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LANGEVIN EQUATION MODELING OF CONVECTIVE BOUNDARY LAYER
DISPERSION ASSUMING HOMOGENEOUS, SKEWED TURBULENCE

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1. INTRODUCTION
Vertical dispersion of material in the convective boundary layer, CBL, is dramatically different than in neutral or stable boundary layers, as has been shown by field (e.g., Briggs, 1993) and laboratory experiments (e.g., Willis and Deardorff, 1976, 1978, 1981). Lagrangian stochastic modeling based on the Langevin equation has been shown to be useful for simulating vertical dispersion in the CBL (e.g., Luhar & Britter, 1989; Weil, 1989). This modeling approach can account for the effects of the long Lagrangian 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 simplified Langevin equation models that assume skewed but homogeneous velocity statistics can capture the important aspects of dispersion from sources in the CBL (Hurley and Physick, 1993). The assumption of homogeneous turbulence has a significant practical advantage, specifically, longer time steps can be used in numerical simulations.

In this paper, we compare two Langevin equation models that use the homogeneous turbulence assumption. We also compare and evaluate three reflection boundary conditions, the method for determining a new velocity for a particle that encounters a boundary. Model results are evaluated using data from Willis and Deardorff's laboratory experiments for three different source heights.

2. LANGEVIN EQUATION MODELS
The two Langevin equations are of the form
\[
\frac{dw}{dt} = a(w) + A(t),
\]
where \( w \) is the velocity of a marked fluid particle, \( a(w) \) is a deterministic force, and \( A(t) \) is a rapidly fluctuating random force. The first model, used by Hurley and Physick (1993), has a non-linear deterministic force \( a(w) \) and a Gaussian random force \( A(t) \), and will be referred to as the nonlinear-Gaussian Langevin equation model. The second model, used by Ermak and Nasstrom (1995), has a linear deterministic force \( a(w) \) and a skewed random force \( A(t) \), and will be referred to as the linear-skewed Langevin equation model.

As discussed by Thomson (1984, 1987), Sawford (1986) and Sawford & Guest (1987), there is a fundamental difficulty in applying a linear-skewed Langevin equation: all the cumulants of the random term are non-zero and when higher order cumulants are important it is difficult to generate such a random variable. For inhomogeneous turbulence it appears this difficulty has not been overcome. However, for the simplified case of homogeneous skewed turbulence Ermak and Nasstrom (1995) have shown that a linear-skewed Langevin equation model can be successfully developed, and that it meets Thomson's (1987) well mixed condition.

An advantage of the linear-skewed Langevin equation model is that it can be integrated explicitly for the case of homogeneous, skewed, unbounded turbulence to yield an exact solution for the time evolution of the particle velocity. The nonlinear-Gaussian Langevin equation is usually solved using a velocity equation accurate to first order in \( \Delta t \).

3. REFLECTION BOUNDARY CONDITIONS
A homogeneous model does not resolve the variation in the statistical properties of the vertical velocity in the surface layer at the bottom of the CBL, or in the entrainment layer at the top, but, rather, treats the interaction with the lower and upper boundaries with reflection of the vertical velocity. In previous Langevin equation models of vertical dispersion in the CBL it has been assumed that the magnitude of the reflected vertical velocity is positively correlated with the magnitude of the incident velocity. In a homogeneous model, this would imply that material approaching the surface from the mixed layer with a strong downdraft velocity is given a strong updraft velocity when it encounters the surface and is quickly returned to the mixed layer. However, as discussed by Lamb (1982), material carried toward the surface in a downdraft tends to stay in the surface layer and move horizontally until it is incorporated in an updraft. Thus, there is no a priori reason to believe that positively correlated incident and reflected speeds are necessarily the best choice for a homogeneous model. We investigated three reflection boundary conditions, one each in which the incident and reflected speeds are (I) positively correlated, (II) negatively correlated and (III) uncorrelated.

Thomson and Montgomery (1994) presented a sound basis for determining reflection boundary conditions. They recognized that a well-mixed spatial and velocity distribution will be maintained if at the height of a boundary, just as at any other height \( z \), the ensemble-average flux of particles with velocity in \( (w, w + dw) \) through \( z \) is proportional to
\[
\phi(w, z) = w n_f(z) P_f(w)dw,
\]
where \( n_f(z) \) and \( P_f(w) \) are the fluid position and velocity distributions, respectively (we are assuming the velocity distribution is independent of height). The probability density function for positive velocities crossing any height \( z \) is proportional to \( A(w, z) \) and is
Similarly, the probability density function for negative velocities crossing any height is

$$P_-(w) = \frac{wP_f(w)}{\int_{-\infty}^{0} wP_f(w)dw}, \quad w < 0.$$  

At the lower boundary, $P_-(w)$ describes the distribution of the ensemble of incident velocities, $w_i$, and $P_+(w)$ describes the distribution of reflected velocities, $w_r$ (the reverse relationship holds at the upper boundary.) However, these distributions do not provide the relationship between a specific $w_i$ and the resultant $w_r$. Thus, any relationship between $w_i$ and $w_r$ that results in these distributions will maintain a well-mixed state.

One method of implementing a reflection method, that results in a positive correlation between the magnitudes of $w_i$ and $w_r$, is to choose a positive $w_r$ (at the lower boundary) such that

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

for a given $w_i < 0$. We will refer to this as reflection method I. Another method (method II) that results in a negative correlation between the magnitude of $w_i$ and $w_r$, is to choose $w_r$ such that

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

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.

In order to improve the numerical accuracy of the reflection calculation, over Thomson & Montgomery's implementation and over our previous implementation, we split the time step at the point a boundary is encountered. We (1) updated particle positions assuming the velocity varied linearly between $w(t)$ and $w(t + \Delta t)$ during $\Delta t$, (2) calculated the particle velocity and time when a boundary was encountered, (3) calculated the reflected velocity using method I, II or III, (4) used the Langevin equation and the reflected velocity to update the velocity at the end of the time step, and (5) updated the position, starting at the boundary, assuming the velocity varied linearly over the remainder of the time step. In this method, particles follow curved (quadratic) $z$ trajectories, and were re-reflected if they again encounter the surface during the remainder of the time step.

We 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 $z = h$. Departure from a uniform spatial distribution decreased with time step size. For $\Delta t = 0.05\tau$, departures from a uniform spatial distribution of less than approximately 1% were obtained using the linear-skewed Langevin equation model, and less than 2% using the nonlinear-Gaussian Langevin equation model. For larger time steps, the departure of the nonlinear-Gaussian model results grew quickly (15% for $\Delta t = 0.2\tau$), but the linear-skewed Langevin equation model performed fairly well (4% for $\Delta t = 0.2\tau$). This difference is due to the fact that the linear Gaussian model uses a first-order-$\Delta t$ velocity equation, while the linear-skewed Langevin equation model uses a more accurate velocity equation (exact for the first three moments of velocity). In these tests, position distributions were calculated using 500,000 particles and 20 bins between the top and bottom boundary, and were averaged from $t / \tau = 1$ to 4.

Fig. 1. Smoothed contours of dimensionless cross-wind-integrated concentration, $C(X,Z)$, versus dimensionless height, $Z$, and downwind distance, $X$, from Willis & Deardorff laboratory experiments for dimensionless source heights, $Z_s$, of (a) 0.067 (top), (b) 0.24 (middle), and (c) 0.49 (bottom). Arrows indicate source location.
Fig. 2. Contours of dimensionless cross-wind-integrated concentration, $C(X,Z)$, versus dimensionless height, $Z$, and downwind distance, $X$, from simulations using linear-skewed Langevin equation model and reflection method II of the Willis & Deardorff experiments for dimensionless source heights, $Z_s$, of (a) 0.067 (top), (b) 0.24 (middle), and (c) 0.49 (bottom).

4. CBL DISPERSION SIMULATIONS

We compared and evaluated the two models and the three reflection methods using simulations of Willis and Deardorff’s (1976, 1978 & 1981) laboratory experiments. Figs. 1a, b, and c show contours of cross-wind-integrated concentration, $C(X,Z)$, versus dimensionless height, $Z = z/h$, and downwind distance, $X = x W^*/U h$ (where $h$ is the boundary layer depth, $W^*$ is the convective velocity scale, and $U$ is the constant mean horizontal wind speed) from Willis & Deardorff experiments for dimensionless source heights, $Z_s$, of (a) 0.067, (b) 0.24, and (c) 0.49. The concentration is non-dimensionalized by the concentration if material were uniformly distributed in the vertical. In all simulations, we used mixed-layer-average velocity statistics determined from the vertical velocity distributions published by Deardorff and Willis (1985): variance $\sigma_v^2 = 0.31w^2$ and skewness $S = w_3 / \sigma_v = 0.78$ (zero mean). A Lagrangian time scale of $\tau = 0.8(h / w^*)$, a time step of $\Delta t = 0.05\tau$, 20 vertical sampling bins, and 100,000 particles were used. It is assumed that there are no horizontal velocity fluctuations, and there are boundaries at the surface and at the height of the capping inversion.

For the linear-skewed model and for all three source heights, method II (negatively correlated incident and reflected speeds) results shown in Fig. 2a, b & c are in better overall agreement with the experimental $C(X,Z)$ (Fig. 1a, b & c) than method I (positively correlated) results shown in Figs. 3a, b & c. In particular, note the better simulation of the lift off of the concentration centerline with downwind distance after it reaches the surface in Figs. 2a, b & c. Results with reflection method III (uncorrelated) are intermediate between the other two reflection methods. (In Figs. 2, 3 & 4, the strong concentration gradient at the boundary layer top is an artifact of the contouring algorithm which used zero values above the model domain.)

For the nonlinear-Gaussian model, method II results shown in Figs. 4a, b & c are in better agreement with measured $C(X,Z)$ patterns in the lower half of the CBL than methods I and III results (not shown) for all three source heights. However, these results show erroneously high concentrations near the top of the
boundary layer. The methods I and III results also exhibited this erroneous feature, to a smaller degree. This feature has also been present in results from inhomogeneous nonlinear-Gaussian model simulations. It has been suggested (Weil, 1989; Du et al., 1994) that it may be due to unrealistic turbulence parameterizations. The fact that this feature does not appear in the simulations with a linear-skewed model, nor in Sawford and Guest's (1987) simulations using an inhomogeneous linear-skewed Langevin model, suggests that this may also be the result of an inherent property of some nonlinear-Gaussian Langevin equation models.

Figs. 5a, b & c compare near-ground concentration versus X for simulations using the linear-skewed model and the three reflection methods to data from the Willis and Deardorff experiments. Figs. 6 a, b, and c show the same comparison using the nonlinear-Gaussian model. Figs. 5 and 6 show that, for both models, the choice of reflection method can significantly affect near-surface concentration. The combination of linear-skewed Langevin equation model and reflection method II (negatively correlated reflection; dotted line; Figs. 5a, b &c) results in the best overall agreement with these experimental data for near-surface concentration. For both Langevin models, reflection method I (positively correlated) results in the poorest agreement overall.

In summary, after comparing results of two Langevin equation models (nonlinear-Gaussian and linear-skewed) using three different reflection methods to laboratory measurements of cross-wind-integrated concentration, the better overall results are from simulations with the linear skewed Langevin equation model using negatively correlated incident and reflected speeds (method II). These results suggest that, for homogeneous Langevin models, application of the negatively correlated incident and reflected speed boundary condition (method II) provides a better representation of dispersion within the CBL. Method II may allow the high velocity descending particles to remain closer to the ground after reflection until slower descending particles approach the ground. This may simulate the observed behavior of fluid carried toward the surface in a downdraft remaining near the surface until incorporated in an updraft.

5. ACKNOWLEDGMENTS
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6. REFERENCES
Fig. 5. Dimensionless near-surface cross-wind-integrated concentration, $C(X,0)$, versus dimensionless downwind distance, $X$, from simulations of the Willis & Deardorff experiments for dimensionless source heights, $Z_0$, of (a) 0.067 (top), (b) 0.24 (middle), and (c) 0.49 (bottom) using linear-skewed Langevin equation model and three different reflection methods.


Fig. 6. The same as Fig. 5, except using nonlinear-Gaussian Langevin equation model.
