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Report Title

Collaborative Research: Lagrangian Modeling of Dispersion in the Stable Boundary Layer and Canopy Environments

ABSTRACT

The objective of this research was to improve our understanding of dispersion in the planetary boundary layer (PBL) by extending our Lagrangian particle dispersion model (LPDM) to the stable boundary layer (SBL) and to PBLs interacting with vegetation canopies. The LPDM was driven by large-eddy simulations (LESs). For the SBL, dispersion simulations of a weakly stable PBL demonstrated the slow dispersion rate caused by the stable stratification and showed that the LPDM produced plume features in good agreement with observations. These included plume "tilting" due to wind direction shear, plume spread, and the downwind concentration distribution. For a neutral PBL with a resolved forest canopy, the LPDM demonstrated enhanced vertical dispersion but reduced effects of directional shear on lateral dispersion by comparison to a reference no-canopy case. More detailed canopy studies were initiated by coupling the LES with a newly developed multi-layer canopy version of the NOAH land-surface model; initial results showed that the modeled canopy-imposed heat source accurately reproduces that obtained from the recent CHATS field experiment.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Weil, J.C., 2008: Linking a Lagrangian particle dispersion model with three-dimensional Eulerian wind field models. J. Appl. Meteor. Climate, V. 47, 2463--2467.

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(c) Presentations

Patton, E.G., 2006: Canopy turbulence and nighttime cooling. Sedona International Workshop on Stable Boundary Layers, Sedona, AZ.

Sullivan, P.P., 2006: Subfilter-scale motions in atmospheric surface layers: what do LES models need? Sedona International Workshop on Stable Boundary Layers, Sedona, AZ.

Weil, J.C., 2006: Lagrangian particle modeling of dispersion in the stable boundary layer. Sedona International Workshop on Stable Boundary Layers, Sedona, AZ.

Weil, J.C., P.P. Sullivan, C.-H. Moeng, and E.G. Patton, 2006: Statistical variability of dispersion in the atmospheric boundary layer. 14th Joint Conference on the Applications of Air Pollution Meteorology with the AWMA, Atlanta, American Meteorological Society, Boston.

Weil, J.C., E.G. Patton, and P.P. Sullivan, 2008: Lagrangian modeling of dispersion in boundary layers with and without a plant canopy. 18th Symposium on Boundary Layers and Turbulence, American Meteorological Society, Boston.

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Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Moeng, C.-H., and J.C. Weil, 2009: Turbulence interaction with atmospheric physical processes. Second International Conference on Turbulence and Interaction - TI2009, Sponsored by ONERA, France, To be held in St. Lucia, June 2009.

Sullivan, P.P., and E.G. Patton, 2008: A highly parallel algorithm for turbulence simulations in planetary boundary layers: Results with meshes up to 1024^3 . 18th Symposium on Boundary Layers and Turbulence (CD ROM), American Meteorological Society, Boston.

Patton, E.G., et al., 2008: The canopy horizontal array turbulence study (CHATS). 18th Symposium on Boundary Layers and Turbulence (CD ROM), American Meteorological Society, Boston.

Patton, E.G., J.C. Weil, and P.P. Sullivan, 2008: A coupled canopy-soil model for the simulation of the modification of atmospheric by tall vegetation. 18th Symposium on Boundary Layers and Turbulence (CD ROM), American Meteorological Society, Boston.

Weil, J.C., E.G. Patton, and P.P. Sullivan, 2006: Lagrangian modeling of dispersion in the stable boundary layer. 17th Symposium on Boundary Layers and Turbulence (CD ROM), American Meteorological Society, Boston.

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Fernando, H.J.S., and J.C. Weil, 2008: An essay: Whither the SBL. Bull. Amer. Meteor. Soc., submitted.

Weil, J.C., E.G. Patton, and P.P. Sullivan, 2009: Lagrangian modeling of dispersion in a weakly stable boundary layer. J. Atmos. Sci., in preparation.

Weil, J.C., E.G. Patton, and P.P. Sullivan, 2009: Lagrangian modeling of dispersion in a neutral boundary layer with and without a plant canopy. J. Atmos. Sci., in preparation.

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FTE Equivalent:	
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Names of Post Doctorates

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Names of Under Graduate students supported

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Names of Personnel receiving masters degrees

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Total Number:

Names of personnel receiving PhDs

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Total Number:

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This is the final report of a collaborative research program by Dr. Jeffrey C. Weil at CIRES, the University of Colorado, and Drs. Edward G. Patton and Peter P. Sullivan at the Microscale and Mesoscale Meteorology Division, National Center for Atmospheric Research.

1. Introduction

Dispersion in the stable boundary layer (SBL) is important for a number of air quality and other problems, but current knowledge of SBL dispersion is deficient due to our limited understanding of the SBL turbulence. This limitation is caused by the weak SBL turbulence, past difficulties in measuring the turbulence, and the broad range of processes complicating the SBL physics. Over the past two decades, large-eddy simulation (LES) has proven to be a powerful tool in simulating turbulence in the planetary boundary layer (PBL). Most of this work has been aimed at the convective PBL, but recent studies have focused on the SBL and have demonstrated the capability to simulate this regime. For modeling dispersion, a key requirement is simulating the stochastic nature of the turbulence, which LES does quite well.

Under previous support from the Army Research Office (ARO), we developed Lagrangian dispersion models for following fluid “particles” in a turbulent flow. The velocities driving the particles were obtained from an LES, and the predicted concentration fields for a convective PBL were shown to be in good agreement with convection tank data (*Weil et al.*, 2004). Under the ARO program just completed, this modeling was extended to the SBL and to PBLs above a canopy. The program consisted of three main studies: 1) dispersion in an SBL with weak-to-moderate stability; 2) dispersion in a neutral boundary layer with a forest canopy at its base; and 3) LES of a dynamic canopy based on a coupled canopy - soil model. In the following, we discuss the key results of these studies.

2. Dispersion in a SBL

In a Lagrangian particle dispersion model (LPDM), one tracks passive particles to obtain the total dispersion and mean concentration field. When using LES to drive these models, we find the particle velocity from the LES “resolved” and “subgrid-scale” (SGS) velocities at the particle position. The SGS velocity is a random value obtained from a stochastic model using the SGS turbulent kinetic energy.

The velocity fields used to drive the dispersion model were obtained from the NCAR LES model (*Moeng and Sullivan*, 1994; *Sullivan et al.*, 1994, 1996; *Patton et al.*, 2005). Two SBL simulations were run with the first (S1) being a high resolution version of the GABLS (Global Energy and Water Cycle Experiment Atmospheric Boundary Layer Study) initiative (*Beare et al.*, 2006). This LES had a grid resolution of ~ 2 m and was forced by a geostrophic wind speed U_g of 8 ms^{-1} and a surface cooling rate of $0.25 \text{ }^\circ\text{Khr}^{-1}$. The forcings led to a surface friction velocity u_* of $\sim 0.28 \text{ ms}^{-1}$ and a stability index $z_i/L = 1.6$, where z_i ($= 200$ m) and L are the SBL height and Monin-Obukhov (MO) length. The above z_i/L classified the SBL as weakly-stable. The second case (S2) was initiated from the first, but with a reduced geostrophic wind (4 ms^{-1}), a grid resolution of ~ 1 m, a $z_i = 62$ m, and a $z_i/L = 2.2$. For reference, we included a neutral boundary layer (NBL, case N1) in which $U_g = 5 \text{ ms}^{-1}$, $u_* = 0.25 \text{ ms}^{-1}$, and $z_i = 615$ m. Table 1 contains a summary of the key PBL variables.

These PBLs exhibited similar overall properties such as an Ekman spiral with a mean wind maximum near z_i and significant wind shear. The velocity variances had maximum values near the surface, and they decreased systematically to small values at the PBL top consistent with observations (*Nieuwstadt*, 1984; *Lenschow et al.*, 1987) and other LESs (*Beare et al.*, 2006). For the SBLs, the Richardson numbers were ≤ 0.22 throughout the boundary layer except close to z_i . In addition, the eddy diffusivity for heat (K_H) had a profile shape similar to the vertical velocity variance σ_w^2 profile and a maximum K_H near $z/z_i \simeq 0.25$. The K_H profile was modeled well by $K_H = \sigma_w^2 \ell_p$, where the ℓ_p is a turbulence length scale parameterized following *Brost and Wyngaard* (1978). Overall, the LES modeled the key features of the weakly stable boundary layer quite well (*Beare et al.*, 2006; *Weil et al.*, 2006).

Case	$u_* (ms^{-1})$	$z_i (m)$	$z_i/L (m)$
S1	0.28	200	1.6
S2	0.13	62	2.2
N1	0.25	615	0
N1c	0.18	612	0

Table 1: Flow parameters for each simulation resulting from the imposed forcing specified. Variables are: u_* the surface friction velocity, z_i the boundary layer depth, and z_i/L the bulk stability parameter where L is the Monin-Obukhov length.

Calculations of the mean concentration fields and dispersion statistics were made for surface and elevated sources in the above PBLs. The results were based on releases with a total of about 70,000 particles. The analysis focused on the dispersion properties as a function of source height z_s , downwind distance x , and stability. The following presents: 1) an overview of the main dispersion features obtained from three-dimensional (3D) views, 2) vertical and lateral dispersion statistics, and 3) the downwind distribution of the surface crosswind-integrated concentration (CWIC, C^y).

Perspective or 3D views of plumes from two source heights in the SBL reveal key traits as shown in Fig. 1, where x is the distance along the PBL averaged wind direction, and y is the lateral or crosswind distance. Near the source, the plume has an anisotropic y - z cross section with little asymmetry in the y direction. With increasing distance, there is an increasing lateral mean plume displacement due to the directional shear or mean wind normal to x ; a positive y deflection occurs at low elevations with clockwise wind turning at the upper elevations. The directional shear also leads to enhanced lateral dispersion, lateral asymmetry, and “tilting” of the plume cross sections at large distances (four most distant planes in Fig. 1). Tilting is a real feature found in plume observations (*Csanady*, 1973; *Smith*, 1965) especially in the SBL, and these results are qualitatively consistent with the observations.

Analysis of the vertical dispersion (σ_z) and displacement statistics focused on their scaling. The vertical inhomogeneity in the mean wind and turbulence suggested that their source height values were most relevant for short-range dispersion. Hence, the σ_z scaled by $\ell_s [= \ell_p(z_s)]$ was examined as a function of the dimensionless travel time or distance $x/(u_s T_{Ls})$, where ℓ_s , u_s , and $T_{Ls} (= \ell_s/\sigma_{ws})$ are the turbulence length scale, mean wind speed, and Lagrangian time scale at the source height. This scaling organized and collapsed the vertical dispersion results (σ_z/ℓ_s) to approximately a single curve in each of two source height regimes: $z_s < 0.25z_i$ and $z_s \geq 0.25z_i$. The key difference between the regimes was the different value (and sign) of the K_H vertical gradient. Figure 2 shows results for the lower height regime.

For reference, Fig. 2 gives the statistical theory predictions (*Taylor*, 1921) applicable to homogeneous turbulence, and shows that for case S1 the simulations are about 30% lower than the theory in the near field, $x/(u_s T_{Ls}) < 2$. The difference between the two results is probably due to the inhomogeneity in the mean wind and turbulence in the simulated PBL and the grid resolution. For a finer concentration sampling grid resolution (factor of 4), the difference between the simulations and theory was only 20%. For case S2, the dimensionless sampling grid resolution was coarser, which probably explains the higher deviation between the simulations and theory in this case. Overall, the agreement between the simulated and theoretical trends is good.

For the lateral dispersion (σ_y), the LPDM results tended towards the statistical theory predictions— $\sigma_y \propto t$ and $\sigma_y \propto t^{1/2}$ —at short- and intermediate times, respectively, and towards $\sigma_y \propto t^{3/2}$ at long times. The enhanced spread at long times was caused by the wind direction shear as discussed above (for Fig. 1) and led to plume tilting. Theories (*Saffman*, 1962; *Smith*, 1965) and observations have shown that at large times the σ_y should vary as $\sigma_y \propto (\partial V/\partial z) \bar{K}_z^{1/2} t^{3/2}$, where V is the mean crosswind velocity and \bar{K}_z is the PBL averaged vertical eddy diffusivity. Figure 3 shows the three regimes of spread for case S1, where the long time ($t^{3/2}$) regime is clearly demonstrated for all source heights and appears to start around $X \sim 0.3$. The results for case S2 (not shown) look similar. In the NBL (Fig. 3b), the spread is similar although the $t^{3/2}$ regime appears to begin near $X \sim 0.5$, and its delay relative to S1 is probably due to the smaller directional shear in the NBL.

For the surface crosswind-integrated concentrations, a surface release is considered first since it forms an upper bound to the surface CWIC for elevated sources, and the results can be compared with observations from the Prairie Grass experiments (*Barad*, 1958). Figure 4 shows the LPDM predictions for the S1 and N1 cases

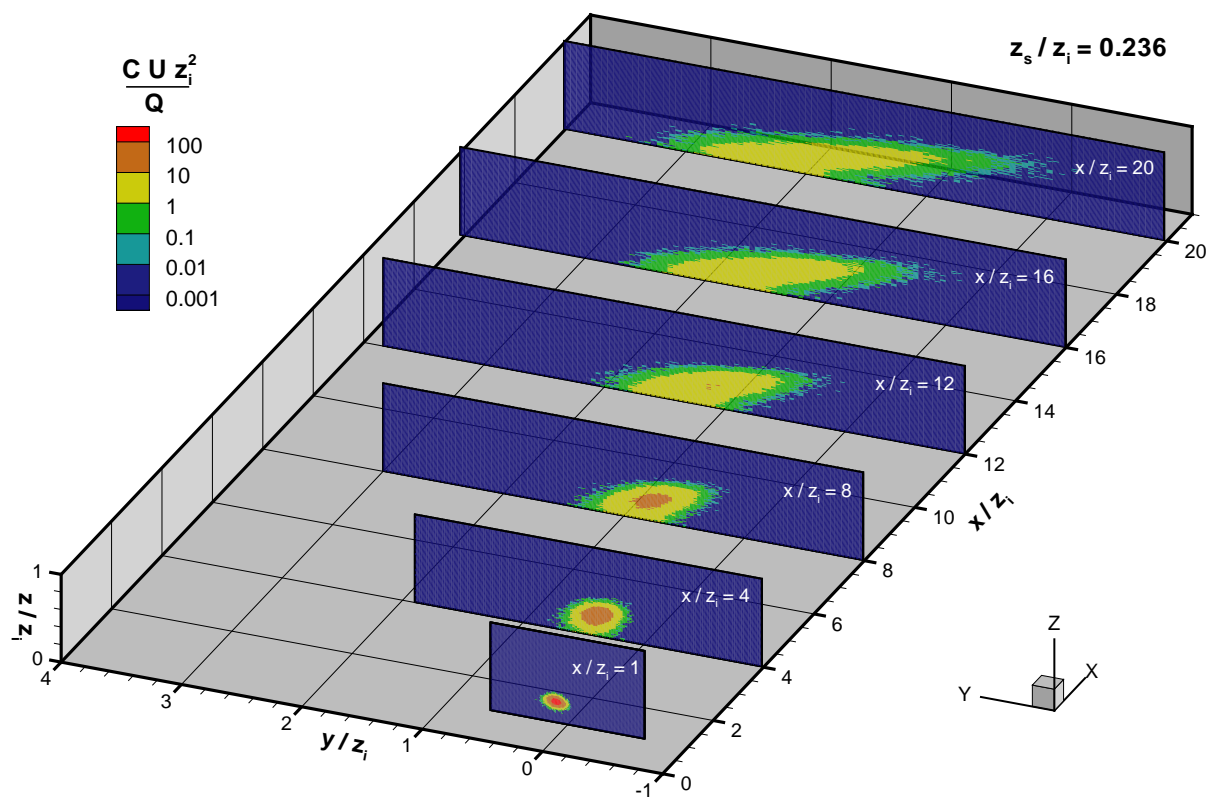
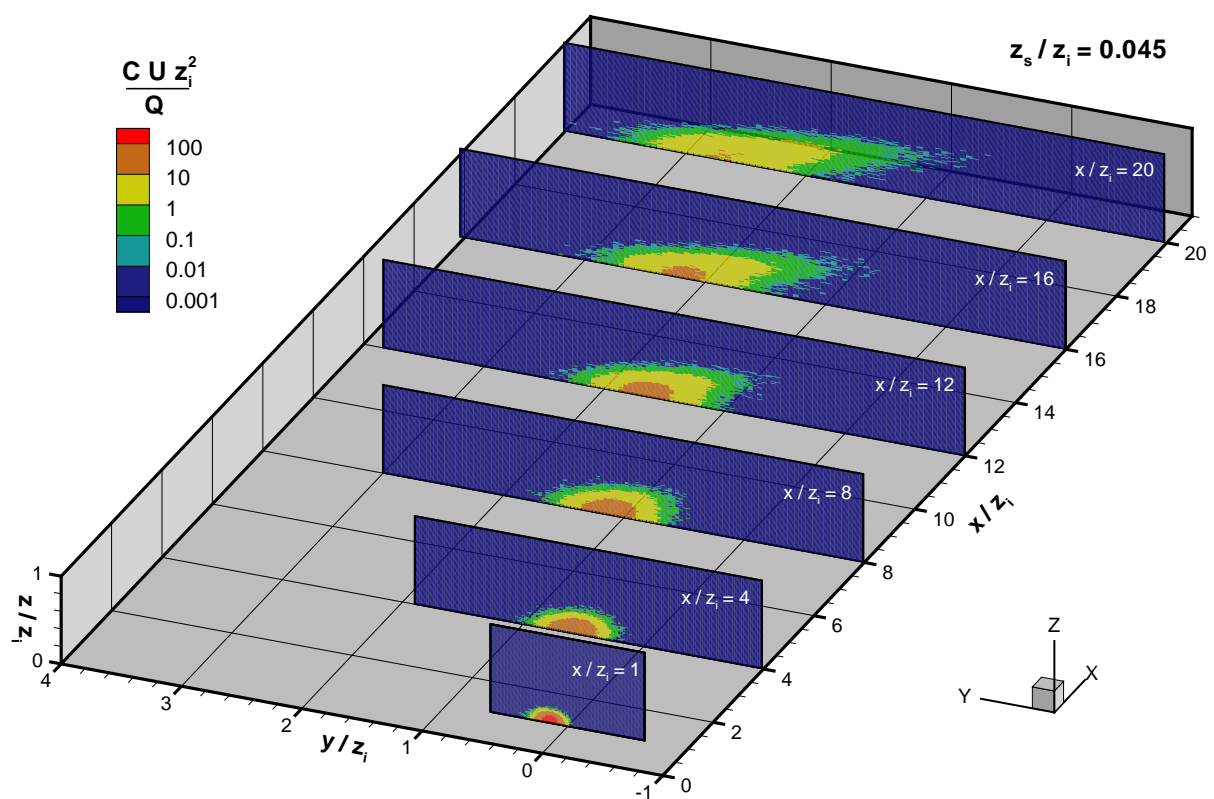


Figure 1: Perspective views of dispersion from two release heights in the SBL with concentration contours given for six crosswind ($y - z$) planes.

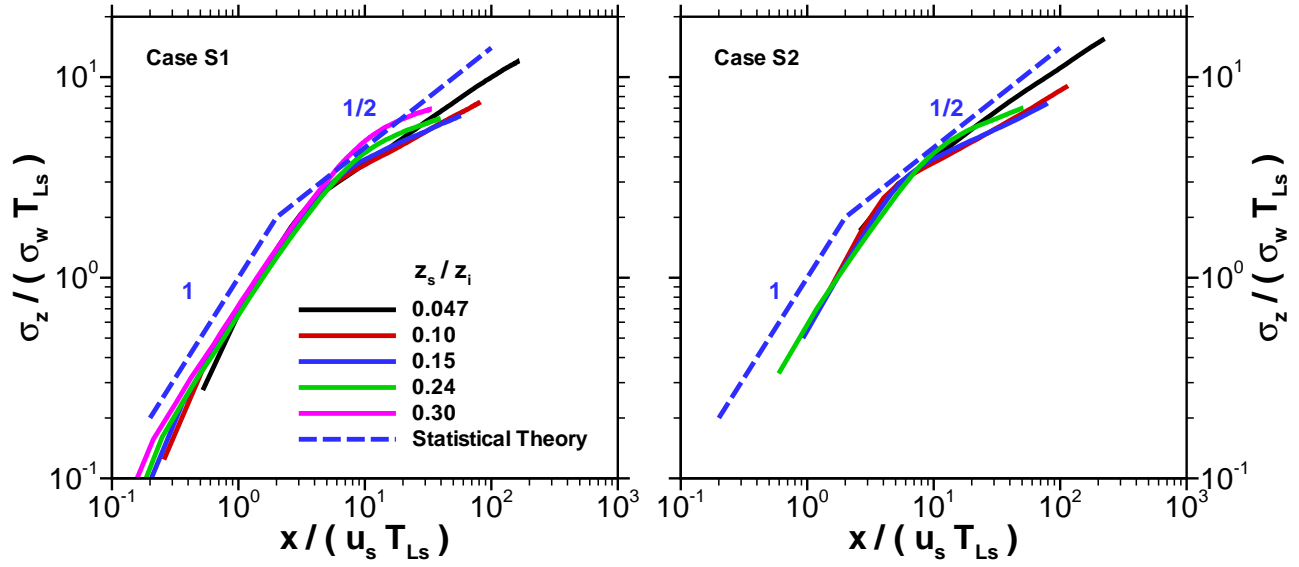


Figure 2: Scaled vertical dispersion as a function of the scaled downstream distance for five source heights in the SBL; results for two stability conditions or PBLs, S1 and S2.

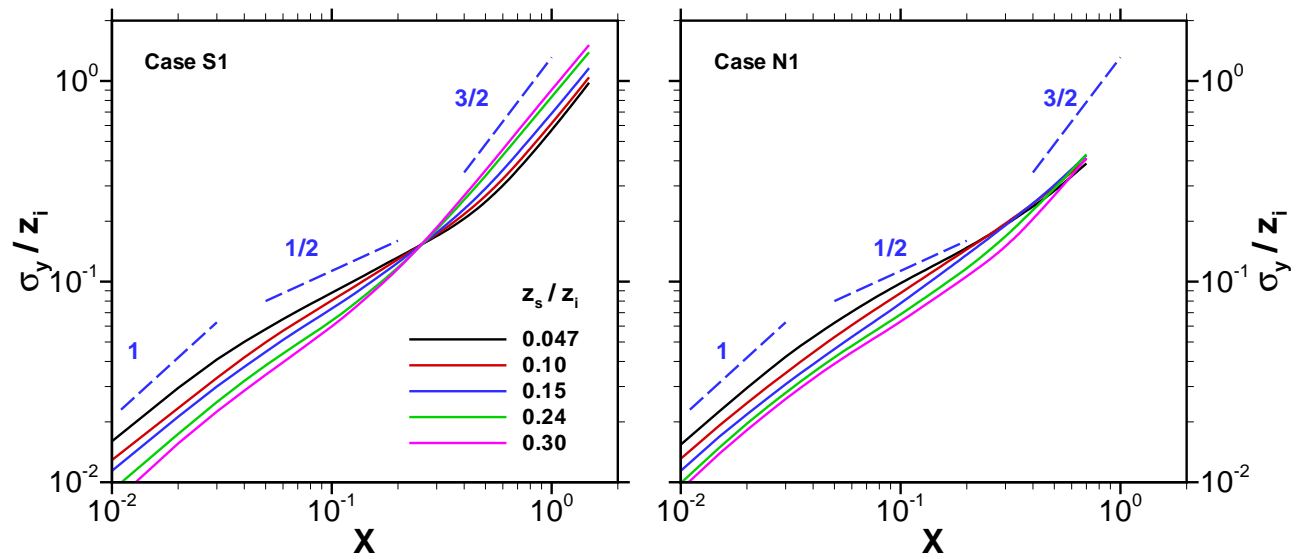


Figure 3: Dimensionless crosswind dispersion versus dimensionless downwind distance for five release heights in the SBL (S1) and NBL (N1).

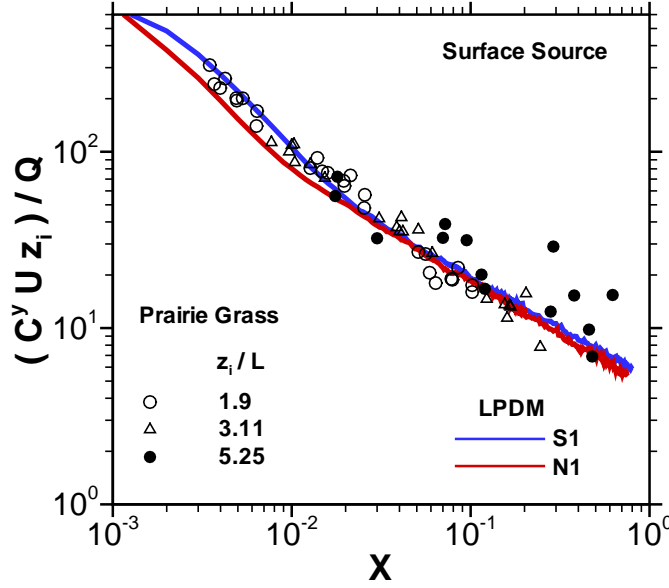


Figure 4: Dimensionless crosswind-integrated concentration (CWIC) at the surface versus the dimensionless distance for surface sources.

along with the Prairie Grass data, where the scaled CWIC ($C^y U z_i / Q$) is given as function of the dimensionless distance $X = u_* x / (U z_i)$, U is the mean wind speed, and Q is the source strength.

Figure 4 shows that the scaled CWIC ($C^y U z_i / Q$) at the surface varies approximately as X^{-1} near the source and as $X^{-1/2}$ far downstream. The LPDM results are in good agreement with the data for the weak-to-moderate stability groups: $z_i / L = 1.9$ and 3.1 . For the more stable case ($z_i / L = 5.25$), the data lie above the curves for $X > 0.07$, as would be expected due to the reduced dispersion in strong stability, which is not handled by the existing LES. Extrapolation of the LPDM long-range result shows that the plume would become well-mixed (with $C^y U z_i / Q = 1$) only very far downstream: $X \simeq 16$ or $x \simeq 80$ km. This demonstrates the very slow dispersion in the SBL.

Papers summarizing these results were presented at the American Meteorological Society (AMS) *17th Symposium on Boundary Layers and Turbulence* in San Diego (May 2006) and at the *Sedona Stable Atmospheric Boundary Layer Workshop* sponsored by ARO, the Arizona State University, and the Defense Threat Reduction Agency (November 2006). A journal article summarizing the results is in preparation. Presentations also were given at the Sedona Workshop on canopy turbulence (Patton) and on subfilter scale motions in the atmospheric surface layer (Sullivan).

3. Dispersion in a Neutral Boundary Layer with a Canopy

Atmospheric motions interacting with tall vegetation generate a roughness sublayer (RSL) in which mean and turbulence variables depart from their usual MO profiles (Finnigan, 2000). The RSL typically occupies the height range $0 \leq z/h \leq 3$ where h is the canopy height. Above the RSL, the mean wind and turbulence follow their MO similarity forms. Early work above forests showed that the eddy diffusivities for heat and moisture were about 2 to 4 times their MO values (Raupach, 1979, 1981). The higher diffusivities were caused by increased scalar mixing resulting from large coherent eddies in the RSL which were generated by the inflection point instability in the mean wind at the canopy top (Raupach et al., 1996; Finnigan, 2000).

The above diffusivities were effectively measures of dispersion from a uniform area source. In this study, we focused on point-source dispersion and investigation of the height and downwind extent of the “canopy effect” on the dispersion. We computed dispersion from sources within and above the canopy using the LPDM driven by an LES that explicitly resolves the canopy through a time-dependent and spatially varying pressure drag force.

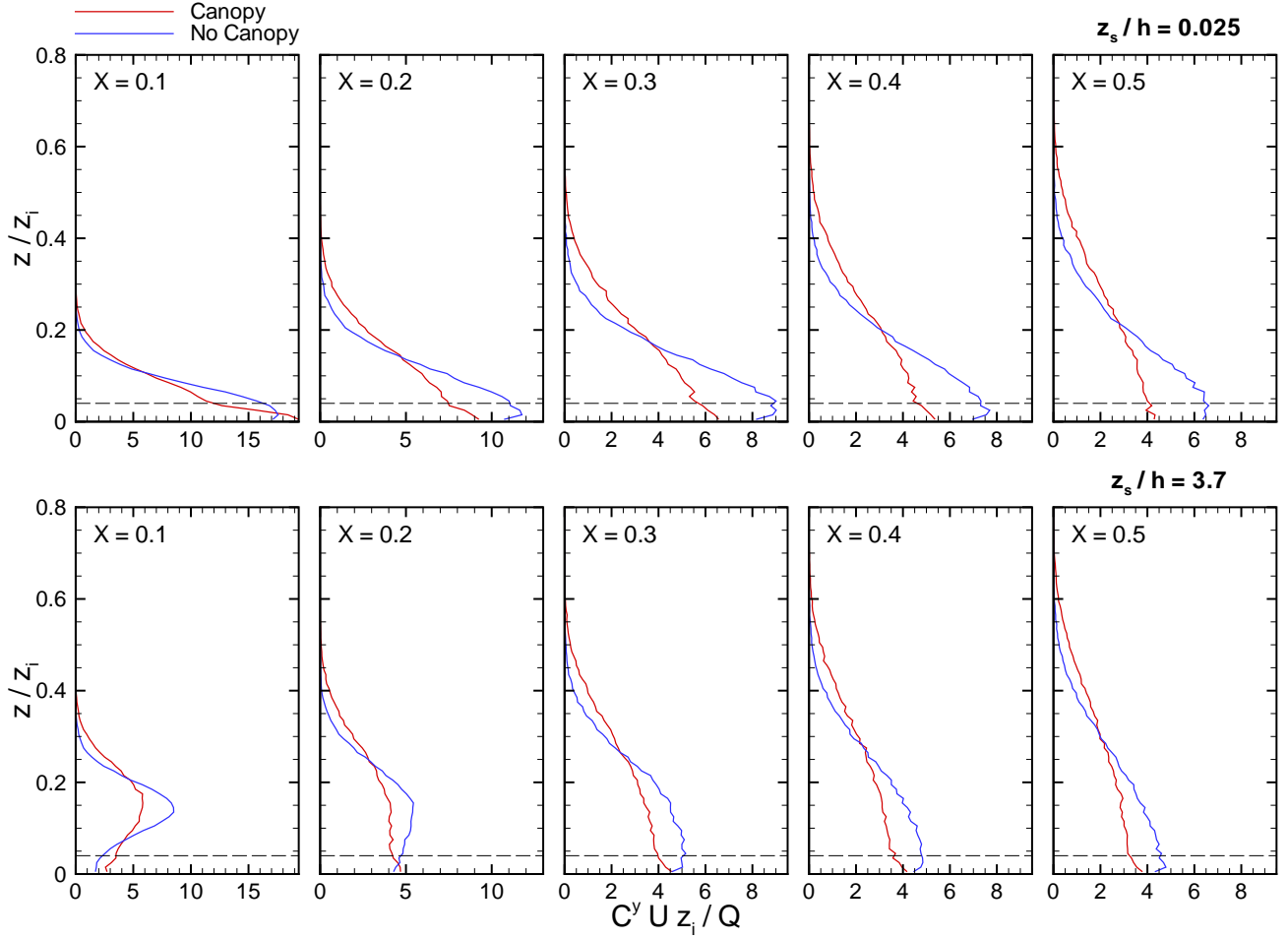


Figure 5: Dimensionless crosswind-integrated concentration profiles versus dimensionless distance in an NBL with and without a canopy. Upper and lower panels for sources within and above canopy, respectively, where canopy height (h) is denoted by dashed line.

For simplicity, the two LES computations were conducted for a neutral boundary layer; one with a canopy (case N1c) and without (case N1). The canopy-resolving LES was implemented as in *Patton et al. (2003)*, with the canopy influence modeled as a mechanical drag that depended on leaf area density and the square of the instantaneous velocity. The canopy was specified to be horizontally homogeneous, but with a leaf density varying with height, similar to a deciduous forest with a relatively dense over-story. The LES conditions for the two NBLs were essentially the same except for inclusion of a 25-m deep canopy in case N1c.

The dispersion analysis focused on vertical profiles of the crosswind-integrated concentration (CWIC) and the particle displacement statistics as a function of downstream distance and source height. As expected, the dispersion and mixing were greater in the NBL with a canopy. Figure 5 demonstrates this with vertical profiles of the dimensionless CWIC as a function of the dimensionless distance X for two source heights: $z_s/h = 0.025$ and 3.7 . The CWIC profiles are clearly broader in the canopy case, and this was true for source heights as large as $7.5h$. Thus, the canopy effect on point-source dispersion extends to greater depths than those for an area source. We believe this is due to the larger turbulence length and time scales in the NBL with a canopy, a view that is supported by an earlier dispersion analysis (*Weil, 1990*). For all sources, the CWIC differences decrease gradually with X as a result of the rather slow dispersion in the NBL.

The vertical and lateral dispersion (σ_y , σ_z) exhibited some similarities as well as differences from those in the SBL. For example, the vertical dispersion scaled as in Fig. 2 collapsed the σ_z/ℓ_s for the different source heights to a nearly single curve. Also, the lateral dispersion tended towards the short- and long-time limits of statistical theory, but did not exhibit the rapid growth ($\sigma_y \propto t^{3/2}$) at large times due to directional shear as found for the SBL.

or the NBL with no canopy (Fig. 3). This growth-rate reduction was caused by smaller directional shear (canopy case), which was about 50% of that in the NBL without a canopy. The canopy role in reducing the directional shear merits further investigation.

Additionally, the mean plume height rose at a faster rate with time in the NBL with a canopy. This is attributed to the different NBL structural properties (mean wind and variance profiles) in the two cases as well as to the greater Lagrangian time scale in the canopy case. A paper summarizing these results was presented at the AMS *18th Symposium on Boundary Layers and Turbulence* in Stockholm, Sweden (June 2008), and further analysis and a journal article are in preparation.

4. LES with Dynamic Canopy

In this work, we coupled the LES with a multi-level canopy model which solves a dynamic radiation/leaf energy balance at every vertical grid-level that will potentially permit simulation of more stable boundary layers and intermittent turbulence. The motivation for this was the earlier work of *Van de Wiel et al.* (2002) who found that a canopy layer was important in generating intermittency (see Section 4.2).

The canopy was included into the NOAH (National Center for Environmental Prediction / Oregon State University / Air Force / Office of Hydrology) land-surface model (*Chang et al.*, 1999), which describes the physics of the soil-water-vegetation system. In addition to the sensible and radiative heat fluxes, NOAH accounts for the moisture/vapor flux from the vegetation and a soil and hydraulic model for moisture supply to the plant roots. In its original form, the canopy in NOAH exchanges heat and moisture as a single “big leaf” and assumes that emitted scalars are vented immediately from the canopy space. Sensible and latent heat fluxes are determined through a coupling between radiation and photosynthesis models and the solution of a leaf energy balance. In the soil, the NOAH model predicts vertical profiles of temperature and moisture using a one-dimensional model with specified lower boundary conditions.

The key feature added to NOAH is a vertically distributed or “multi-level” canopy. NOAH remains as a 1-D column model and is implemented at every horizontal location in the LES domain, but the canopy extends vertically into the flow domain. Therefore, the vertical distribution of the light environment, atmospheric temperature, moisture and wind fields drive the system. We accomplished this by merging a number of already developed models to vertically extend NOAH’s current “big-leaf” canopy model.

For example, the canopy light environment model stems from MEGAN (*Guenther et al.*, 1995) which uses specified leaf scattering and reflection coefficients combined with the assumption of a spherical leaf angle distribution to calculate the absorption and scattering of direct/diffuse radiation by both sunlit and shaded leaves (*Goudriaan and van Laar*, 1994; *Leuning et al.*, 1995). Stomatal conductance is calculated using a photosynthesis-based formulation following GEM (*Niyogi et al.*, 2008) where a photosynthesis - carbon assimilation - transpiration model (*Collatz et al.*, 1991, 1992) is coupled with the Ball-Berry model (*Ball et al.*, 1987; *Leuning*, 1990).

Following *Leuning et al.* (1995), the ‘isothermal’ form of the Penman-Monteith combination equation (*Monteith*, 1965; *Jones*, 1976) is used to partition net radiation absorbed by the leaves into latent heat exchange at each level based upon the appropriate combination of leaf boundary layer and stomatal resistance along with the moisture gradient between the leaf and the atmosphere. Sensible heat exchange between the leaf and its surroundings can be then determined from the leaf energy balance equation. This method allows for the heat/radiation load on the leaf to determine the leaf’s temperature.

Development of the multi-level canopy version of NOAH and its coupling to the LES code has been completed. These models have undergone two levels of evaluation. The first evaluation involved driving the canopy model with measured atmospheric conditions taken during the CHATS campaign (*Patton et al.*, 2008). This evaluation has been completed and showed that the modeled canopy heat source distribution matches that found from the CHATS data (Figure 6). The second test evaluates the coupled model in its non-canopy-resolving mode to simulate the effects of a horizontally-varying soil moisture content on the turbulence structure of the convective PBL. The results of this simulation were compared with those of a previously coupled NOAH - LES model

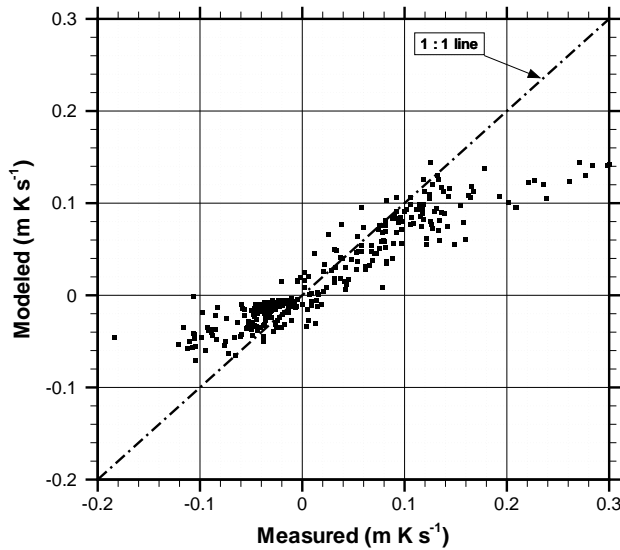


Figure 6: An evaluation of the multi-level canopy model as driven by data from the Canopy Horizontal Array Turbulence Study (CHATS) taken in a California walnut orchard in the Spring of 2007 (Patton *et al.*, 2008). Presented are the terms in the vertically-integrated heat budget ($\int_0^h \left[\frac{\partial \theta}{\partial t} + \frac{\partial}{\partial z} \overline{w'\theta'} \right] dz$), where the first two terms are taken from the CHATS measurements (labeled as: measured) and the third (\bar{S}_θ) is the model prediction (labeled as: modeled). The points represent hourly-averaged data spanning the entire last month of the CHATS campaign (when there were leaves on the trees). Satisfactory agreement is achieved using model parameters (leaf width, length, scattering and absorbing efficiencies, etc) specific to a “broad-leaf” forest, and could be improved through tuning these parameters specifically to walnuts.

(Patton *et al.*, 2005) to demonstrate consistency of the results (not shown).

We anticipate a third test (to be completed) will be a simulation of a weakly stable boundary layer to demonstrate the viability of the simulated mean and turbulence profiles. We also anticipate extended utility from this multilevel-canopy model through its inclusion into the Weather Research and Forecast (WRF) model (NOAH is already the primary land-surface model in WRF), which will permit incorporating spatially distributed vegetation and its influence on turbulence and momentum, heat, moisture, and other trace gases on weather and climate prediction.

5. References

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