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6. AUTHOR(S)
Jeffrey C. Weil

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Cooperative Institute for Research in Environmental Sciences, University of Colorado

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13. ABSTRACT (Maximum 200 words)
The research objective was to improve our understanding of dispersion in the planetary boundary layer, with focus on the convective boundary layer (CBL), using Lagrangian "particle" models coupled with large-eddy simulation (LES) fields. A one-particle model for the mean concentration field was enhanced by a theoretically-improved treatment of the LES subgrid-scale (SGS) velocities. The new model agreed with laboratory and field data and surface layer similarity theory. Investigations of stability effects on CBL dispersion showed that the dispersion rate decreased with a decreasing stability index $-z_i/L$, which was attributed to the greater wind shear and the smaller turbulence scales in the surface layer. Using our two-particle model, we investigated relative dispersion in the CBL and found that it behaved in a quasi-homogeneous manner for all source heights except those near the surface; the latter was due to the vertical inhomogeneity in the dissipation rate. A study of concentration fluctuations revealed the large (factor of $\sim$ 10) variability caused by velocity field fluctuations; the predicted concentration variability matched the trends in field observations from CBL sources.

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1. Introduction

Dispersion in the planetary boundary layer (PBL) is important for a number of problems including air quality, hazardous chemical releases, and battlefield obscurant clouds. Knowledge of the mean concentration (C) field and dispersion is insufficient to address the above problems because of the large variability in the concentration. The mean field must be supplemented by predictions or measurements of the fluctuating field, e.g., the root-mean-square (rms) concentration σ_c. For short averaging times and downwind distances (≤ 5 km), σ_c/C can range from 1 to 10 (Lewellen and Sykes, 1986; Mylne and Mason, 1991).

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 Lagrangian dispersion models for following fluid "particles" or particle pairs in a turbulent flow. Two general approaches were developed. In the first, the Lagrangian velocities for particle tracking were obtained from a purely stochastic model, which required the Eulerian velocity statistics as input. The model was applied successfully to determine the mean concentration fields from point and area sources in the convective boundary layer (CBL) (Weil, 1989, 1990). In addition, a code was developed for the relative dispersion and σ_c in homogeneous turbulence based on Thomson's (1990) two-particle model.

The second approach was a more general Lagrangian model in which the velocities for particle tracking were obtained from the time-dependent velocity fields from a large-eddy simulation (LES). An initial version of this model, produced under an earlier grant (Weil, 1995), was developed for a CBL with strong convection and produced mean concentration fields that were qualitatively similar to the Willis and Deardorff (1976, 1978) convection tank data. However, deviation of the vertical concentration profile from a vertically well-mixed state at large distances suggested that an improved treatment of the LES subgrid-scale (SGS) velocities was necessary (Weil, 1995).

Under the ARO program just completed, the Lagrangian models based on LES fields were further developed, improved, and tested. First, for the mean concentration field, we developed an improved Lagrangian stochastic model (LSM) for treating the SGS velocities and investigated the dispersion characteristics over a range of stability in the CBL. Second, we extended our two-particle model for relative dispersion to include the time-dependent LES fields and studied relative dispersion over a range of source heights. Third, we investigated the variability in concentration from a point source by computing the concentration fields from a number of spatially-separated sources in the CBL. We discuss the results of these studies below and additional related work.

2. Modeling of the Mean Concentration Field

In Lagrangian models, one tracks single particles to obtain the mean concentration field. For the mean field, there have been two major activities: 1) development of a theoretically improved and better performing LSM for the SGS velocities, and 2) determining the variation of dispersion properties with stability for CBL sources.

2.1. Improved Lagrangian Stochastic Model for SGS Velocities

The use of LES velocity fields in Lagrangian dispersion modeling was pioneered by Lamb (1978) and adopted more recently by Weil et al. (1997, 2000, 2001). The velocity following a particle is decomposed as

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

where $\mathbf{u}_r$ is the LES resolved velocity at the particle position $\mathbf{x}_p(t)$ at time t, and $\mathbf{u}_s$ is a random SGS velocity; the bold-faced symbol denotes a vector.

The approach in our earlier (Weil et al., 2000, 2001) and current (Weil et al., 2003a) models is to adapt Thomson's (1987) LSM to include LES fields. The analysis removes the resolved velocity from the LSM treatment since it is already included in Eq. (1). The primary difference between the new and old models is the form of the random forcing term, $(C_0\epsilon)^{1/2}d\xi$, where ϵ is the turbulence dissipation rate, $d\xi$ is a Gaussian random process, and C_0 is the Lagrangian structure function constant ($\simeq$ 2 to 6). In the old model, we used the total dissipation rate (ϵ), which is parameterized by the LES. However, since the stochastic model only treats the SGS velocity, it was argued that the full ϵ overestimates the random forcing. This would be "double-counting" especially in regions where the SGS turbulent kinetic energy (TKE) is an appreciable fraction of the total TKE, i.e., near the ground.

In the old and new models, the total Lagrangian velocity u_L following a particle is the sum of the u_r and a random SGS velocity u_s. The criterion guiding the new model is that the Lagrangian autocorrelation function for the summed velocity $u_r + u_s$ should be the same as that for u_L; i.e., the velocity should decorrelate in the same manner whether it is decomposed into u_r and u_s or not. The net result is that the decorrelation time scale for the SGS velocity is T_L, the Lagrangian time scale for the total velocity u_L. The resulting dissipation rate ϵ_s used in the SGS treatment is $\epsilon_s = \epsilon\overline{\sigma_s^2}/(\overline{\sigma_s^2} + \overline{\sigma_{ra}^2})$, where $\overline{\sigma_s^2}$ and $\overline{\sigma_{ra}^2}$ are the horizontally-averaged values of the SGS variance and the average resolved velocity variance. Thus, only a fraction of the total dissipation rate is used in the SGS random forcing.

A paper summarizing the formulation and results will be submitted shortly to the *Journal of the Atmospheric Sciences* (Weil et al., 2003a). The new model is an improvement over our earlier model primarily for surface and near-surface releases, and it also is in much better agreement with observations than a Lagrangian model that neglects the SGS velocities; the latter approach was adopted by Gopalakrishnan and Avissar (2000). The models were compared with convection tank data, field data, and surface layer similarity (SLS) theory (van Ulden, 1978), which applies to a surface source. The analysis focused on the vertical and downwind variation of the crosswind-integrated concentration (CWIC) or C^y. The dimensionless CWIC, C^yUz_i/Q, was examined as a function of the dimensionless distance $X = w_*x/(Uz_i)$, where U is the mean wind speed in the CBL, z_i is the CBL depth, w_* is the convective velocity scale, x is the downwind distance, and Q is the source strength.

Figure 1 shows predictions of the dimensionless surface CWIC for a surface release and compares them with SLS theory and data from the Willis and Deardorff (1976) tank experiment. For a commonly-accepted $C_0 = 3$, the new model (Fig. 1b) agrees better with

SLS theory and measurements than the old model (Fig. 1c) and much better than the model with a zero SGS velocity (Fig. 1a). We also found that the new model is not strongly sensitive to C_0 for C_0 values ranging from 1 to 6 (Fig. 2), where the accepted range is $2 \leq C_0 \leq 6$ (Du et al., 1995; Sawford, 1991; Thomson, 1987; Wilson and Sawford, 1996). In contrast, the old model exhibited best agreement for $C_0 = 1$ and progressively poorer agreement with SLS theory and data as C_0 increased from 1 to 6. The new model also gave good predictions of the evolution of the CWIC vertical profile with downstream distance (Fig. 3).

2.2. Variation of Dispersion Properties with Stability

An investigation was conducted of the stability effects on dispersion, which has been a long-standing problem in atmospheric diffusion. The "stability index" characterizing the importance of convective and shear-generated turbulence is $-z_i/L$ as first suggested by Deardorff (1972), where L is the Monin-Obukhov (M-O) length. The LES fields were obtained using the Moeng and Sullivan (1994) model for the two most unstable CBLs and a modified form of that model (Sullivan et al., 1994) for weak convection; the last case was added during this ARO program. The LES fields were generated by P.P. Sullivan and C.-H. Moeng at NCAR. The cases of strong, moderate, and weak convection correspond to $-z_i/L = 106$, 16, and 5.5, respectively. The LESs were made using a 5 km $\times$ 5 km $\times$ 2 km domain with 96^3 grid points.

Dispersion calculations for elevated sources were made with source heights (z_s) matching those in the Willis and Deardorff (1976, 1978, 1981) experiments: $z_s/z_i = 0.07$, 0.24, and 0.5. The results for strong convection ($-z_i/L = 106$) agreed well with experimental data on the CWIC contours, the mean plume height ($\overline{z}_p$), and the surface CWIC versus downstream distance. Figure 1b shows the agreement for the surface CWIC for $z_s/z_i = 0.07$. As the stability index decreased, the dispersion rate decreased as found from more compact CWIC contours and a decreased rate of rise of $\overline{z}_p$ with distance. The slower dispersion rate was due to the greater wind shear and the larger TKE dissipation rate (ϵ), which led to smaller turbulence time and length scales in the surface layer ($z/z_i \leq 0.1$). The results for the old SGS model are summarized in Weil et al. (2000); results for the new model (Section 2.1) are quite similar (Weil et al., 2003b).

For a surface source, the variation of $\overline{z}_p/z_i$ with X showed that all curves collapsed to essentially the same one for $X < 0.1$ but exhibited a natural ordering by stability ($-z_i/L$) for larger X; i.e., the $\overline{z}_p$ for strong convection was largest followed by that for moderate and weak convection. The dependence of the surface C^y on X and stability was generally consistent with the $\overline{z}_p/z_i$ variation. Figure 4 presents the mean dimensionless CWIC at the surface (solid line) as a function of X for strong convection. It shows that the model: 1) is in close agreement with SLS theory, 2) follows the average trend of the field data (Prairie Grass, CONDORS) rather well, and 3) asymptotes to the CWIC for a vertically well-mixed plume far downstream ($X = 4$). The observations correspond to $-z_i/L \geq 40$ and 100 for Prairie Grass (Nieuwstadt, 1980) and CONDORS (Briggs, 1993), respectively, and the concentration averaging time was 10 min (Prairie Grass) or 30 min (CONDORS) (see Weil et al., 2001, 2003b).

For an elevated source in the surface layer, the CWIC distribution with X was expected to have the same shape for a given stability, but the maximum CWIC (C^y_{max}) and the distance (X_{max}) to the maximum should vary with the source height. Thus, for a fixed z_i/L, a self-similar distribution of C^y/C^y_{max} versus X/X_{max} was expected. Figure 5 confirms this for the three $-z_i/L$ cases. A comparison of the modeled surface CWIC with field data downwind of a 115-m source showed good agreement between the two (Fig. 6); most of the data corresponded to $5 \leq -z_i/L \leq 14$ (Weil et al., 2003b).

Additional support for the stability dependence of the turbulence and dispersion properties was given by two analyses. First, the correlation length scale (Λ_z) for vertical velocity fluctuations in the surface layer showed that the Λ_z for moderate and weak convection was $\sim 25\%$ to 40% smaller than that for strong convection. Second, results from an analytical trajectory model (Durbin, 1983) exhibited a systematic reduction in the $\overline{z}_p/z_i$ versus X with decreasing $-z_i/L$; this was primarily due to the corresponding reduction in T_L at the source height (see Weil et al., 2001).

3. Relative Dispersion and Concentration Variance

The two-particle model previously developed for relative dispersion and σ_c^2 in the CBL (Weil, 1995) was applicable only to frozen-field turbulence, i.e., for a single LES time step or file. During the past ARO program, the model was further developed to include the time-dependent LES fields, and an investigation was conducted of the source height dependence of the three components of the relative dispersion—σ_{rx}, σ_{ry}, σ_{rz}.

For short times ($t \ll z_i/w_*$), all three components exhibited a nearly $t^{3/2}$ dependence consistent with Batchelor's (1950) theory for homogeneous turbulence. At large times ($t > z_i/w_*$), the dispersion approached a $t^{1/2}$ dependence for the horizontal components (σ_{rx}, σ_{ry}) and a constant for the vertical component. The latter was due to particle trapping by the elevated inversion and the vertical homogenization of the concentration within the CBL. For strong convection and release heights $z_s \geq 0.07 z_i$, the relative dispersion followed a similarity form for $t \leq z_i/w_*$ by scaling the results using the CBL variables (w_*, z_i) and a normalized dissipation rate at the source height. The applicability of Batchelor's (1950) theory and the similarity form for these release heights is due to the strong vertical mixing in the CBL. For lower releases ($z_s < 0.07 z_i$), the relative dispersion followed a different form due to the vertical inhomogeneity in the dissipation rate within the surface layer. The results for moderate convection ($-z_i/L = 16$) were similar to those for strong convection except that the effects of turbulence inhomogeneity extended to greater heights. This work as well as a similar analysis for the single-particle or absolute dispersion was presented at an American Meteorological Society Symposium (Weil et al., 1999).

Further work on the two-particle model to obtain the ensemble-mean variance σ_c^2 was postponed due to development of an alternative approach for determining the concentration variability as discussed below.

4. Concentration Variability

The variability in the time-averaged concentration field was studied for CBL sources having the same emission time (28 min) as for the ensemble-mean calculations (Section

2.2). A realization of the average concentration field was generated by tracking particles from a single source in fine time resolution; particles were released every 20 s. The total number of particles emitted for a single source was about the same as for the ensemble-mean calculations so that the concentration accuracy was similar in the two cases. Thirty (30) independent realizations were obtained. The individual sources used in the calculations were separated by z_i in the y direction and by Uz_i/w_* in the x direction, where the x separation corresponds to a travel time of z_i/w_*. The calculations were performed for the most unstable CBL ($-z_i/L = 106$) and three source heights: $z_s/z_i = 0.0005$, 0.07 and 0.32 (Weil et al., 2003c).

For a surface source ($z_s/z_i = 0.0005$), the modeled mean CWIC at the surface was presented and discussed earlier (Fig. 4). Figure 7 shows the individual concentration realizations (points) along with SLS theory and the computed mean concentration. The difference or scatter in the realizations is due to differences in the resolved velocity fields for the individual sources. The CWIC scatter is smallest close to the source due to the small resolved velocities near the surface, and the spread increases systematically for $0.1 \leq X \leq 1$ as the resolved velocities increase due to an increase in particle height above the surface. The points below the predicted mean correspond to strong and persistent updrafts, whereas those above the mean correspond to particles emitted initially into downdrafts or weak updrafts.

Figure 8 is a superposition of Figs. 4 and 7 and shows that the computed CWIC variability captures most of the scatter in the field data for $X > 0.2$. This is very encouraging and shows that the variability in the resolved velocity field is the principal cause of the observed CWIC variability. The computed variability does not capture all of the observed scatter probably because the LES run is for one case ($U = 3$ m/s, $z_i = 1000$ m, $w_* = 2$ ms^{-1}, etc.), whereas the field data comprise a variety of conditions. For the CONDORS data, the range of conditions was: $1.6 \leq U \leq 3.2$ m/s, $870 \leq z_i \leq 1600$ m, and $0.84 \leq U/w_* \leq 1.6$. In addition to differences in conditions, there is uncertainty (or experimental error) in the observed U, z_i, heat flux, and other variables that would contribute to the observed scatter. Also, 30 realizations may be insufficient to capture all of the variance. Nevertheless, we believe that the calculations are an encouraging step, and the computed variance captures most of the observed scatter.

For an elevated source in the surface layer ($z_s/z_i = 0.07$), the modeled mean surface CWIC near the source ($X \leq X_{max}$) is substantially reduced relative to that for a surface release (Fig. 9) as would be expected. However, beyond X_{max} ($\simeq 0.1$ to 0.2), the mean CWICs for the two source heights are essentially the same and agree with data from the Willis and Deardorff (1976) experiment. For $X > 0.2$, the concentration variability for the elevated source (Fig. 10) is similar to that for the surface release, but it is substantially greater than that from the surface release for shorter distances. The latter should be expected since the particles from an elevated source are initially driven by nonzero resolved velocities, which vary widely. This contrasts with the essentially zero initial resolved velocities for a surface release.

Figure 11 shows the modeled mean and individual realizations of C^y and observations from the CONDORS experiment for a more elevated source, $z_s/z_i = 0.32$. As expected, the mean C^y_{max} and X_{max} are smaller and larger, respectively, than for those at the lower source height ($z_s/z_i = 0.07$); the mean CWIC for a surface release and $z_s/z_i = 0.07$ are shown for reference. In addition, there is more variability in the C^y for $X < 1$ by comparison to Fig. 10. This is probably caused by the larger values and greater range of the resolved velocities, especially the vertical component, at this higher release height. The modeled CWIC variability (Fig. 11) is as large or greater than that found in the CONDORS data; differences in the scatter could be due to the use of 30 realizations in the modeling versus only five 30-min periods in the observations. Nevertheless, we believe that the overall results are encouraging and useful. There are many statistics from the CWIC field as well as the plume (y and z) displacements that can be gleaned from these calculations.

The large scatter in Fig. 11 helps to explain the low correlation found between modeled and observed surface concentrations from tall stack releases in the CBL (e.g., Weil et al., 1992). The modeled values are estimates of the ensemble-mean concentration whereas the observations are individual realizations from field experiments.

5. Other Activities Under ARO Program

In collaboration with scientists from NCAR, the Johns Hopkins University, and the Pennsylvania State University, J. Weil participated in the Horizontal Array Turbulence Study (HATS) near Kettleman City, CA (September, 2000). The objective was to obtain subfilter-scale (SFS) fluxes and variances of turbulence quantities that are modeled in LES; the data were obtained from an array of sonic anemometers at two heights in the surface layer. It was found that the SFS motions were sensitive to the relative values of the spectral peak wavelength Λ_w of the vertical velocity and the filter cutoff scale Δ_f. In particular, the results showed that over a wide range of Δ_f and Λ_w, the SFS quantities collapsed to nearly universal curves when plotted as a function of Λ_w/Δ_f (Sullivan et al., 2003). The results have important implications and serve as useful benchmarks for future SFS or SGS models.

The HATS results also have bearing on the short-range ($X \leq 0.2$) behavior of the Lagrangian model in Fig. 4. Relative to SLS theory, the model underestimation of C^y is believed due to the assumed isotropic stress tensor in the stochastic SGS model, which is important for near-field dispersion. The HATS results showed that the SGS variances are anisotropic and match measurements from the neutral surface layer: $\sigma_u^2/\sigma_{is}^2 \simeq 1.5$, $\sigma_v^2/\sigma_{is}^2 \simeq 1$, and $\sigma_w^2/\sigma_{is}^2 \simeq 0.5$, where σ_{is}^2 is the isotropic velocity variance. A halving of the SGS vertical velocity variance in the model would increase the near-source CWIC by about 40%, thus providing a better match to SLS theory at short range.

J. Weil also participated in the 1997 Lövanger International Workshop on Turbulence and Diffusion in the Stable Boundary Layer (SBL), which was sponsored in part by ARO. A contribution on dispersion in the SBL was made to the workshop summary (Weil, 1999, in Nappo and Johannson, 1999).

J. Weil also has been advising two researchers on the use of the Lagrangian dispersion model driven by LES fields: 1) Si-Wan Kim, a postdoctoral researcher at NCAR, who is investigating fumigation into the CBL from stabilized plumes aloft, and 2) Marta Antonelli, a doctoral candidate at the University of Genoa and an NCAR visitor, who is studying dispersion in the CBL during highly convective conditions

($-z_i/L = 106,\ 250,\ 350$) with weak winds: $\sigma_u/U = 0.26,\ 0.50,\ 0.70$.

6. Publications Under this Program

Journal Articles and Published Proceedings

Sullivan, P.P, T.W. Horst, D.H. Lenschow, C.-H. Moeng, & J.C. Weil, 2003: Structure of subfilter-scale fluxes in the atmospheric surface layer with application to large-eddy simulation modeling. *J. Fluid Mech.*, **482**, 101-139.

Weil, J.C., 1999: Vertical dispersion in the stable PBL. In: Nappo, C.J., and P.-E. Johansson, 1999: Summary of the Lövanger international workshop on turbulence and diffusion in the stable boundary layer. *Bound.-Layer Meteor.*, **90**, 345–374.

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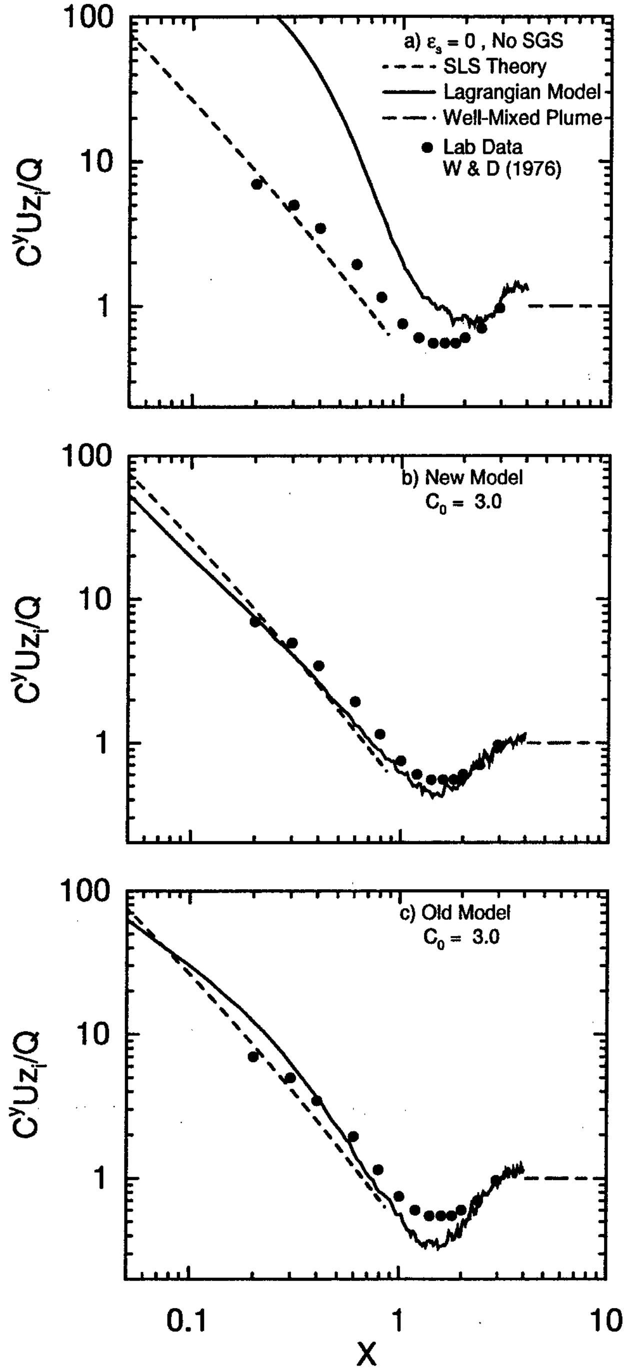

Figure 1: Dimensionless CWIC at the surface versus dimensionless downwind distance for a surface source and three SGS modeling approaches: a) no SGS velocity, b) new model with $\epsilon_s = \epsilon\overline{\sigma_s^2}/(\overline{\sigma_s^2} + \overline{\sigma_{ra}^2})$, and c) old model with $\epsilon_s = \epsilon$; $-z_i/L = 106$.

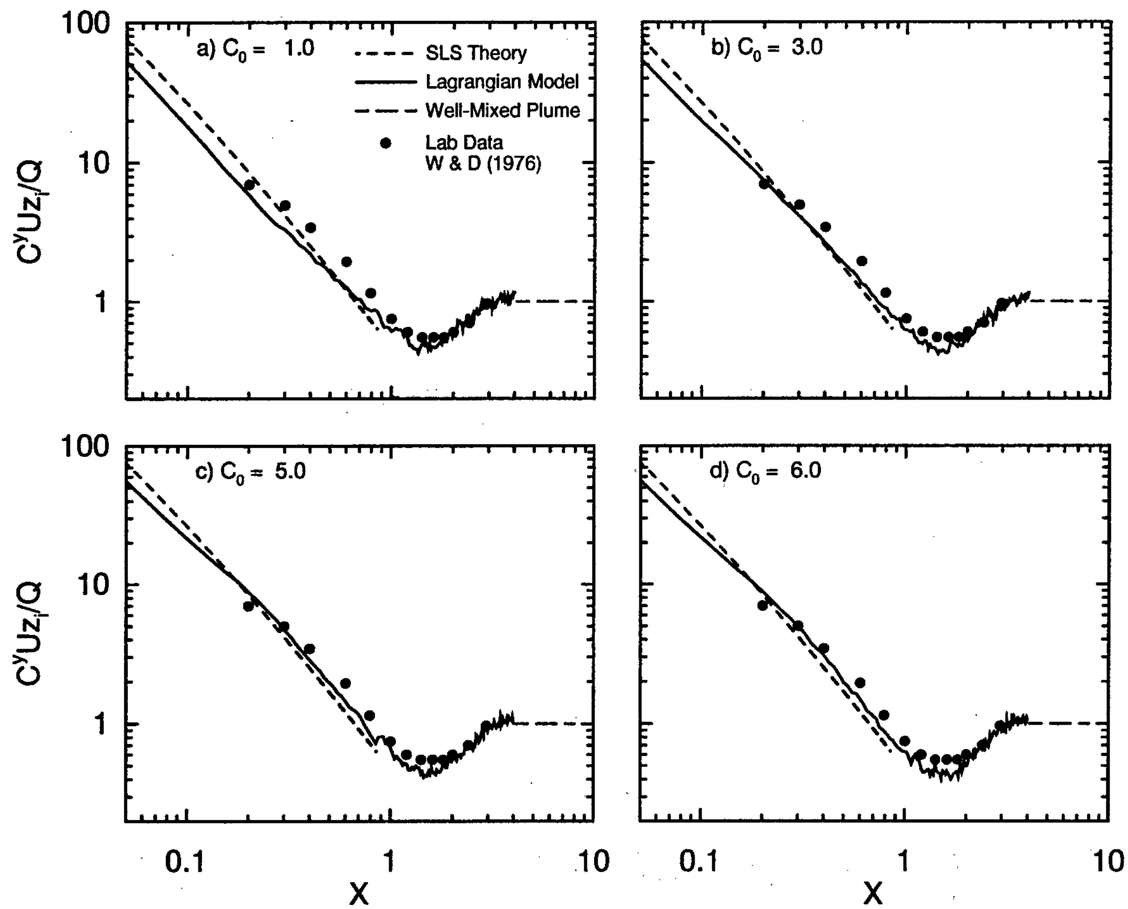

Figure 2: Dimensionless CWIC at the surface versus dimensionless downwind distance for a surface source and the new model; C_0 is the parameter in a) to d) and $-z_i/L = 106$.

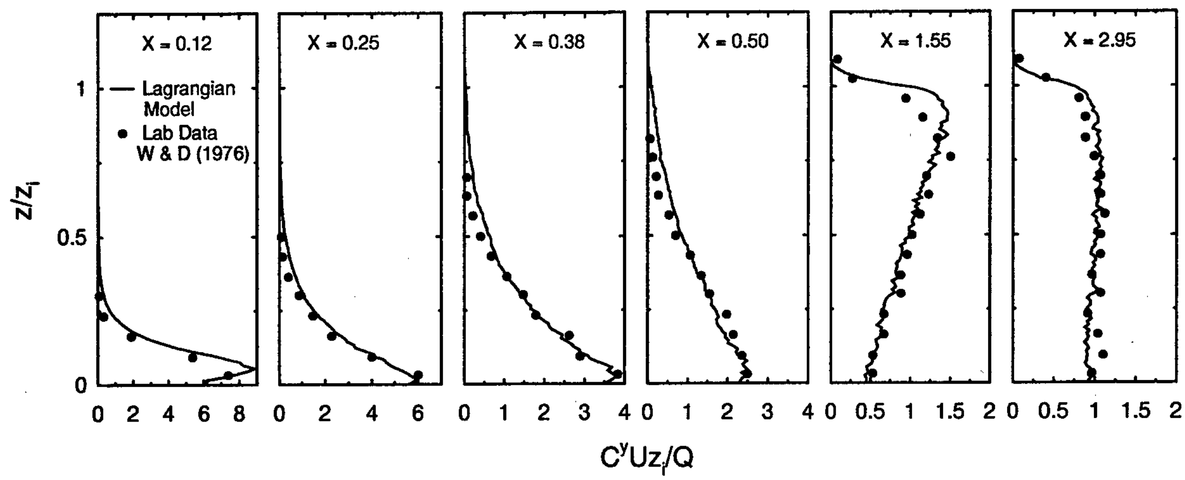

Figure 3: Evolution of vertical profiles of the dimensionless CWIC for an elevated source in the surface layer, $z_s/z_i = 0.07$, and $-z_i/L = 106$.

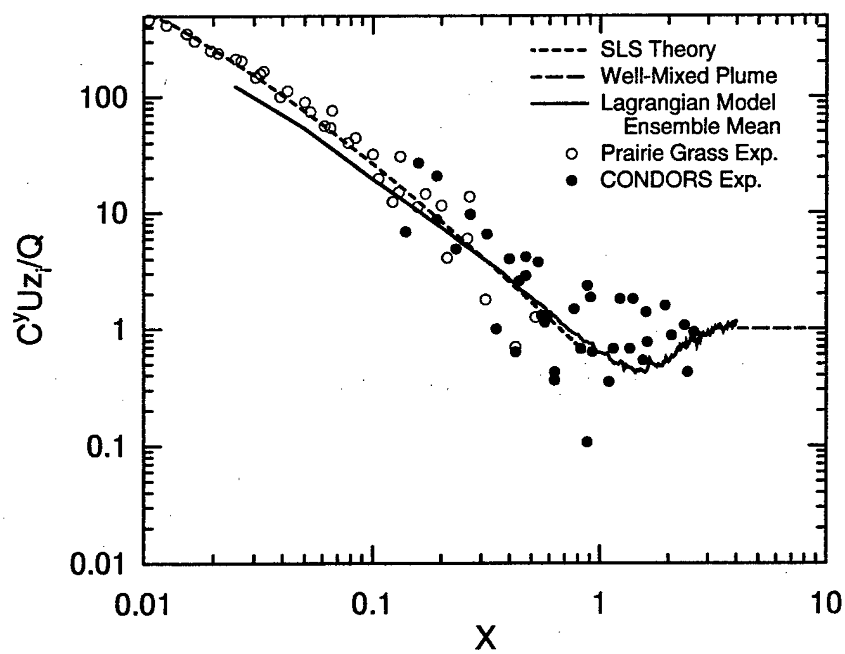

Figure 4: Dimensionless CWIC at the surface versus dimensionless downwind distance for a surface source in the CBL; mean modeled CWIC compared with SLS theory and field data. Prairie Grass data from Nieuwstadt (1980) and CONDORS data from Eberhard et al. (1988) and Briggs (1993).

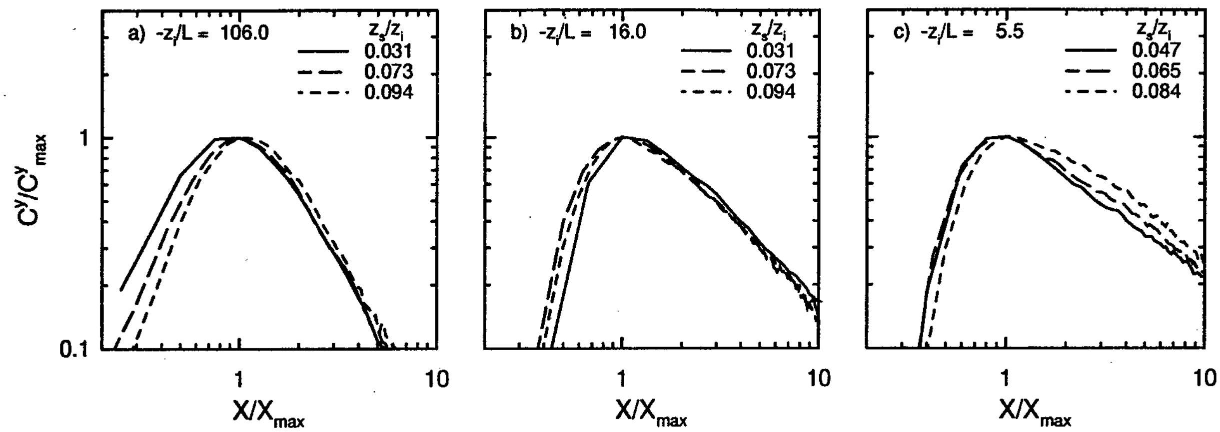

Figure 5: Surface CWIC scaled by its maximum value as a function of dimensionless distance (X) scaled by the distance to the maximum for three source heights in the surface layer and three CBL cases.

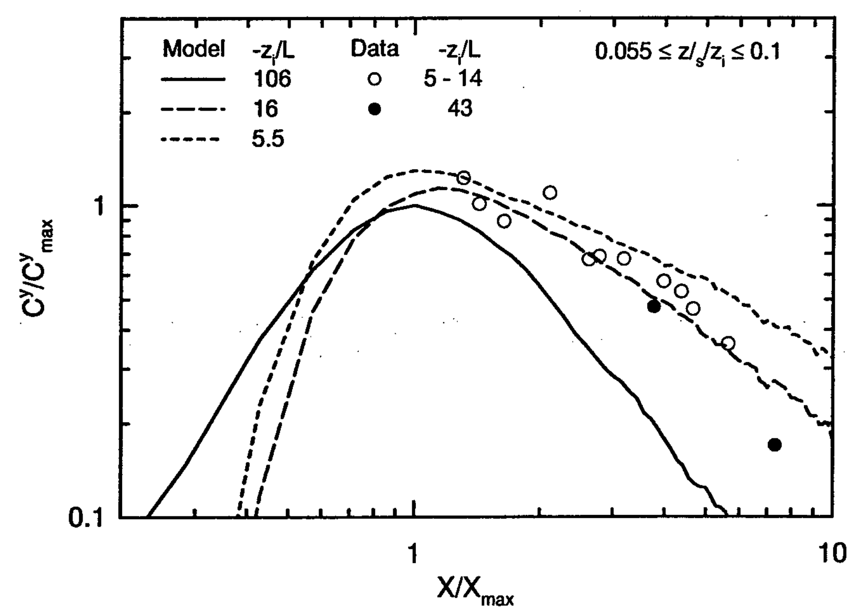

Figure 6: Modeled mean surface CWIC nondimensionlized by the maximum surface CWIC, C^y_{max}, as a function of X/X_{max}, where the C^y_{max} and X_{max} here correspond to the case $-z_i/L = 106$; the field data (Gryning and Lyck, 1984) are downwind of a 115-m source in the CBL surface layer.

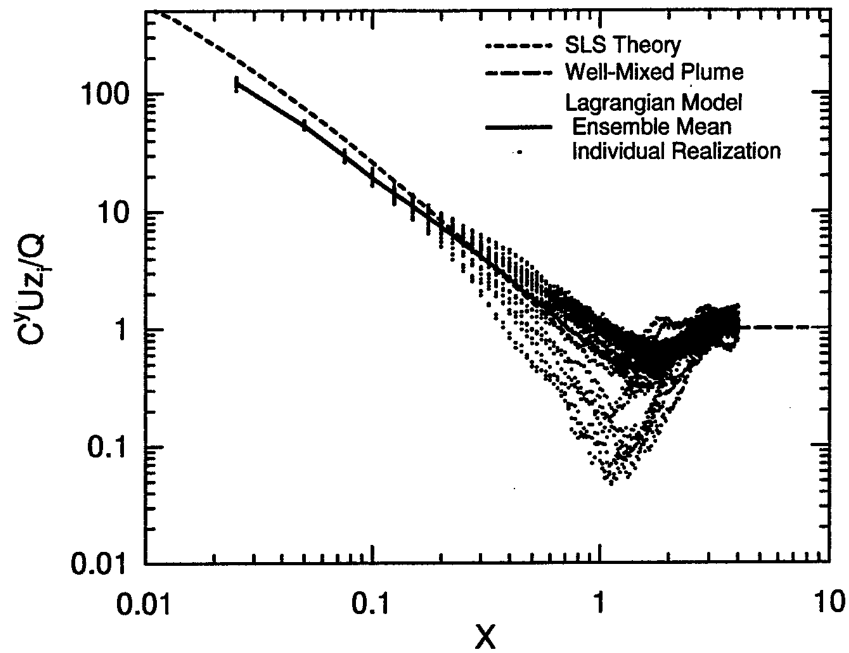

Figure 7: Dimensionless CWIC at the surface versus dimensionless downwind distance for a surface source in the CBL; modeled mean and individual realizations of the CWIC.

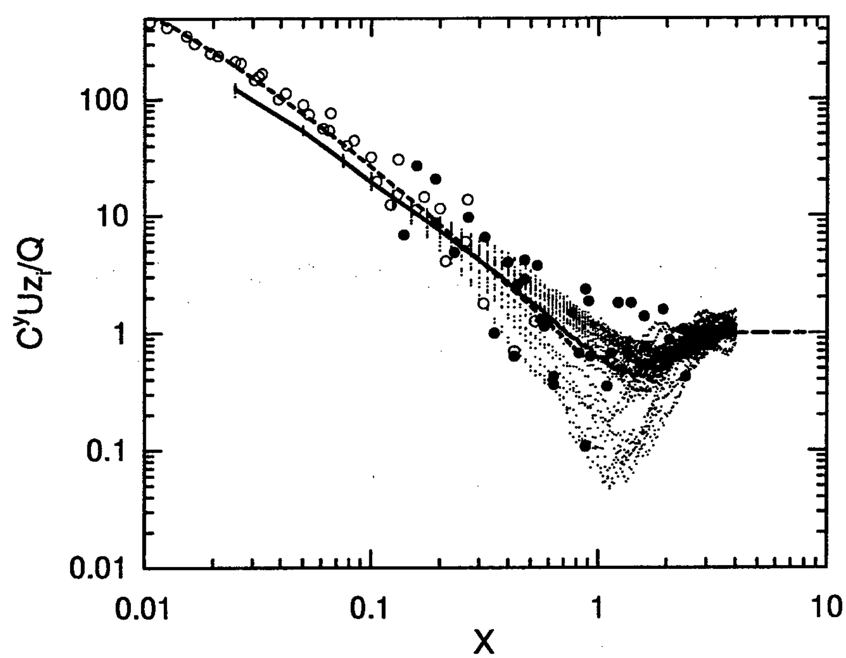

Figure 8: Dimensionless CWIC at the surface versus dimensionless downwind distance for a surface source in the CBL; superposition of Figs. 4 and 7.

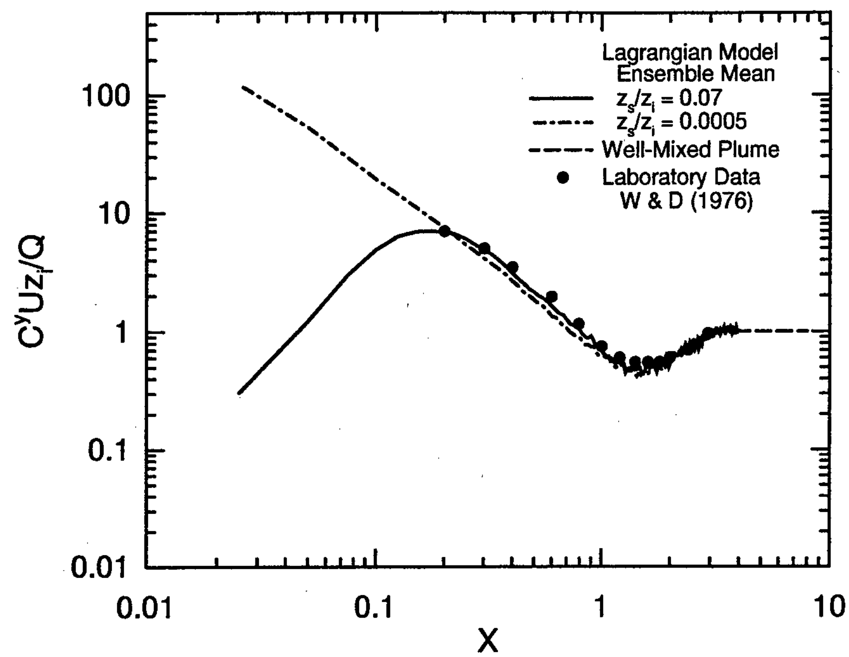

Figure 9: Dimensionless mean CWIC at the surface versus dimensionless downwind distance for a surface source and an elevated source ($z_s/z_i = 0.07$) in the surface layer.

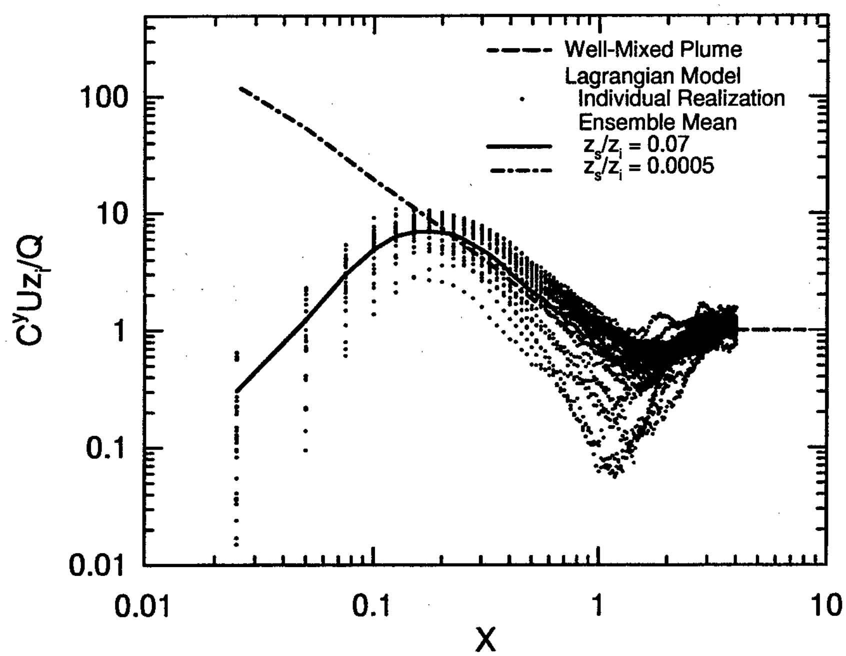

Figure 10: Dimensionless CWIC at the surface versus dimensionless downwind distance for an elevated source ($z_s/z_i = 0.07$) in the surface layer; modeled mean and individual realizations of the CWIC.

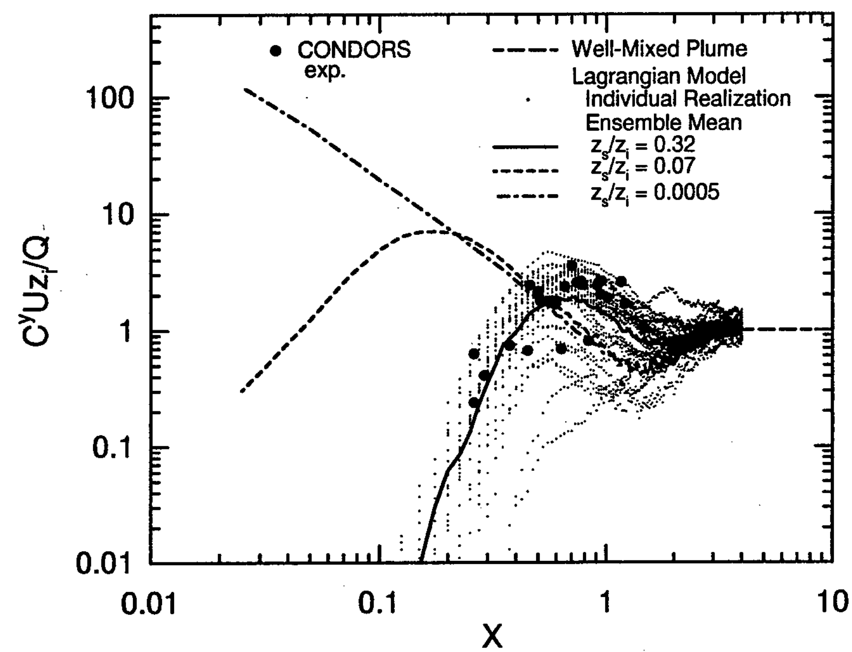

Figure 11: Dimensionless CWIC at the surface versus dimensionless downwind distance for an elevated source, $z_s/z_i = 0.32$, in the CBL; modeled mean and individual realizations of the CWIC.