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COMPARISON OF REFLECTION BOUNDARY CONDITIONS FOR LANGEVIN EQUATION MODELING OF CONVECTIVE BOUNDARY LAYER DISPERSION

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1. INTRODUCTION

Lagrangian stochastic modeling based on the Langevin equation has been shown to be useful for simulating vertical dispersion of trace material in the convective boundary layer or CBL (e.g., Luhar & Britter, 1989). This modeling approach can account for the effects of the long velocity correlation time scales (associated with large-scale turbulent structures), skewed vertical velocity distributions, and vertically inhomogeneous turbulent properties found in the CBL. It has been recognized that Langevin equation models assuming skewed but homogeneous velocity statistics can capture the important aspects of diffusion from sources in the CBL, especially elevated sources (Hurley and Physick, 1993).

We compare three reflection boundary conditions using two different Langevin-equation-based numerical models for vertical dispersion in skewed, homogeneous turbulence. One model, described by Ermak and Nasstrom (1995), is based on a Langevin equation with a skewed random force and a linear deterministic force. The second model, used by Hurley and Physick (1993), is based on a Langevin equation with a Gaussian random force and a non-linear deterministic force. The reflection boundary conditions are all based on the approach described by Thomson & Montgomery (1994).

2. REFLECTION BOUNDARY CONDITIONS

Thomson and Montgomery (1994) based their approach to particle reflection at boundaries on the concept that a well-mixed spatial and velocity distributions will be maintained if each particle that encounters, for example, the lower boundary is reflected with a velocity that is chosen so that the ensemble-average upward and downward particle flux is the same as if there were an imaginary region of fluid below the boundary. Since the net flux at the boundary must be zero, this criteria reduces to

$$-\int_{-\infty}^{0} w_i P_f(w_i) dw_i = \int_{0}^{\infty} w_r P_f(w_r) dw_r \qquad (1)$$

where $P_f(w)$ is the fluid velocity distribution at the boundary, w_i is the incident (downward) velocity and w_r is the reflected (upward) velocity (the same relationship with w_i and w_r interchanged applies at the upper boundary.) The probability distribution of reflected (positive) velocities is proportional to the flux of particles with an upward velocity w and is

$$P_+(w) = AwP_f(w), \quad w > 0,$$

where A is a positive normalization constant. The analogous distribution for incident (negative) velocities is

$$P_-(w) = -AwP_f(w), \quad w < 0.$$

The criteria given by Eq. (1) provides a relationship between the ensemble of incident velocities and the ensemble of reflected velocities, but does not provide the relationship between a specific w_i and the resultant w_r. Thus, any relationship between w_i and w_r that meets the Eq. (1) criteria will maintain the well-mixed condition. (We will then apply these relationships under well-mixed and non-well mixed conditions.)

One method (method I) of implementing Eq. (1), that results in a positive correlation between the magnitudes of w_i and w_r, is to choose w_r such that

$$\int_{0}^{w_r} P_+(w) dw = \int_{w_i}^{0} P_-(w) dw.$$

When $P_f(w)$ is Gaussian (or any other function symmetric about $w = 0$), this method reduces to the well-known reflection boundary condition $w_r = -w_i$. Another method (method II) that results in a negative correlation between the magnitude of w_i and w_r, is to chose w_r such that

$$\int_{0}^{w_r} P_+(w) dw = \int_{-\infty}^{w_i} P_-(w) dw.$$

A third method (method III) is to randomly select a reflected velocity value from the distribution P_+ at the lower boundary (P_- at the upper boundary).

We implemented these methods by constructing tables of w versus cumulative probability using 256 bins from $w = -12\sigma_w$ to $12\sigma_w$ with evenly spaced intervals of w, and linearly interpolating between values.

3. COMPARISON OF REFLECTION METHODS

We first tested each of the three reflection methods with each Langevin equation model to determine the time step required to maintain a well-mixed distribution. We performed simulations with a velocity skewness of 1, Lagrangian time scale $\tau = 0.5(h / \sigma_w)$, and an initial uniform spatial distribution of particles between boundaries at $z = 0$ and $z = h$. Departures from a uniform spatial distribution of less than approximately 5% were obtained using a time step $\Delta t = 0.05\tau$, and 1% using a time step $\Delta t = 0.01\tau$. (Position distributions were calculated using 500,000 particles and 40 bins between the top and bottom boundary, and were averaged from $t / \tau = 1$ to 4.)

We then compared the three reflection methods using simulations of dispersion from a continuous point source in the CBL. Using data from Willis and Deardorff's (1981) laboratory experiment (see Fig. 1) from a source at non-dimensional height $Z_s = 0.49$, we compared non-dimensional cross-wind-integrated concentrations, $C(X,Z)$, versus non-dimensional height, $Z = z/h$, and downwind distance, $X = xw_* / Uh$, where h is the boundary layer depth, w_* is the convective velocity scale, and U is the mean horizontal wind speed. We used average velocity statistics for the lower half of the mixed-layer determined from the vertical velocity distributions published by Deardorff and Willis (1985): variance $\sigma_w^2 = 0.35w_*^2$ and skewness $S = \overline{w^3} / \sigma_w^3 = 0.65$ (zero mean). A Lagrangian time scale of

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$\tau = 0.9(h / w_*)$, a time step of $\Delta t = 0.02\tau$, 20 vertical sampling bins, and 500,000 particles were used.

Figs. 2 and 3 compare near-ground concentration versus X for simulations using the Ermak-Nasstrom and Hurley-Physick models, respectively, and the three reflection methods. For both Langevin models, reflection method II (negatively correlated incident and reflected speeds) results in a larger peak near-ground concentrations, with the peak concentration closer to the observed peak (C=1.8). Method I (positively correlated) results in the lowest peak near-ground concentrations. Method III (uncorrelated) is intermediate between the other two. Method II also moves the downwind location of the peak near-ground concentration slightly toward the source in better agreement with the observations. Farther above the surface, the different reflection methods have less of an effect, as expected.

These initial results suggest that application of the negatively correlated incident and reflected speed boundary condition (method II) within a homogeneous Langevin equation model provides a better representation of the dispersive behavior within the CBL than either of the other two methods. We speculate that method II allows the high velocity descending particles to remain closer to the ground after reflection until slower descending particles approach the ground, resulting in a larger peak near-ground concentration.

4. ACKNOWLEDGMENTS

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5. REFERENCES

Deardorff, J.W. and G.E. Willis, 1985: Further results from a laboratory model of the convective planetary boundary layer, *Bound.-Layer Meteorol.*, **32**, 205-236.

Ermak, D.L. and J.S. Nasstrom, 1995: Numerical simulation of the Langevin equation for skewed turbulence. Preprint, *11th Symposium on Boundary Layers and Turbulence*, Charlotte, NC, 27-31 March 1995. American Meteorological Society, Boston.

Hurley and Physick, 1993: A skewed homogeneous Lagrangian particle model for convective conditions. *Atmos. Environ.*, **27A**, 619-624.

Luhar, A.K. and R.E. Britter, 1989: A random walk model for dispersion in inhomogeneous turbulence in a convective boundary layer. *Atmos. Environ.*, **23**, 1911-1924.

Thomson, D.J. and M.R. Montgomery, 1994: Reflection boundary conditions for random walk models of dispersion in non-Gaussian turbulence. *Atmos. Environ.*, **28**, 1981-1987.

Willis, G.E. and J.W. Deardorff, 1981: A laboratory study of dispersion from a source in the middle of the convective mixed layer. *Atmos. Environ.*, **15**, 109-117.

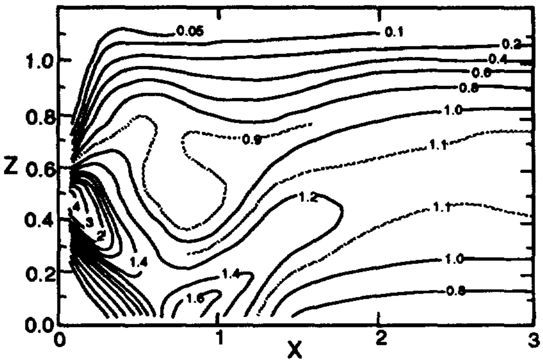

FIG. 1. Contours of non-dimensional concentration versus non-dimensional height and downwind distance from Willis & Deardorff (1981) laboratory experiment.

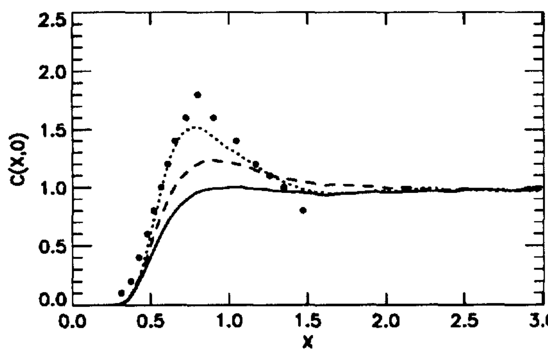

FIG. 2. Near-ground non-dimensional concentration versus non-dimensional downwind distance for simulations using the Ermak-Nasstrom model and the three reflection methods: method I (solid line), method II (dotted line), method III (dashed line). Circles are data from Willis & Deardorff (1981).

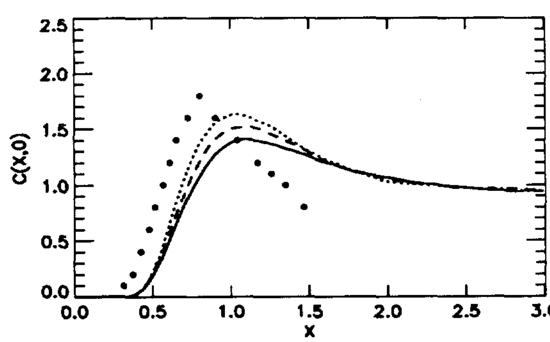

FIG. 3. Same as Fig. 2, but using the Hurley-Physick model.

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