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<p>An existing Lagrangian stochastic model for dispersion in the convective boundary layer (CBL) was extended in two main ways. First, a model for the mean field dispersion in a rapidly-evolving CBL was developed and calculations of the crosswind-integrated concentration (CWIC) were carried out for a range of conditions. Second, a Lagrangian model for the CWIC and the mean and root-mean-square concentrations was developed that uses the velocity fields from large-eddy simulations as input. Calculations of the CWIC fields were made for three source heights and showed good agreement with the convection tank measurements of Willis and Deardorff (1976, 1978, 1981).</p>				
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**LAGRANGIAN STOCHASTIC MODELING OF DISPERSION IN THE
PLANETARY BOUNDARY LAYER**

FINAL REPORT

J. C. WEIL

4 APRIL 1995

U.S. ARMY RESEARCH OFFICE

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1. Introduction

Dispersion of battlefield obscurant clouds, hazardous materials, and air pollutants occurs in the planetary boundary layer (PBL). Like PBL turbulence, dispersion is a stochastic phenomena, which means that the scalar concentration should be described statistically through a probability distribution. The distribution can be described by a shape function (e.g., a gamma distribution), in which the most important variables are the ensemble-mean concentration C and the root-mean-square (rms) fluctuating concentration σ_c ; the latter characterizes the width of the distribution.

For many PBL dispersion problems, concentration fluctuations are large in that σ_c/C can be $\sim 1 - 10$ for short averaging times (seconds to tens of minutes) and short downwind distances (≤ 5 km). Recent field measurements have demonstrated large σ_c values from near surface releases (Mylne and Mason, 1991; Yee et al., 1993). Laboratory experiments have shown that σ_c/C due to elevated sources can be as large as 6 near the surface for simulated averaging times of a few minutes (Deardorff and Willis, 1988). Large fluctuations in aerosol concentrations also have been found in obscurant clouds (Hanna, 1984). Thus, the C field alone is insufficient to determine the probability of seeing through a smoke screen, i.e., C must be supplemented by predictions of σ_c .

The stochastic nature of dispersion and the complications of PBL turbulence require a suitable modeling approach. Under previous support from the Army Research Office (ARO), we developed a Lagrangian stochastic model in which one follows passive particles or particle pairs through a turbulent flow given the Eulerian velocity statistics. The mean concentration was found from the probability density function (p.d.f.) of particle position, which was evaluated numerically from the particle trajectories. The model was applied successfully to dispersion of point and area source emissions in the convective boundary layer (CBL) (Weil, 1989, 1990a, 1990b). For σ_c , we constructed a numerical code based on Thomson's (1990) two-particle model for homogeneous turbulence.

Under the ARO program just completed, this modeling has been extended in two ways. First, we developed a model for mean-field dispersion in a rapidly-evolving CBL and carried out calculations of C for a range of conditions (Weil, 1992). Second, we constructed a new Lagrangian model for the C and σ_c fields in the PBL using the velocity fields from large-eddy simulations (LES) as input; calculations have been made for point sources in the CBL. A third goal was exploratory calculations of the C field for sources in the stable boundary layer, but this was postponed due to the extensive efforts required for the second project task.

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In the following, we briefly summarize results for the rapidly-evolving CBL (Section 2) and the Lagrangian dispersion model using LES fields (Section 3). We also discuss additional investigations related to the research including: 1) the vertical flux distribution or “footprint” from a surface scalar source, and 2) the relative dispersion of ice crystals in cumulus clouds (Section 4).

2. Dispersion in a Rapidly-Evolving CBL

The focus of this problem was on dispersion in the early morning where the CBL depth h and surface heat flux $\overline{w\theta_o}$ increased rapidly with time t . The effect of the unsteady turbulence field on the crosswind-integrated concentration- (CWIC, C^y) field was considered in two parts: 1) changes in the turbulence with transport time, and 2) changes in the CBL conditions at the release time over about a 1-h period. Dispersion was modeled for nonstationary inhomogeneous turbulence with the rms vertical velocity σ_w parameterized by $\sigma_w = w_*(t)f(z/h(t))$, where w_* is the convective velocity scale and f is a similarity function. A parabolic profile for f^2 was used along with a constant Lagrangian time scale, $\tau = 0.7h/w_*$. Calculations of the CWIC were made for a sinusoidal variation of $\overline{w\theta_o}(t)$ with $h(t)$ determined from Carson’s (1973) model; an initial h (i.e., h_o) of about 300 m was assumed with a tripling of h in an hour.

Calculations of the hourly-averaged CWIC were made for both steady and unsteady conditions and for source heights (z_s) at $z_s/h_o = 0, 0.25, 0.75$, and 1. In both conditions, the region of high CWIC ($C^y U h_o / Q \geq 1$) was limited typically to dimensionless distances $X = w_* x / U h_o < 1.5$, where x is the downwind distance and U is the mean wind speed. In the steady case, the $C^y U h_o / Q$ approached 1 throughout the CBL for $X \geq 3$, whereas in the unsteady case, the C^y field continued to decrease for $X \geq 1.5$ due to the increase in h . As might be expected, the reduction in the near field CWIC ($X < 1.5$) increased as z_s did, indicating that the higher release heights “felt” the moving upper boundary sooner than did the lower releases.

Relative to unsteady Gaussian turbulence, the results for unsteady skewed turbulence exhibited enhanced dispersion for $z_s/h_o = 0, 0.25$ and somewhat reduced dispersion for $z_s/h_o = 0.75, 1$. This was consistent with the C^y fields for skewed and nonskewed turbulence in steady conditions and was attributed to the bias in the p.d.f. of vertical velocity caused by skewness (Weil, 1990a). In the unsteady case, the most noticeable effect of the skewness occurred for $z_s = 0$ where there was a significant “lift off”—an elevated maximum in C^y —and a local relative maximum in the mean plume height ($\langle Z \rangle$) with X . This differed from the unsteady Gaussian case where a local $\langle Z \rangle$ maximum did not occur presumably because h increased sufficiently rapidly to obscure the phenomena.

For steady conditions, the vertical profiles of C^y for the different source heights collapsed to the same profile, $C^y \simeq Q/Uh$, for $X > 3$. However, for the unsteady CBL, the collapse to a single (nonuniform) distribution of C^y for the various source heights did not occur until $X \simeq 5$. The above results were summarized in Weil (1992).

3. Lagrangian Dispersion Modeling Using LES Velocity Fields

The Lagrangian one- and two-particle models were generalized to permit particle tracking and predictions of the concentration field using time-dependent velocity fields from LES. The LES input included: 1) the resolved velocity fields to describe the particle motion due to the large-scale eddies, and 2) the subgrid-scale turbulent kinetic energy (TKE). The inhomogeneity and skewness of CBL turbulence exist mostly on the large scales, whereas the subgrid-scale eddies are closer to being homogeneous and isotropic. The subgrid eddies are treated by our stochastic particle models.

The LES data are from the Moeng and Sullivan (1994) simulations over a $5 \text{ km} \times 5 \text{ km} \times 2 \text{ km}$ domain with 96^3 grid cells. The data were generated for three CBLs representing a wide range of instability as characterized by $h/|L|$, where L is the Monin-Obukhov length and measures the depth over which surface friction effects are important. The results were obtained for highly-, moderately-, and weakly-convective CBLs corresponding to $h/|L| = 110, 14$ and 1.5 , respectively. For the two most unstable cases, $w_* \simeq 2 \text{ m/s}$, $h \simeq 1000 \text{ m}$, and $\overline{w\theta_0} = 0.24 \text{ }^\circ\text{Km/s}$. The LES fields were stored at 10 s intervals, which is about 0.02 times the eddy-turnover time h/w_* . The LES results were generated by P.P. Sullivan and C.-H. Moeng at NCAR.

The highly convective case ($h/|L| = 110$) was obtained to minimize the influence of surface friction so that our dispersion modeling could be done in a CBL that approximated the conditions in the convection tank experiments of Willis and Deardorff (1976, 1978, 1981). In the tank experiments, there was no surface shear.

In the Lagrangian model, the total velocity vector \mathbf{u} of a particle is decomposed as

$$\mathbf{u}(\mathbf{x}_p(t), t) = \mathbf{u}_r(\mathbf{x}_p(t), t) + \mathbf{u}_s(\mathbf{x}_p(t), t) \quad (1)$$

with

$$d\mathbf{x}_p = \mathbf{u}dt, \quad (2)$$

where \mathbf{u}_r is the resolved velocity at the particle position $\mathbf{x}_p(t)$ and \mathbf{u}_s is a random subgrid-scale velocity. The \mathbf{u}_s is found from the subgrid TKE e_s using Thomson's (1987) approach. The dissipation rate ϵ is required and is parameterized as $\epsilon \propto e_s^{3/2}/\ell$, where ℓ is a length scale dependent on the grid size and stratification (Moeng, 1984). Two formulations for \mathbf{u}_s have been used: one based on the local e_s and ignoring its gradients,

and a second using the horizontally-averaged e_s (\bar{e}_s) and including its vertical gradient. The best results were obtained for the first method and only those are discussed here. A third formulation has been devised and is discussed below.

The statistical approach requires that one track a large number of "independent" particles, which means that the initial velocity fields should be independent. To achieve this, particles were released from 16 sources in a horizontal plane with a source separation of $\sim 1.1h$; in addition, the initial subgrid-scale velocities were independent randomly-selected variables. Due to the wide variability in the instantaneous velocity fields, the particle displacement statistics and concentration fields were averaged over 20 release times t_s in the interval $0 \leq t_s \leq 3.8h/w_*$. The C fields discussed below are based on approximately 10^4 particle trajectories.

Results for the C field from the single-particle model with $h/|L| = 110$ have been obtained and show fair-to-good agreement with the Willis and Deardorff (1976, 1978, 1981) laboratory data. Figure 1 shows contours of C^yUh/Q as a function of z/h and X for three release heights approximating those used in the experiments. The general contour behavior is similar to that found in the experiments especially the downward tilting of the contours from the elevated sources in Figs. 1b,c. The contours from the near-surface source (Fig. 1a), while exhibiting a qualitatively similar pattern to the laboratory data, do not show a clear lift-off of the maximum CWIC from the surface as found in the experiments. However, the vertical profiles of C^yUh/Q in Fig. 2a (see $X = 2$) do show the lift-off phenomena.

Figure 2 shows vertical profiles of C^yUh/Q for two release heights and three downwind distances. The profiles illustrate two key points: 1) the tendency for an elevated maximum CWIC to occur near $X = 2$ for both releases as found in the laboratory experiments, and 2) an approximate vertically well-mixed plume with $C^yUh/Q \simeq 1$ at $X = 3$. The well-mixed distribution for a vertically-inhomogeneous turbulence field, which exists in the CBL, is expected for a properly formulated Lagrangian model (Thomson, 1987). The results for $X = 3$ show that a well-mixed distribution is achieved over the bulk of the CBL, but there is a departure from this behavior for $z/h \lesssim 0.2$.

The suspected cause for the high CWIC values in the lowest 20% of the CBL is the form of the stochastic subgrid model. The model used here ignores the instantaneous three-dimensional inhomogeneity in the e_s field. The e_s and its gradients are largest near the surface and thus should make their most significant contribution to the velocity field there. An inhomogeneous three-dimensional subgrid model based on Thomson's (1987) approach has been coded and currently is being debugged.

Figure 3 compares predictions of the dimensionless mean plume height $\langle Z \rangle/h$ and

surface $C^y U h / Q$ values with the Willis and Deardorff laboratory data for three source heights. Overall, the predicted trends with z_s/h and X agree well with the data. The modeled surface CWIC values (Fig. 3b) tend to overestimate the observations for $X > 1$, which may be due to the subgrid model formulation. The behavior is consistent with the high surface-layer CWIC values found in Fig. 2 ($X = 3$) and will be re-examined using the new subgrid model.

Results for the CWIC field also have been generated for the moderately-convective case, $h/|L| \simeq 14$. The results were expected to depart only slightly from those in Figs. 1 - 3, but the departures were more significant. This could be attributed to the subgrid model since e_s and its gradients are larger for $h/|L| \simeq 14$ (than for 110) due to the greater contribution of surface shear. The C field results are being summarized in a paper being prepared for publication (Weil et al., 1995).

The two-particle model for the relative dispersion σ_r and the rms concentration σ_c has been coded and run for a test case to ensure that σ_r satisfies the appropriate limits: $\sigma_r \propto t^{3/2}$ for $t \ll h/w_*$ and $\sigma_r \sim \text{constant}$ for $t > h/w_*$. The test case uses a single LES input file corresponding to an instantaneous velocity field. For test purposes, the model was run under the assumption of a frozen velocity field, and the results showed that σ_r did satisfy the above limits. Further calculations with the model were postponed pending completion of the current single-particle and C field computations; the two-particle work will be resumed upon completion of these computations.

4. Additional Investigations

In research related to the mean concentration field in the PBL, the Lagrangian single-particle model was used to predict the vertical flux distribution or "footprint" downwind of a surface scalar source. Model results for the atmospheric surface layer were in good agreement with those of a simpler model which was field tested; the results covered conditions ranging from unstable to stable and were summarized in Horst and Weil (1992). In addition, vertical flux distributions were generated for the entire CBL where the simpler model is inapplicable. Results showed that the horizontal profile of the flux at different heights collapsed to a nearly universal curve in the lower half of the CBL. This has important implications for modeling and measurement of the flux distribution. Ultimately, the results will be used to determine the surface flux distribution of trace species from aircraft measurements of fluxes. This work was summarized in Weil and Horst (1992).

We also investigated the relative dispersion of ice crystals in cumulus clouds. Although this is a non-boundary layer problem, a unique opportunity existed to test the stochastic two-particle model with a large number of dispersion measurements obtained

under similar conditions. In the experiments, a vertical area source of ice crystals was created in a cloud by releasing dry ice pellets from an airplane along a horizontal line. The dispersion normal to the source was measured as a function of time. A comparison of the average observed relative dispersion with the model showed good agreement. The observations implied a rather large initial dispersion which suggested that $\sigma_r \propto t$ for short times ($t < \tau$, where τ is the Lagrangian time scale) rather than $\sigma_r \propto t^{3/2}$ as given by Batchelor's (1950) theory. At long times ($t > \tau$), the model and observations both showed that $\sigma_r \propto t^{1/2}$. In addition, the p.d.f.s of the individual dispersion realizations showed an evolution from a broad positively skewed distribution at early times to a narrower and more symmetrical one at late times. This research was summarized in Weil et al. (1993).

5. Publications Under this Program

Journal Articles and Published Proceedings

Horst, T.W., and J.C. Weil, 1992: Footprint estimation for scalar flux measurements in the atmospheric surface layer. *Bound.-Layer Meteor.*, **59**, 279–296.

Weil, J.C., and T.W. Horst, 1992: Footprint estimates for atmospheric flux measurements in the convective boundary layer. *Precipitation Scavenging and Atmosphere-Surface Exchange*, Vol. 2, S.E. Schwartz and W.G.N. Slinn, Coords., Hemisphere Publishing, 717–728.

Weil, J.C., R.I. Sykes, and A. Venkatram, 1992: Evaluating air quality models: review and outlook. *J. Appl. Meteor.*, **31**, 1121–1145.

Weil, J.C., R.P. Lawson, and A.R. Rodi, 1993: Relative dispersion of ice crystals in seeded cumuli. *J. Appl. Meteor.*, **32**, 1055–1073.

Weil, J.C.: Concentration fluctuations in plumes: observations and models. In: *Wind Climate in Cities*, J.E. Cermak, A.G. Davenport, E.J. Plate, and D.X. Viegas, Eds., Kluwer Academic Publishers, 457–484.

Weil, J.C., C.-H. Moeng, and P.P. Sullivan, 1995: Lagrangian modeling of dispersion in the convective boundary layer using LES velocity fields. *J. Atmos. Sci.*, in preparation.

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Horst, T.W., J.C. Weil, and M.Y. Leclerc, 1991: Footprint estimation for atmospheric flux measurements. *Preprints 7th Symposium on Meteorological Observations and Instrumentation*, Amer. Meteor. Soc., Boston.

Horst, T.W., and J.C. Weil, 1992: Application of the flux footprint to scalar flux measurements within the atmospheric surface layer. *Preprints 10th Symposium on Turbulence and Diffusion*, Amer. Meteor. Soc., Boston, 305–308.

Weil, J.C., L.A. Corio, and R.P. Brower, 1991: Dispersion modeling of highly buoyant plumes in the convective boundary layer. *Preprints 7th Joint Conference on Applications of Air Pollution Meteorology*, Amer. Meteor. Soc., Boston, 105–108.

Weil, J.C., 1992: Dispersion in a rapidly evolving convective boundary layer. *Preprints 10th Symposium on Turbulence and Diffusion*, Amer. Meteor. Soc., Boston, 204–207.

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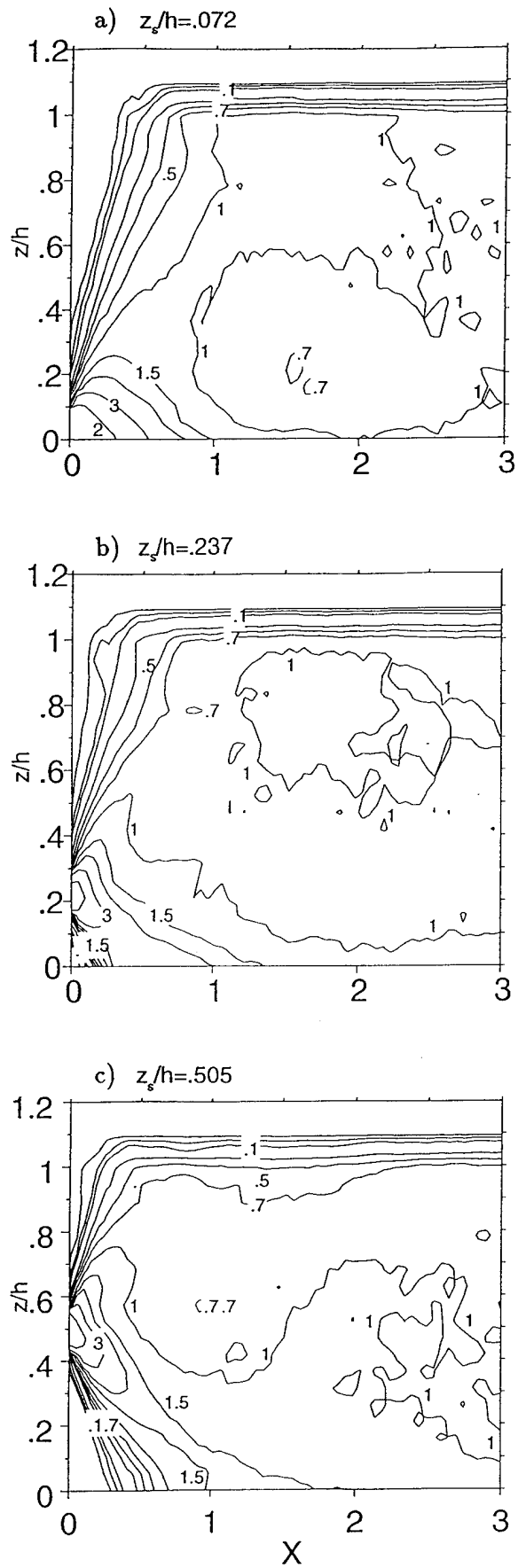
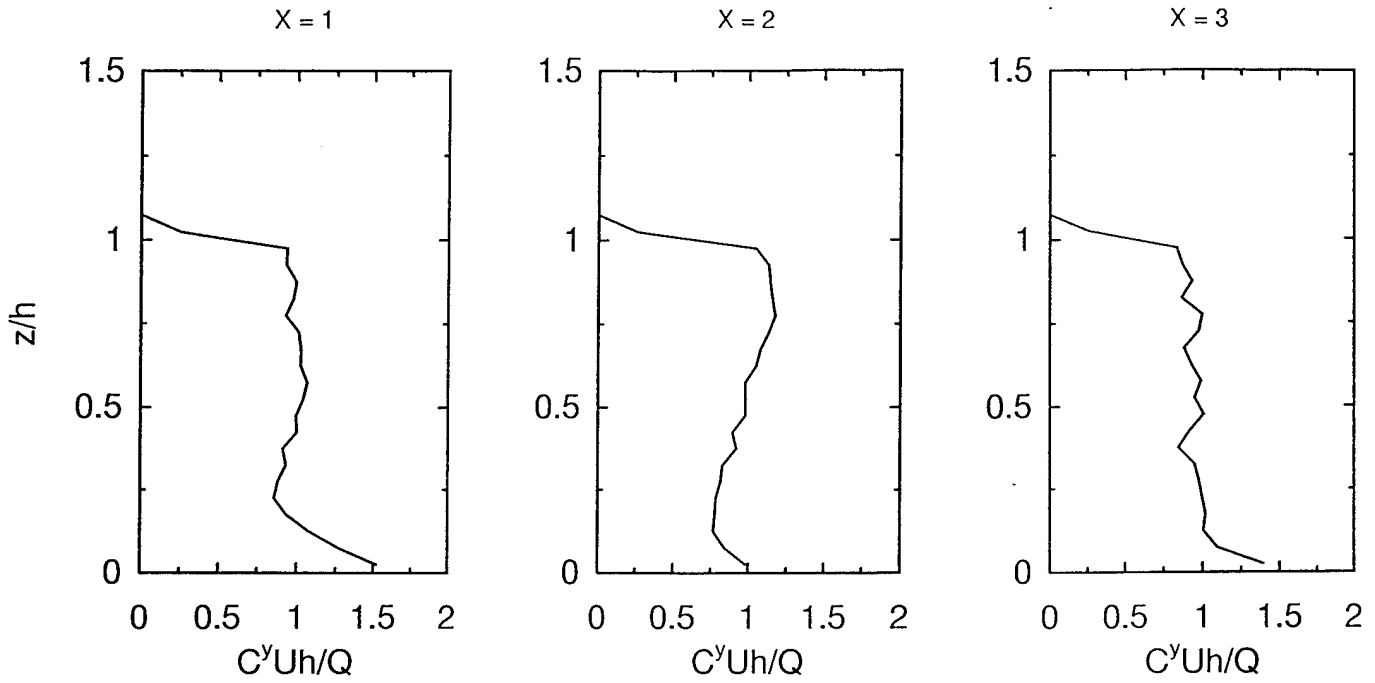


Figure 1. Predicted contours of the dimensionless crosswind-integrated concentration $C^y U h / Q$ as a function of the dimensionless height and dimensionless distance X .

a) $z_g/h=0.072$



b) $z_g/h=0.237$

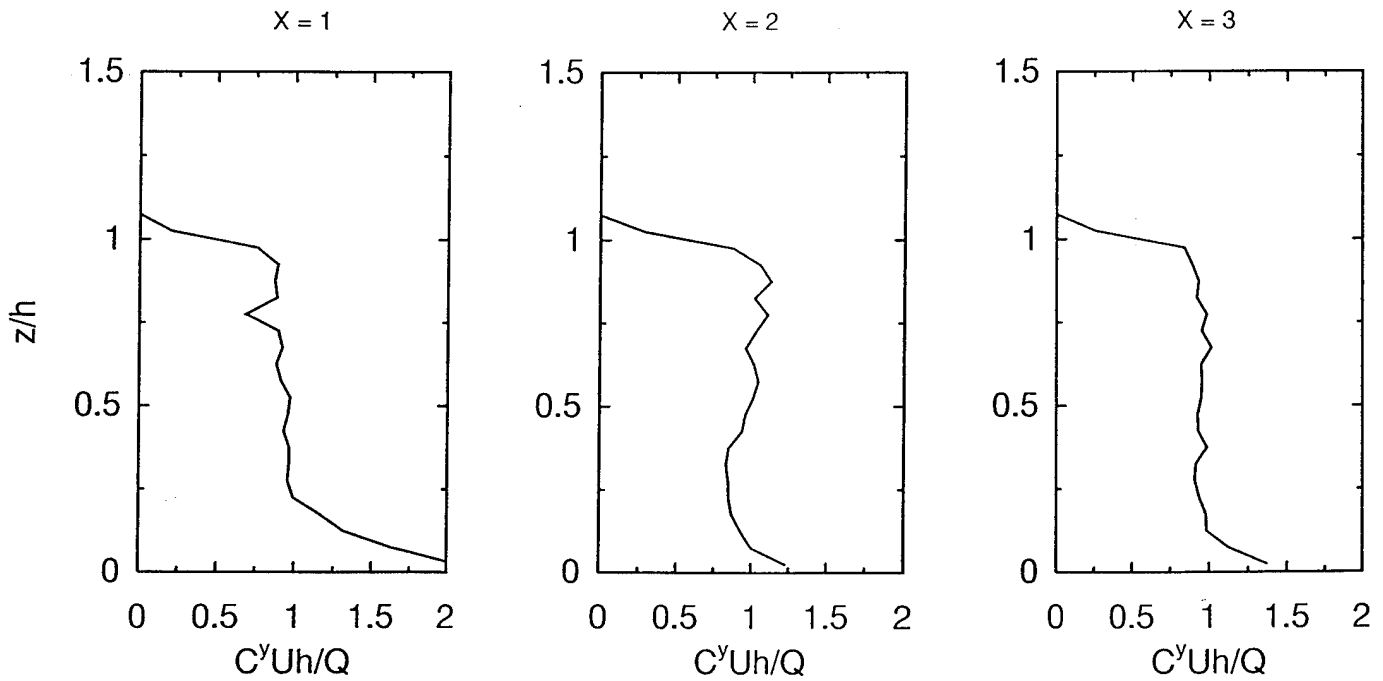


Figure 2. Predicted vertical profiles of the dimensionless crosswind-integrated concentration for three dimensionless distances.

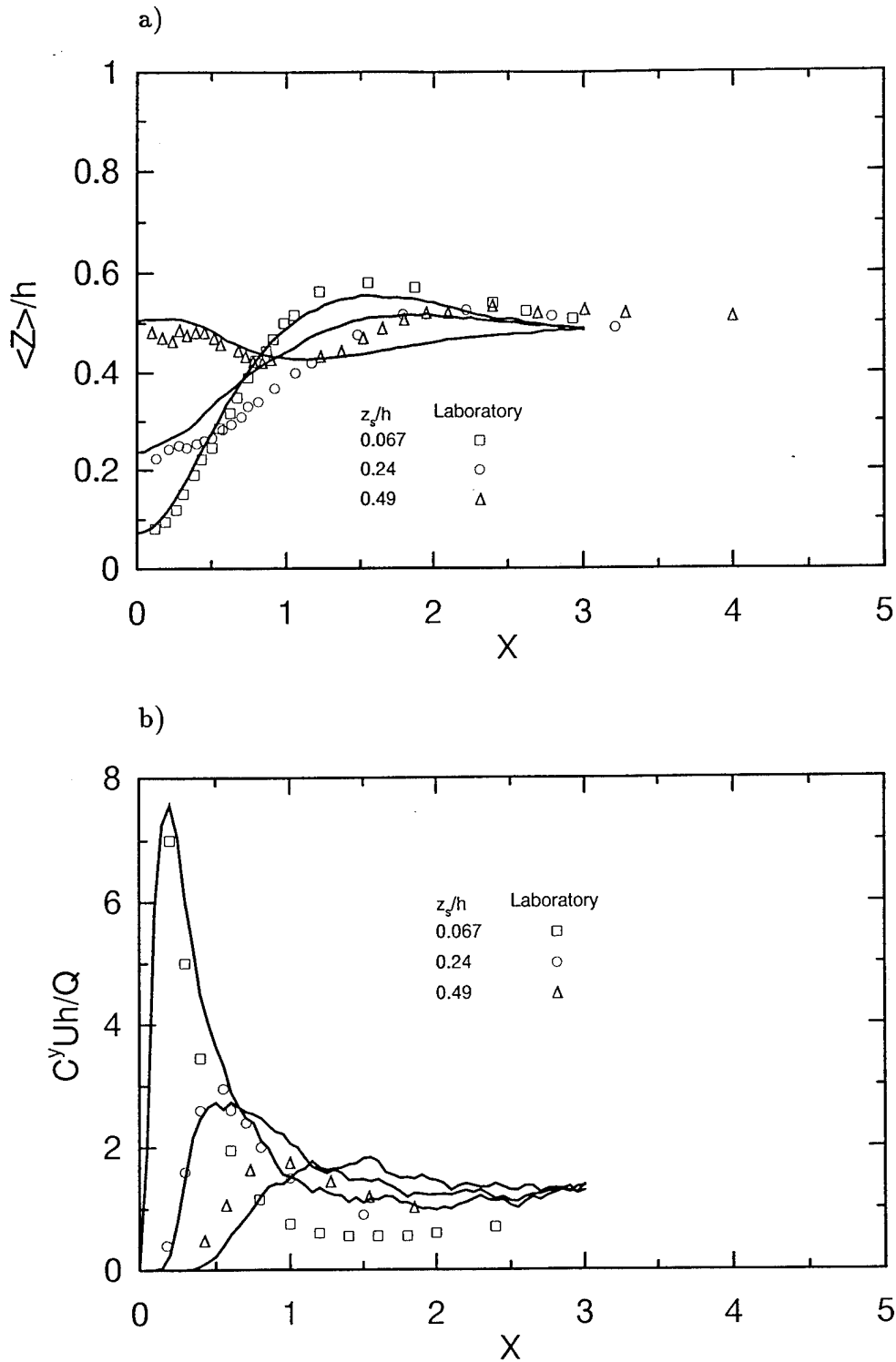


Figure 3. Comparison between model predictions (lines) and laboratory measurements of a) dimensionless mean plume height and b) dimensionless crosswind-integrated concentration at the surface as a function of the dimensionless distance for three source heights. Laboratory data are from Willis and Deardorff (1976, 1978, 1981).