles transmitted is the highest possible, namely,

$$\frac{F_0^\infty(z_{i+})}{F_0^\infty(z_{i-})}$$

(or unity if this is smaller). In this case, the particles approaching the interface from the side with the smaller incident flux are always transmitted.

As a check on the above, we can derive the central result, that is, the conservation of the flux $F_w^\infty(z)$ following a particle, in a different way. In the limit of large τ, the one-dimensional random walk model satisfying the well-mixed condition takes the form

$$\frac{dw}{dt} = \frac{\phi}{p_a}$$

with

$$\frac{\partial \phi}{\partial w} = -\frac{\partial}{\partial z}(w p_a)$$

and $\phi \to 0$ as $w \to \pm\infty$; that is,

$$\frac{dw}{dt} = \frac{1}{p_a}\int_w^\infty \frac{\partial}{\partial z}[w' p_a(z, w')]\, dw' = \frac{1}{p_a}\frac{\partial}{\partial z}F_w^\infty(z)$$

(see, e.g., Thomson 1987). We then have

$$\frac{d}{dz}F_w^\infty(z) = -w p_a \frac{dw}{dz} + \frac{\partial}{\partial z}F_w^\infty(z)$$

$$= -p_a\frac{dw}{dt} + \frac{\partial}{\partial z}F_w^\infty(z) = 0.$$

Of course the turbulence may be small scale in the interface, and the assumption that τ is much larger than the residence time in the interface may be invalid. If so, it may be appropriate to add a random component in determining the particle behavior. However, to ensure that a well-mixed distribution of tracer remains well-mixed, it is important to ensure that, if the particles impinging on the interface come from a well-mixed distribution—that is, if the particles impinging on the interface have a velocity pdf proportional to $f_i(w)$—then the velocity distribution of particles leaving the interface should be chosen to be that appropriate for a well-mixed distribution of particles [i.e., chosen from a distribution with pdf proportional to $f_e(w)$]. This condition is of course satisfied by the large τ approach described above. One possibility is that, when the particle reaches the interface, w is chosen at random from the distribution with pdf $f_e(w)/\int f_e(w)\, dw$. This gives a transmission probability from below of $\int_0^\infty f_e\, dw/\int_{-\infty}^\infty f_e\, dw = F_0^\infty(z_{i+})/[F_0^\infty(z_{i+}) - F_{-\infty}^0(z_{i-})]$. There are clearly many possibilities that are intermediate between making the exit velocity determined by the incident velocity as in the large τ approach above and making it completely independent of the incident velocity. Note that for any such model the fraction of particles transmitted must still lie between the bounds established for the case with τ much greater than the residence time in the interface.

Which model is best in general can be resolved only by considering the physics at the interface and is not addressed by the arguments presented here. However, in the absence of other information, the approach in Eqs. (2)–(5) seems plausible. This gives the maximum possible transmission probability and should be adequate in situations where the rate of diffusion is limited not by the detailed physics of the interface but by the rates of diffusion on either side of the interface. This seems likely to be true in most situations although it is hard to give precise criteria for validity. It can fail only if the diffusivity within the interface is substantially smaller than the diffusivities occurring both above and below the interface.

In applying the above ideas, we note that ideally the particle velocity [which in most random walk implementations is held constant over a time step, with z evolving according to $z(t + \Delta t) = z(t) + w\,\Delta t$] should change at the instant the particle reaches the interface, with $z(t + \Delta t)$ calculated in a way that accounts for the change in velocity in the middle of the time step.

Note the above analysis follows quite closely the ideas for treating impermeable boundaries discussed by Thomson and Montgomery (1994). In fact, impermeable boundaries can be regarded as a special kind of interface, namely, one with no turbulent diffusion (and in fact no fluid) on one side of the boundary. Also, although we assumed that the interface is stationary, the above results can be applied to moving interfaces by working in a frame of reference fixed in the interface. Finally, we note that, although we have allowed for the possibility of a mean velocity (relative to the interface), it may be easier in practice to consider a split time step model where the particle position is updated in two separate steps that account for the turbulence and mean flow, respectively. In this case the interface can be treated as if there is no mean flow in the turbulence step, and ignored in the mean flow step. This approach will still ensure that a well-mixed distribution of particles is preserved.

3. The Gaussian case

Let us consider Gaussian conditions with no mean vertical velocity (or with the mean vertical velocity treated separately) and with vertical velocity standard deviation $\sigma_w(z)$. In this case $F_w^\infty(z)$ is proportional to $\sigma_w(z)\exp[-w^2/2\sigma_w^2(z)]$ and so our preferred approach [Eqs. (2)–(5)] reduces to the following. For a particle approaching from below with velocity w_i, we calculate

$$\sigma_w^2(z_{i+})\left[\frac{w_i^2}{\sigma_w^2(z_{i-})} + \log\frac{\sigma_w^2(z_{i+})}{\sigma_w^2(z_{i-})}\right]. \qquad (6)$$

This is the value of w_t^2 obtained from (2). If this is negative, then w_i is less than w_c as determined by (5) and so, as implied by (3), we apply perfect reflection to the particle. If it is positive, we allow the particle to cross the interface with its velocity changing at the moment it crosses the interface to that given by the square root of (6). The treatment of particles entering the interface from above is similar. The particles approaching from the side with the smaller value of σ_w are always transmitted.

An alternative approach that is simple to implement and that is intermediate between making the exit velocity determined by the incident velocity and making it completely independent of the incident velocity is as follows. For a particle approaching from below, allow particles to be transmitted at random with probability $\sigma_w(z_{i+})/\sigma_w(z_{i-})$ (or unity if this is less) and multiply their velocities by $\sigma_w(z_{i+})/\sigma_w(z_{i-})$ at the moment of crossing. Otherwise, apply perfect reflection to the particle. The treatment of particles approaching from above is, of course, similar. This approach satisfies the criterion discussed above that, if the particles impinging on the interface have a velocity pdf proportional to $f_i(w)$, then the velocity distribution of particles leaving the interface should be chosen from a distribution with pdf proportional to $f_e(w)$. Like the approach based on (2)–(5), this method maximizes the transmission probability, with the particles approaching from the side with the smaller value of σ_w always being transmitted. The approach will also work in non-Gaussian cases provided $p_a(z_{i+}, w)$ has the same shape as $p_a(z_{i-}, w)$. Wilson (1980) used this method to treat a smooth change in σ_w by approximating it by a series of small discontinuities (see also Leclerc et al. 1988).

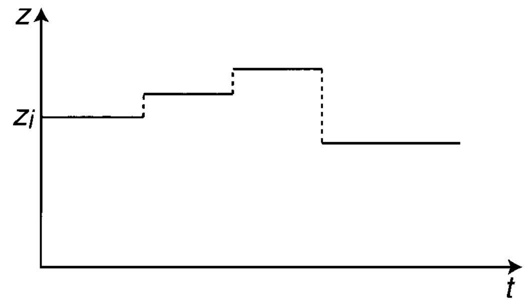

FIG. 4. Illustration of possible discontinuous evolution of boundary layer depth in a model.

4. Jumps in z_i

In practical models where z_i is the boundary layer top, it is often the case that the model boundary layer top moves in jumps rather than continuously (see Fig. 4). In such cases, z_i is constant at most times and so the theory discussed above can be used. However, the turbulence properties change discontinuously in time at the places marked by dashed lines in Fig. 4. At such places it should be ensured that, if the particles approaching the discontinuity are well mixed [i.e., $p(z, w, t_-) \propto p_a(z, w, t_-)$], then so are the particles leaving the discontinuity [i.e., $p(z, w, t_+) \propto p_a(z, w, t_+)$]. This can be ensured by, for example, conserving $\int_w^\infty p_a(z, w', t)\, dw'$ as each particle crosses (e.g., for the Gaussian case, by keeping w/σ_w fixed) or by "reinitializing" each particle with a random velocity whose distribution has pdf proportional to $p_a(z, w, t_+)$.

5. The 3D case

So far we have treated the problem as if it is one-dimensional with the interface horizontal and the vertical motion being unaffected by the horizontal motion. In the general case, we can again use the principle that, if the particles impinging on the interface come from a well-mixed distribution, then the velocity distribution of particles leaving the interface should be appropriate for a well-mixed distribution of particles. For a stationary interface with normal $\mathbf{n}$ and with $\mathbf{x}_+$ and $\mathbf{x}_-$ denoting points on the two sides of the interface, $\mathbf{x}_+$ being on the side to which $\mathbf{n}$ points, this can be expressed as the requirement that, if the velocities impinging on the interface have a distribution with pdf proportional to

$$\begin{cases} |\mathbf{u}\cdot\mathbf{n}|p_a(\mathbf{x}_-, \mathbf{u}), & \text{if } \mathbf{u}\cdot\mathbf{n} > 0, \\ |\mathbf{u}\cdot\mathbf{n}|p_a(\mathbf{x}_+, \mathbf{u}), & \text{if } \mathbf{u}\cdot\mathbf{n} < 0, \end{cases}$$

then the particles leaving the interface should have a velocity pdf proportional to

$$\begin{cases} |\mathbf{u}\cdot\mathbf{n}|p_a(\mathbf{x}_+, \mathbf{u}), & \text{if } \mathbf{u}\cdot\mathbf{n} > 0, \\ |\mathbf{u}\cdot\mathbf{n}|p_a(\mathbf{x}_-, \mathbf{u}), & \text{if } \mathbf{u}\cdot\mathbf{n} < 0. \end{cases}$$

Moving interfaces can be treated by using a frame of reference fixed in the interface as in section 2 above, and time discontinuities can be treated using the obvious 3D extension of the approach given in section 4.

If, as discussed in section 2 above, we regard an impermeable boundary as a special kind of interface, then the above condition is satisfied, in particular, by the method proposed by Wilson and Flesch (1993). Wilson and Flesch were concerned with flow above a horizontal boundary for the case of Gaussian turbulence in which the vertical and horizontal velocities at a fixed point are correlated. They proposed reversing the fluctuating part of the horizontal velocity as well as the vertical velocity when a particle hits the boundary. Physically, one can think of the horizontal momentum change of the particles being balanced by the drag force on the ground.

In practical models, one might have a situation where the boundary layer top is horizontal, but z_i changes discontinuously with the horizontal coordinates x and y and with time and where one needs to consider horizontal as well as vertical motions. We will briefly consider how the above can be applied to this case. We will not assume that the horizontal velocity $\mathbf{u}_H$ is unaffected by the vertical motion (this clearly will not be the case in general since the horizontal velocity will be affected by which side of the interface at $z = z_i$ the particle finds itself on), but we will assume that $\mathbf{u}_H$ and w are independent when measured at a fixed point. This last assumption, although inconsistent with the turbulence dynamics in general, is not likely to lead to large errors in the calculation of dispersion and is adopted in many practical dispersion models. The simplest approach is as follows. First, we consider the vertical velocities. At the discontinuity at the boundary layer top, treat w as in sections 2 and 3. At discontinuities caused by z_i changing with x, y, or t, treat the vertical velocity as for the time discontinuities discussed in section 4. The treatment of horizontal velocities at time discontinuities or at the interface $z = z_i$ can also be based on the approach in section 4—that is, conserving $\int p_a\, d\mathbf{u}_H$, where p_a refers here to the distribution of horizontal velocities. The treatment of horizontal velocities at places where z_i changes discontinuously with x and y is in principle more complex and should be based on the ideas in sections 2 and 3 (i.e., conserving $\int \mathbf{u}\cdot\mathbf{n} p_a\, d\mathbf{u}$ rather than $\int p_a\, d\mathbf{u}$ where $\mathbf{n}$ is normal to the interface). However, in practice (at least in atmospheric dispersion applications) the horizontal advection across the discontinuity will probably be dominated by the mean flow, and so details of the procedure adopted are probably of less importance.

6. Diffusion models

We have mainly been concerned with random walk dispersion models where the position and velocity of the particle obey a coupled set of stochastic differential equations. However, in some cases, it is simpler to model dispersion using the particle position only. For example, if the mean vertical velocity is zero, the evolution of z can be modeled by the stochastic differential equation

$$dz = \frac{\partial K}{\partial z}dt + \sqrt{2K}\, d\xi, \tag{7}$$

where K is the eddy diffusivity and $d\xi$ is the increment of a Wiener process—that is, $d\xi$ is Gaussian with mean zero and variance dt with the values of $d\xi$ at different times being independent. Such models are equivalent to solving the diffusion equation (see, e.g., Durbin 1983; Boughton et al. 1987; Luhar and Rao 1993). In the same way as for the models considered above, it would be useful to be able deal with a discontinuity in K.

Let K_+ and K_- be the values of K immediately above and below the interface. Suppose without loss of generality that $K_+ < K_-$ and that there is an impermeable perfectly reflecting boundary at $z = 0$. Now consider a new coordinate system z', which is linearly compressed above the interface and defined by

$$z' = \begin{cases} z, & 0 \le z \le z_i, \\ (z - z_i)\left(\dfrac{K_-}{K_+}\right)^{1/2} + z_i, & z \ge z_i, \end{cases}$$

and introduce a revised eddy diffusivity K' defined by

$$K' = \begin{cases} K, & 0 \le z \le z_i, \\ K\dfrac{K_-}{K_+}, & z \ge z_i. \end{cases}$$

Then K' is continuous at the interface and, away from the interface, z' evolves according to

$$dz' = \frac{\partial K'}{\partial z'}dt + \sqrt{2K'}\, d\xi. \tag{8}$$

If (8) is applied and nothing special is done at the interface (i.e., a forward step is used and the interface is ignored), then we know from the form of (8) that the

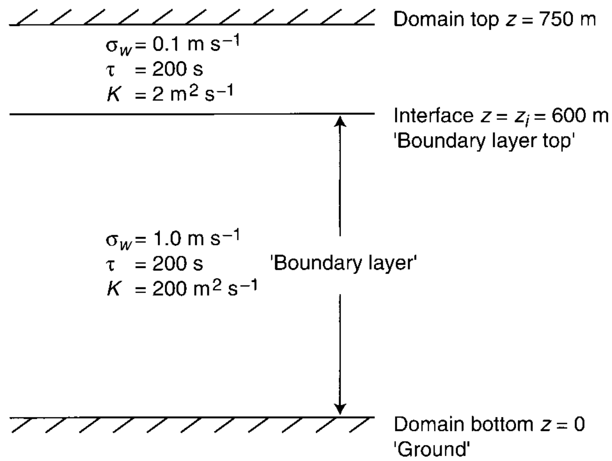

FIG. 5. Illustration of the geometry and parameter values used in the simulations to test the preservation of the well-mixed state.

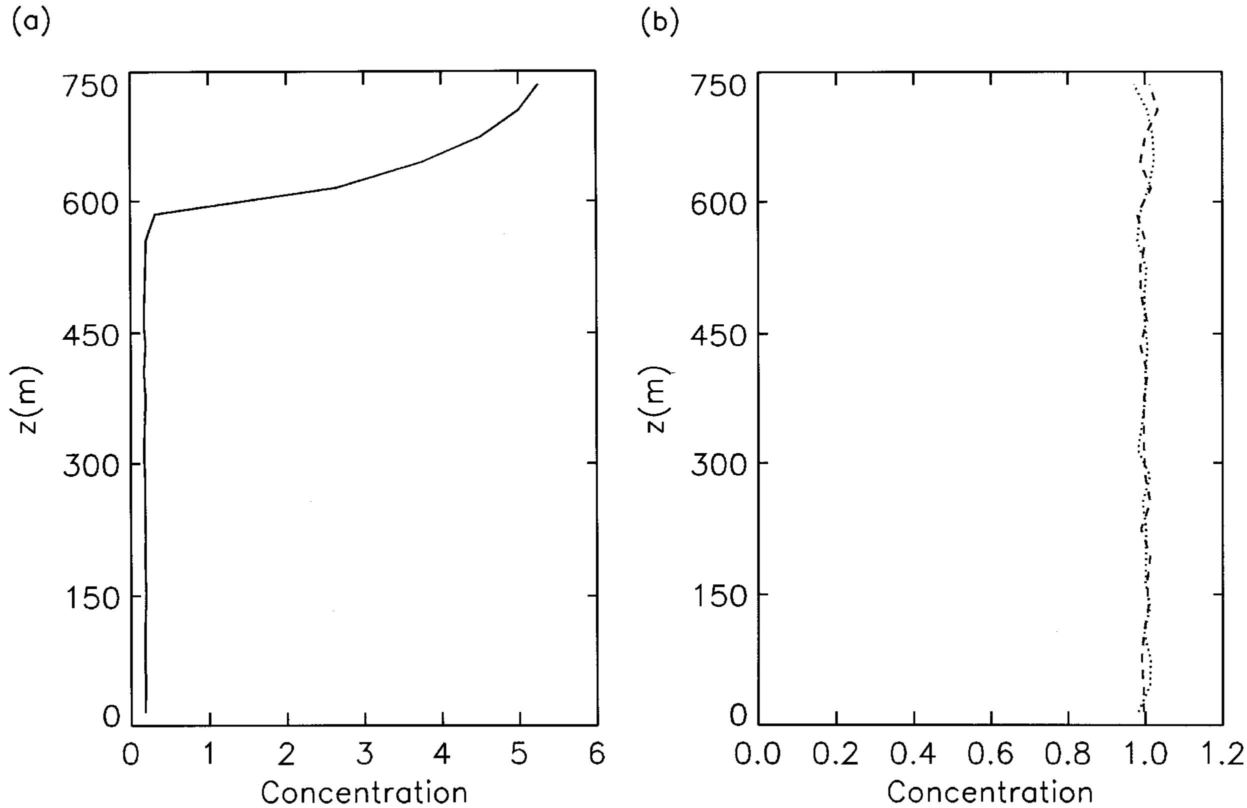

FIG. 6. Large time concentration profiles for a (z, w) model with p_a assumed Gaussian and $\Delta t = 0.02\tau$. The solid line (Fig. 6a) shows the result of not doing anything special at the boundary layer top while the dashed and dotted lines (Fig. 6b) show results from the methods described in the first and second paragraphs of section 3, respectively. Concentrations are normalized to equal unity when well mixed in the vertical.

density of particles in z' space will have a well-mixed state that is uniform. This is undesirable because then the density in z space above the interface will be $(K_-/K_+)^{1/2}$ times that below. However, it can be corrected as follows. As well as having an ensemble of particles evolving according to (8) and ignoring the interface, we introduce a second ensemble (which we call ensemble B, the original ensemble being ensemble A) for which particles are confined to the region below the interface. If m_A and m_B are the masses of particles in the two ensembles in the region below the interface when the particles are well mixed, then the concentration (mass per unit vertical length) of all particles in the well-mixed state is

$$\begin{cases} \dfrac{m_A}{z_i} + \dfrac{m_B}{z_i}, & 0 \le z \le z_i, \\ \dfrac{m_A}{z_i}\left(\dfrac{K_-}{K_+}\right)^{1/2}, & z \ge z_i. \end{cases}$$

This is uniform if $m_A/(m_A + m_B) = (K_+/K_-)^{1/2}$. However, we still have an undesirable situation with some particles trapped forever beneath $z = z_i$ while others are allowed to pass through. This can be corrected, however, by allowing particles below the interface to change at random between the two ensembles (particles above the interface are all in ensemble A). If the time step Δt is the same just above and just below the interface, this can be done most easily by deciding which ensemble a particle belongs to when it reaches the discontinuity. A particle approaching from below should be given a probability of $m_A/(m_A + m_B) = (K_+/K_-)^{1/2}$ of belonging to ensemble A. One can also view this as allowing particles below the interface to decide afresh which ensemble they belong to at the start of every time step. This procedure will not work if Δt changes discontinuously at the interface. A difference in time step across the interface means that particles just below the interface have a different probability per unit time of being able to change ensemble depending on whether or not they have just come from above the interface. Because particles from above are all from ensemble A while the other particles form a mixture, this will bias the results.

The above approach can be summarized as follows (where we now drop the restriction that $K_+ < K_-$). The time step is chosen such that it changes continuously across the interface. For a particle approaching from below, the particle is transmitted with probability $(K_+/K_-)^{1/2}$ (or unity if this is smaller) and, if it is transmitted, its ‘‘velocity’’ is multiplied by $(K_+/K_-)^{1/2}$ at the

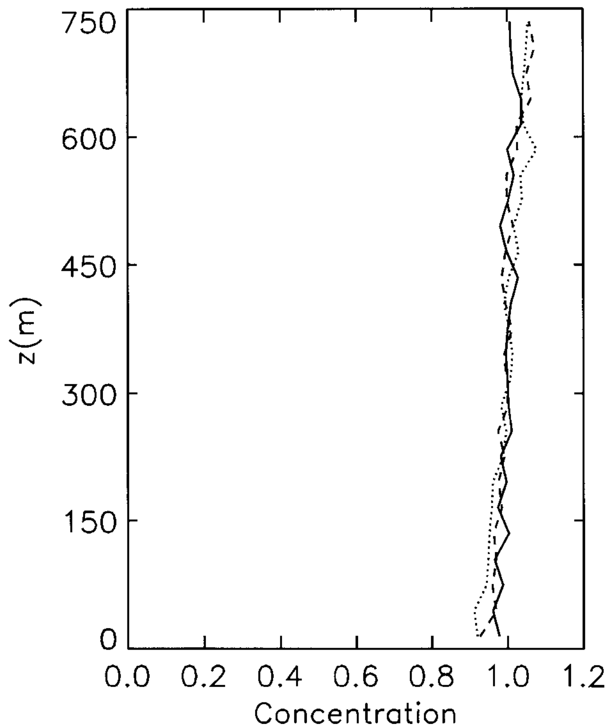

FIG. 7. Large time concentration profiles for a (z, w) model with a skewness of 0.6 within the boundary layer and Gaussian turbulence above using the method described in section 2 [Eqs. (2) to (5)]. The solid, dashed, and dotted lines show results for $\Delta t = 0.02\tau$, 0.05τ, and 0.1τ, respectively. Concentrations are normalized to equal unity when well mixed in the vertical.

moment of crossing, with the particle continuing at this new velocity until the end of the time step. If it is not transmitted, it is perfectly reflected, with the particle again continuing to move at its new velocity until the end of the time step. The treatment of particles approaching from above is similar and the particles approaching from the side with the smaller value of K are always transmitted.

The above approach can also be derived as follows. Suppose, as above, that the time step Δt is the same on both sides of the interface. Although the particle velocities depend on Δt and so are not physically meaningful, we can regard the model as giving Gaussian velocity distributions with $\sigma_w^2 = 2K/\Delta t$. [This is not immediately clear if $\partial K/\partial z$ is nonzero. However, if the time step Δt is sufficiently small so that K cannot change by a large fraction over a time step, then the mean "drift" velocity $\partial K/\partial z$ is much less than $\sigma_w = (2K/\Delta t)^{1/2}$ and so can be ignored to leading order. Note that it is not correct to allow for $\partial K/\partial z$ by giving p_a a nonzero mean since (7) is designed for situations with zero mean velocity. Although the mean velocity of particles leaving z at the start of a time step is $\partial K/\partial z$, the mean velocity of particles arriving at z at the end of the time step has the opposite sign due to the larger velocities of particles arriving from the side where K is larger. In some average sense the mean velocity for well-mixed particles is still zero.] Hence, we can apply the approaches discussed in sections 2 and 3 with

$$p_a(z, w) \propto \left[\frac{\Delta t}{2K(z)}\right]^{1/2} \exp\left[-\frac{1}{2}\frac{w^2}{2K(z)/\Delta t}\right].$$

The approach described at the end of section 3 then corresponds to that derived above.

The above could be extended relatively easily to 3D cases (and trivially to time discontinuities), but we will not consider this here.

7. Simulations

A number of simulations were conducted to demonstrate that the above approaches do indeed preserve the correct well-mixed state. These simulations were restricted to one-dimensional situations and were conducted with the geometry shown in Fig. 5. For simplicity we use the language appropriate to a boundary layer with a discontinuity at the boundary layer top, as this is likely to be the most common situation to which the ideas presented here are applied. Values of σ_w and τ (for simulations in which the particle state is characterized by z and w) and values of K (for diffusive simulations in which the particle state is characterized by z only) are also shown. Various values of the time step Δt were tried. The quantity τ is the model Lagrangian timescale, defined here so that the random term in the equation for the evolution of w has variance $2\sigma_w^2\Delta t/\tau$. At the domain boundaries perfect reflection was applied for the simulations with p_a assumed Gaussian and for the diffusive simulations, while the method of Thomson and Montgomery (1994) was used for cases where p_a was assumed skew. Within both the boundary layer and the layer above, particles were stepped forward in time by applying the model appropriate for the specified turbulence [following Thomson (1987) for the (z, w) model calculations and using (7) for the diffusive cases]. For the (z, w) model simulations, w was incremented each time step using a forward step with σ_w, etc., evaluated at the last calculated value of z. Then, except when domain boundaries or the boundary layer top were encountered, z was incremented using the just-calculated value of w. One can think of this as w and z leapfrogging each other in time, with w being incremented instantaneously at the start of the time step and then being held constant for the duration of the time step while z changes. In all cases 20 000 particles were followed, and the particles were initially distributed uniformly in space with [in the case of (z, w) models] the particle velocities distributed according to the assumed form of p_a. Concentration profiles were allowed to evolve for 1 h, and then results were obtained by time averaging the concentration profile over the following hour—more specifically by averaging together the results obtained every 6 min between 66 min and 120 min after the

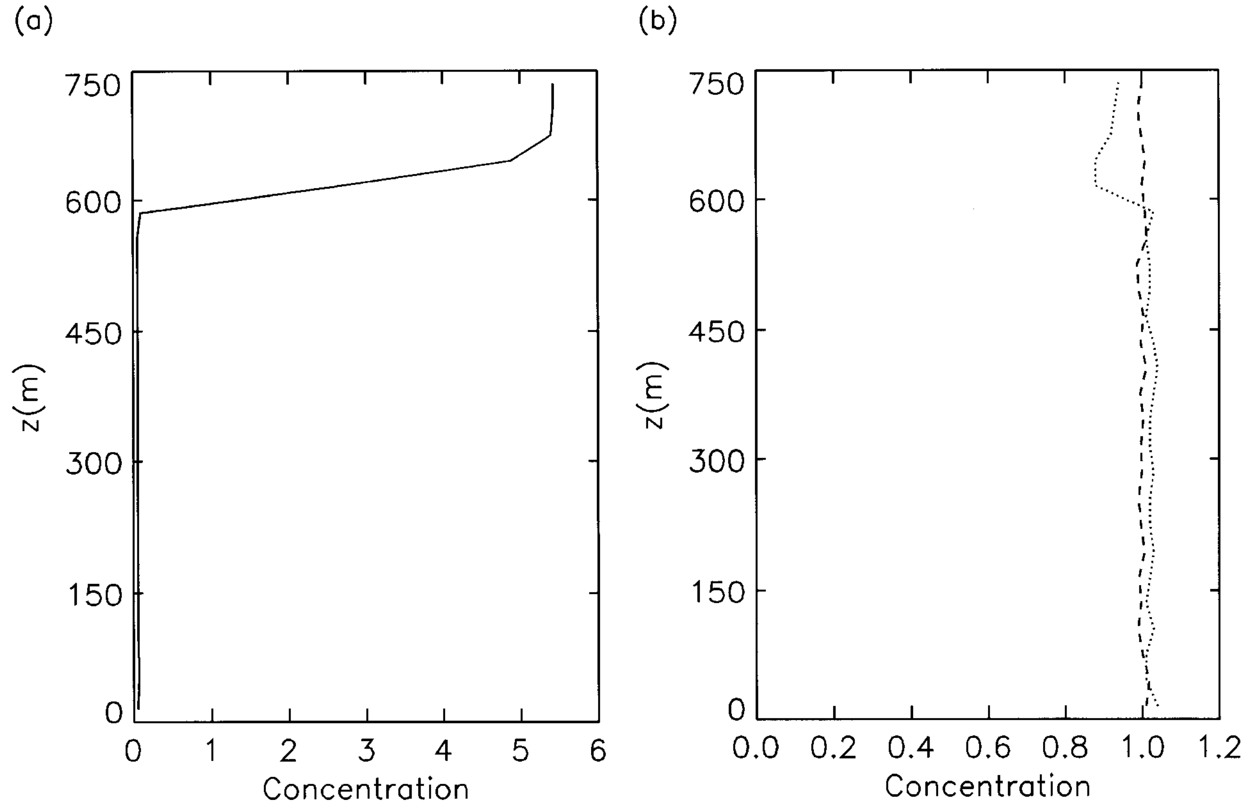

FIG. 8. Large time concentration profiles for the diffusion model (7). The solid line (a) shows the result of not doing anything special at the boundary layer top, the dashed line (b) shows the results from the method described in section 6, and the dotted line (b) shows the results obtained using the section 6 method with the modification that the time step takes a different value above and below the boundary layer top. The time step Δt was taken to be 4 s, with the exception of the simulation shown by the dotted line for which Δt was doubled (to 8 s) for particles below the boundary layer top. Concentrations are normalized to equal unity when well mixed in the vertical.

particles were released. The averaging is useful in reducing noise. An hour is comparable to the time required for a particle to diffuse across the upper layer and longer than the time required to diffuse across the lower layer. Hence, this should be long enough to uncover any problems. The concentration profiles were evaluated by counting particles in boxes that were 30 m high.

Figure 6 shows three cases using a (z, w) model with p_a assumed Gaussian and $\Delta t = 0.02\tau$ (4 s). The first curve shows the result of not doing anything special at the boundary layer top (i.e., leaving w unchanged as the particle crosses). Particles accumulate in the layer above the boundary layer top in an unacceptable way. The other two curves show the two methods described in section 3. These methods lead to acceptable results. For larger time steps (not shown), the first method described in section 3 gives a slight accumulation just above the boundary layer; the concentration is about 4% and 8% too large for time steps of 0.05τ and 0.1τ, respectively. The second method in section 3 seems more robust for larger time steps with no significant problems occurring for $\Delta t = 0.05\tau$ and 0.1τ.

Figure 7 shows results assuming a skew form for p_a in the boundary layer and a Gaussian p_a above the boundary layer and using a (z, w) model with the boundary layer top treated as in section 2 [Eqs. (2)–(5)]. Here, p_a was represented as the sum of two Gaussians (as in Baerentsen and Berkowicz 1984; Luhar and Britter 1989; Weil 1989; Hurley and Physick 1993) with the mean μ of each Gaussian related to its standard deviation σ by $|\mu| = \sigma$ and the skewness chosen to be 0.6. Results are shown for Δt equal to 0.02τ, 0.05τ, and 0.1τ. For $\Delta t = 0.02\tau$ the results again seem satisfactory, although not as good as for the Gaussian simulations. For larger Δt, the results are worse with accumulation near the top of the domain and depletion near the ground. It seems likely that this is due as much to the reflection boundary condition at the ground as to what is happening at the boundary layer top. (This is not meant to imply an error in the surface boundary condition—the boundary condition *is* consistent with the assumed velocity distribution. The problem arises because, for a finite time step, the velocity distribution produced by the model will depart from that assumed, even in the absence of boundaries.)

Finally, three diffusive simulations are presented in Fig. 8. The first shows the unacceptable particle accumulation that occurs when (7) is applied and nothing

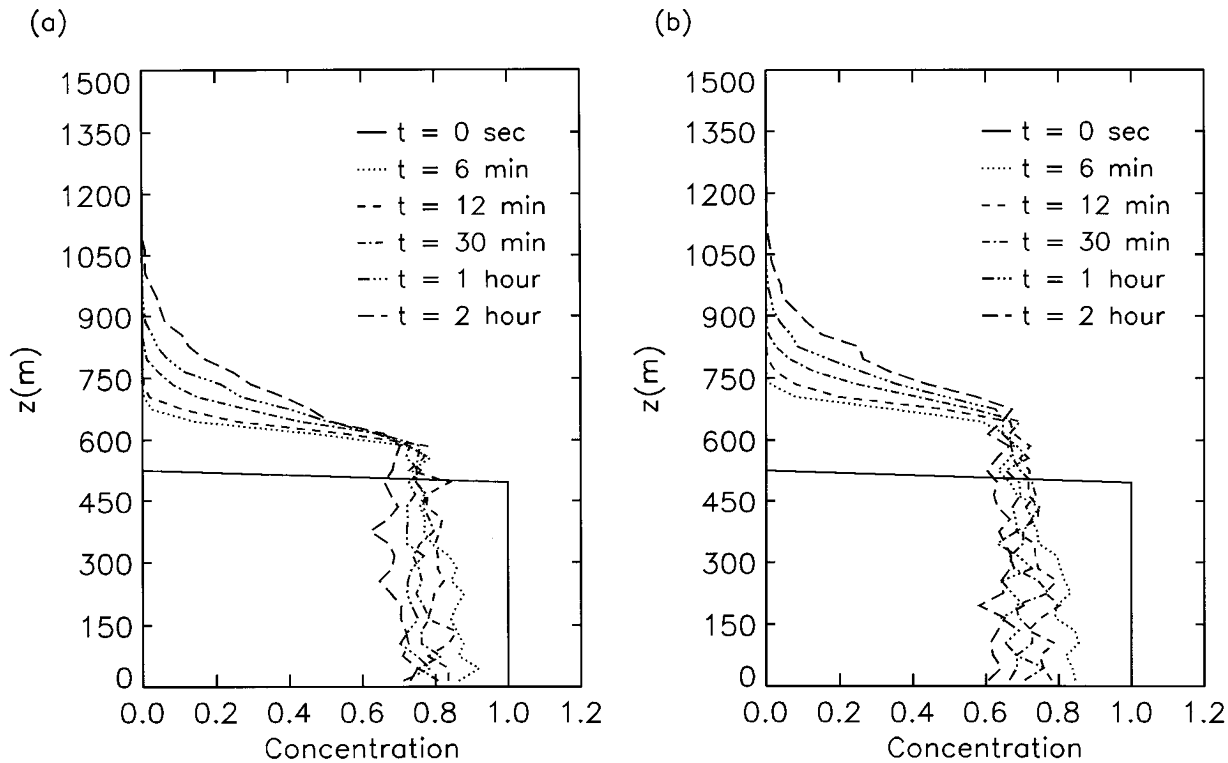

FIG. 9. Evolution of the concentration profile for the diffusive model with material initially distributed uniformly up to 510 m above the ground with zero concentration above: (a) shows results with a jump in diffusivity at the boundary layer top (600 m); (b) shows the evolution for the case of a continuous eddy-diffusivity profile that changes between the boundary layer and free-troposphere values over the height range 540 m to 660 m. Concentrations are normalized to equal unity when well mixed up to 510 m.

special is done at the boundary layer top (i.e., a forward time step is used and the boundary layer top is ignored). The second shows the satisfactory results obtained from the method described in section 6. The third simulation is identical to the second except that we have altered Δt to illustrate that the method fails if Δt varies across the boundary layer top. In the first two simulations we took Δt to be 4 s, while in the simulation with Δt varying across the boundary layer top, we took $\Delta t = 4$ s for particles starting their time step above the boundary layer top and $\Delta t = 8$ s for those below.

In addition to the above simulations designed to test the "well-mixed condition," we performed some simulations to investigate the rate at which particles escape from the boundary layer. The first simulation was, with two exceptions, identical to that using the section 6 approach with constant Δt presented above. The two exceptions are that the upper boundary was removed to allow particles to diffuse upward indefinitely and that particles were initially well mixed up to 510 m instead of within the entire domain. Figure 9a shows the evolution of the concentration profile showing the particles rapidly mixing up to the top of the boundary layer and then, more slowly, escaping from the boundary layer. To test whether the rate of escape is appropriate we repeated the simulation with the K profile replaced by a continuous profile with K changing linearly with height in a transition region between 540 m and 660 m above the ground. This necessitated the use of a smaller time step in order to prevent K changing by a large fraction in any one time step. The time step chosen is given by

$$\Delta t = \begin{cases} \max[\min(\Delta t_1, \Delta t_2), \Delta t_3], \\ \quad \text{in regions where } K \text{ is constant,} \\ \Delta t_3, \\ \quad \text{in the transition region where } K \text{ changes,} \end{cases}$$

where $\Delta t_1 = 4$ s, Δt_2 is given by $2K\,\Delta t_2 = (\text{distance to transition region}/3)^2$, and $\Delta t_3 = 0.1$ s (tests showed that, with the upper boundary restored, this choice of Δt was sufficiently small to maintain a well-mixed distribution). The results are shown in Fig. 9b. Although there are differences between Fig. 9a and 9b in the vicinity of the boundary layer top, it is clear that the rates at which particles escape are comparable, with the concentration profiles above the boundary layer differing by no more than a vertical displacement of order the thickness of the transition region. Note that the small value of Δt required for the simulation with the continuous K profile means that the simulation took about 10 times as much computer time. This illustrates an important advantage to be gained by treating such situations as discontinu-

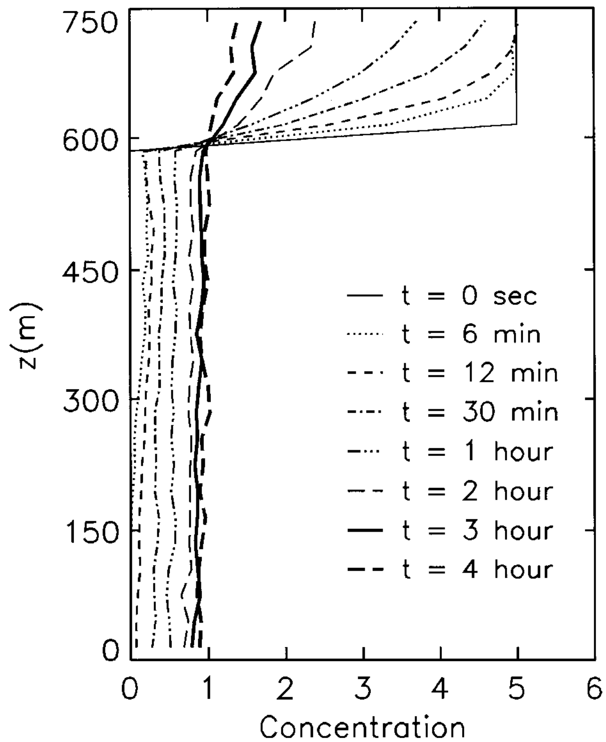

FIG. 10. Evolution of the concentration profile for a situation where material that is initially distributed uniformly above the boundary layer is entrained into the boundary layer. Concentrations are normalized to equal unity when well mixed in the vertical.

ities. The 4-s time step used away from the boundary layer top is probably unnecessarily small in both calculations. If this was increased, the fractional saving in computer time would be even greater. Two further simulations (not shown) were conducted in which the height over which K changed was reduced to 60 m and 30 m. As the boundary layer top becomes sharper, the calculations become increasingly expensive in terms of computer time because of the need to reduce the time step. The results provide convincing evidence that as the boundary layer top becomes sharper the results converge to those obtained with a discontinuity in K (Fig. 9a). We did not attempt to demonstrate any such convergence for the (z, w) models. However, if we consider the case where τ is large within the inversion (discussed in the first part of section 2), then the method of derivation (which involves detailed consideration of what happens within the interface and does not just involve the well-mixed condition) gives confidence that results should converge. In situations with small τ or where the model for treating the discontinuity involves a random component, there is less reason for confidence here. It would be of interest to conduct some simulations to test this.

As a final example, Fig. 10 illustrates how the proposed interface condition is able to simulate the entrainment of a plume from a less-turbulent layer into a more-turbulent one. Parameters are as for the simulation in Fig. 7 with $\Delta t = 0.05\tau$ (10 s). The initial concentration field is uniform in the region above the boundary layer top and zero below. The instantaneous profiles show quite rapid entrainment in the early stages followed by an approach toward a well-mixed profile.

We finish with a note of warning. In the case with the continuous K profile, Δt needs to be sufficiently small to prevent the value of K at a particle's location changing by a large fraction over a time step. In trying to make the time step as large as possible while remaining consistent with this constraint, we experimented with allowing particles just below the region over which K changes to have a large time step if they were moving away from the boundary layer top, but a small time step otherwise—that is, Δt depending on the random number to be used in the time step. In retrospect, it is easy to see that this hopelessly biases the random numbers and leads to accumulation problems.

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