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Large-Eddy Simulation of the Stable Boundary Layer and Implications for Transport and Dispersion

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Abstract

Large-eddy simulation (LES) of the evolving stable boundary layer (SBL) provides unique data sets for assessing the effects of stable stratification on transport and dispersion. The simulations include the initial development of the convective boundary layer (CBL) in the afternoon, followed by the development of an SBL after sunset with a strong, surface-based temperature inversion. The structure of the turbulence is modified significantly by negative buoyancy associated with the temperature inversion. The magnitude of velocity variances is reduced by an order of magnitude compared to that in the CBL, and the vertical velocity variance is damped further as the static stability preferentially damps vertical motions. The advanced subgrid-scale turbulence model allows simulation of intermittently enhanced periods of turbulence in the SBL that are often observed. During these turbulent episodes, mixing is increased within the SBL. Air pollution models that account only for the long-term mean structure of the SBL do not include the effects of these episodes. In contrast, our LES results imply that material released near the surface and mixed to higher elevations would be transported by stronger winds and in different directions, due to the vertical shear of horizontal wind speed and direction. Material released at altitude in the SBL will tend to be mixed downward toward the surface during these turbulent episodes in a fumigation-like scenario at night.

1 Introduction

Results from large-eddy simulation (LES) of the atmospheric boundary layer are used to evaluate transport and dispersion under stable and unstable atmospheric conditions. (In this paper, we use dispersion to refer to small-scale transport by turbulent eddies, and, as such, is much like diffusion; on the other hand, we use transport to refer to advection by the mean flow). Since impact assessments usually treat the stable boundary layer (SBL) as the worst case scenario, we will concentrate on LES results for an SBL case. The LES techniques used here are able to resolve fine-scale features of the SBL flow, and the associated spatially varying and intermittent turbulence. Traditional Reynolds-averaging approaches for characterizing turbulence used in most air pollution models are not well suited for unsteady turbulence in the SBL.

The simulations address the transition from the convective boundary layer (CBL) that develops during the afternoon to the SBL that develops after sunset. In the CBL, turbulent transport arises primarily from large, thermally-driven eddies that develop in response to surface heating. As the surface heating is replaced by surface cooling after sunset, the CBL collapses. The much-reduced turbulent transport comes from shallow, shear-driven eddies. In simulations using a previous subgrid-scale (SGS) model, the collapse of the CBL happened too rapidly (Cederwall [1]). Our advanced SGS model allows energy to be transferred both upscale and downscale, which provides a more realistic simulation of the evolving SBL (Cederwall & Street [2]).

2 Modeling Approach

Our LES model is based on a previous model designed for atmospheric boundary layer studies (Wyngaard & Brost [3]; Nieuwstadt & Brost [4]). It uses a second-order accurate leapfrog scheme for time integration, that is non-dissipative and employs an Asselin filter to control the computational modes (Asselin [5]). We have reduced the value of the damping factor from 0.1 to 0.02 to minimize the impact on the fine-scale velocity. A second-order accurate scheme is used for advection that conserves velocity variance (Piacsek and Williams [6]), and has very little numerical diffusion. Thus, we added a fourth-order dissipation term to control non-linear instabilities.

The subgrid scale model is an extension of the one developed by Salvetti & Banerjee [7]. We modified their SGS model for application to the atmospheric boundary layer by replacing the Smagorinsky viscosity scheme with a time-evolving SGS turbulent kinetic energy (TKE) scheme (Deardorff [9]) so that effects of atmospheric stability and turbulent transport of SGS TKE can be incorporated. The SGS model is a two-parameter approach that dynamically evaluates coefficients for the eddy viscosity and the modified Leonard term, and allows backscatter (upscale transfer) of energy (Cederwall & Street, [2], [8]). Corresponding dynamic equations have been developed for the SGS heat flux.

The numerical grid is oriented west-east for the x-direction (the nominal surface wind direction), and south-north for the y-direction. The grid resolution for the simulations is 20m in the horizontal directions and 5 m in the vertical direction. Results analyzed here are from a small domain of 32 grid points in each horizontal direction, and 80 grid points in the vertical direction; the small domain was used for purposes of computer efficiency while conducting numerous sensitivity studies. (Although the depth of the simulated CBL is smaller than typically observed, the simulated turbulence structure scales with observations, and provides the desired afternoon conditions prior to the evening transition. The structure of the resulting SBL is similar to observations.) Periodic boundary conditions are used in the horizontal direction. The momentum forcing at the top of the model is a constant geostrophic wind of 10.4 m/s. A weak temperature inversion is initially prescribed at the upper fourth of the model levels. Similarity is used at the bottom boundary, with a roughness length of 10 cm. The prescribed surface heat flux for the CBL is 75 W/m^2. The surface heat flux is then decreased linearly over a 1-hour period to -25 W/m^2 to represent the period around sunset, and held constant at a -25 W/m^2 during the rest of the simulation.

3 Results

3.1 Vertical Profiles of Mean Quantities and Turbulence Structure

Vertical profiles of temperature and winds for the simulated CBL agree well with observations which show small vertical gradients in the mixed layer below the capping inversion. This is due to the large amount of turbulence, especially in the vertical direction. The simulated turbulence structure shows the dominance of the vertical velocity variance within the mixed layer, while the horizontal velocity variances dominate near the ground. The SBL after several hours of cooling shows a strong, surface-based temperature inversion (Figure 1), as typically observed. In contrast to the CBL, the vertical velocity variance is a minimum in the SBL, and the turbulence is due primarily to horizontal velocity fluctuations and is a maximum near the ground where generation by wind shear

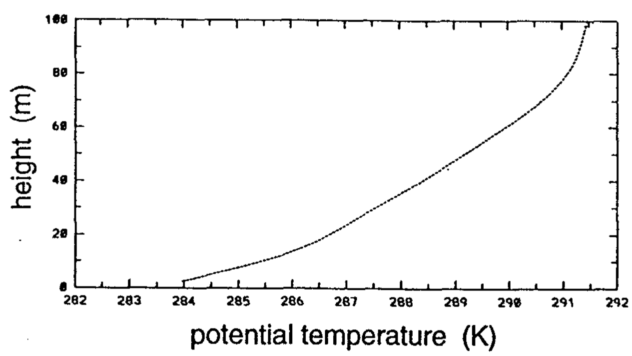

Figure 1. Vertical profile of mean potential temperature in the SBL.

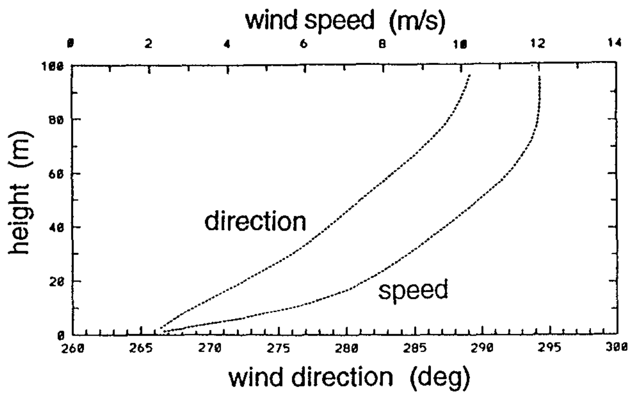

Figure 2. Vertical profile of mean wind speed and direction in the SBL.

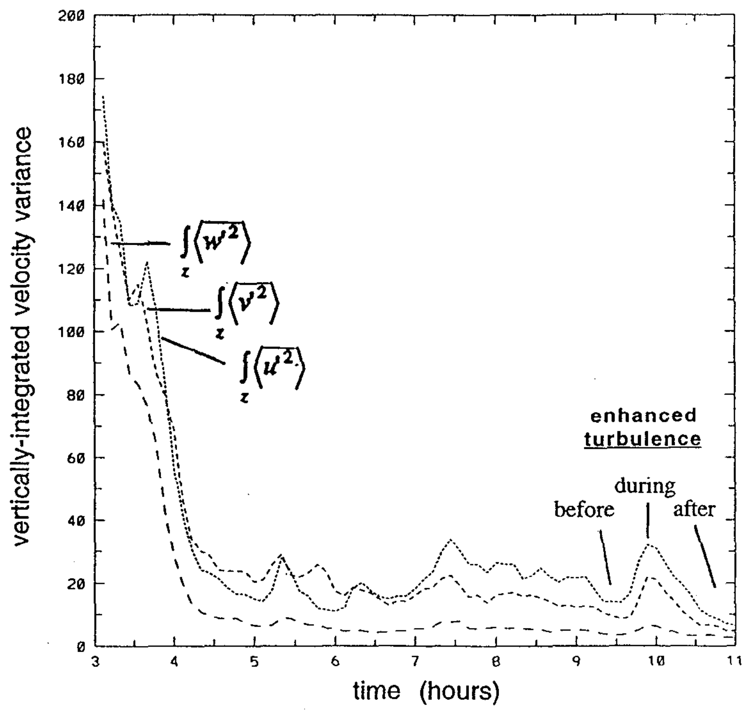

Figure 3. Time history of vertically-integrated velocity variances.

is the greatest (see Figure 2). The vertically-integrated velocity variances in Figure 3 provide a clear picture of the evolution of turbulence after sunset. The collapse of the mixed layer and its associated large amount of turbulence occurs rather completely during the 1-hour transition period of surface heating to surface cooling. The turbulence is not fully suppressed during the continued cooling. Instead, there are temporally varying levels of turbulence throughout the night.

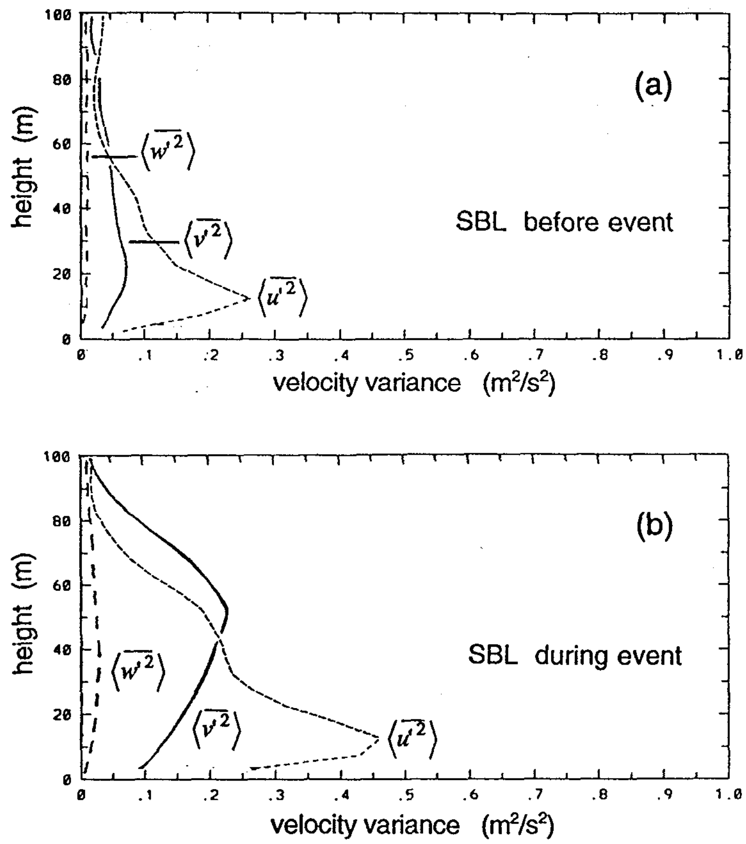

Figure 4. Vertical profiles of velocity variance (a) before and (b) during the enhanced turbulence event in the SBL.

As noted in Figure 3, there is an event of enhanced turbulence at hour 10 of the simulation after several hours of surface cooling. The vertical profiles of velocity variance before and during this event show the deepening of turbulence activity throughout the SBL, especially in the horizontal velocity components (see Figure 4). After the event, the turbulence is greatly reduced in all components, and is confined mainly to a shallow layer near the ground. Spectral analysis of the velocity components shows that the enhanced turbulence occurs at all scales, but that the spectral peak is moved towards smaller scales. In contrast, the strong reduction of turbulence after the event takes place more in the smaller scales, with the spectral peak occurring at scales larger than those before the event.

3.2 Transport and Dispersion in the Simulated Wind Fields

The simulation of an enhanced period of turbulence in the SBL is of particular interest since traditional air pollution dispersion models cannot explicitly treat such intermittent events, and yet the SBL is often the worst-case scenario addressed in hazard assessment. We evaluated the effects of intermittently enhanced turbulence by releasing groups of 75 marker particles every second in the LES-generated wind fields to represent individual sources of air pollution, and tracking them for five minutes. Thus there was a population of 22,500 particles for each source. The particles were advanced with a one-second time step. The transport wind was determined by trilinear interpolation of values at the corners of the volume containing the particle. Almost all of the velocity variance is resolved, except very near the ground, so no additional perturbation was added to the transport velocity to account for SGS turbulence. The release positions were centered on a specified release point for the individual source, with 5 positions in each of the horizontal directions equally spaced across 10 m, and repeated 3 times in the vertical direction, equally spaced across 1 m. After some time, particles were transported horizontally beyond the model grid. The use of periodic boundary conditions allowed us to handle this situation, as was done by Kemp and Thomson [10].

The variation in transport and dispersion in the SBL depends strongly on height, due to the strong wind shear and the variation in strength of turbulence. For this reason, we chose five release heights (10m, 30m, 50m, 70m, and 90m) at the same horizontal location to study the differences in transport and dispersion. The location of marker particles after 5 minutes is shown in Figure 5 for the simulated flow before the enhanced turbulence event. Note that the vertical scale is much smaller than the horizontal scale. The height dependence of speed and direction of transport is clearly evident. There is no strong variation in dispersion with height. The location of marker particles released during the enhanced turbulence event tells a different story. Within the middle portion of the SBL, there is much greater dispersion, as seen in Figure 6. This leads to significantly reduced concentration of released material which can be estimated from the marker particles, as done by Kemp and Thomson [10].

For purposes of comparison, marker particles were also released within the CBL, but at just two heights (20m and 60m). The vertical transport by large convective eddies is seen in Figure 7a. The small vertical gradient of wind direction within the well-mixed CBL is evident in Figure 7b, when compared to that in the SBL (see Figure 5b and 6b). The CBL offers a much different environment for transport and dispersion; this is captured in our simulated wind fields.

4 Discussion

Large-eddy simulation provides realizations of atmospheric flows that are observed under both stable and unstable atmospheric conditions. The simulated wind fields can be used to study transport and dispersion under a variety of atmospheric conditions, without the need to make assumptions about the turbulence, which is explicitly resolved by the LES. The SBL is of interest due to its frequent use as a worst-case scenario in hazard assessment, and yet our

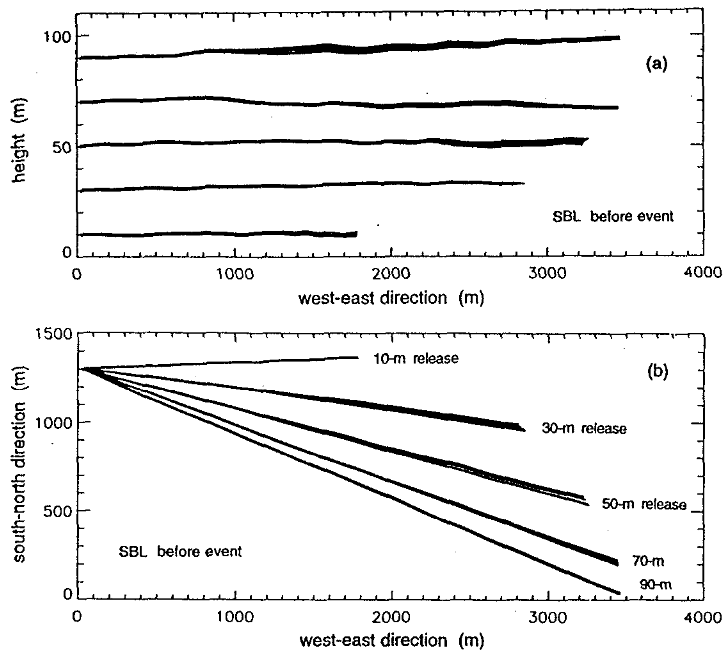

Figure 5. Location of marker particles for 5-minute release before SBL event in (a) x-z plane, and (b) x-y plane.

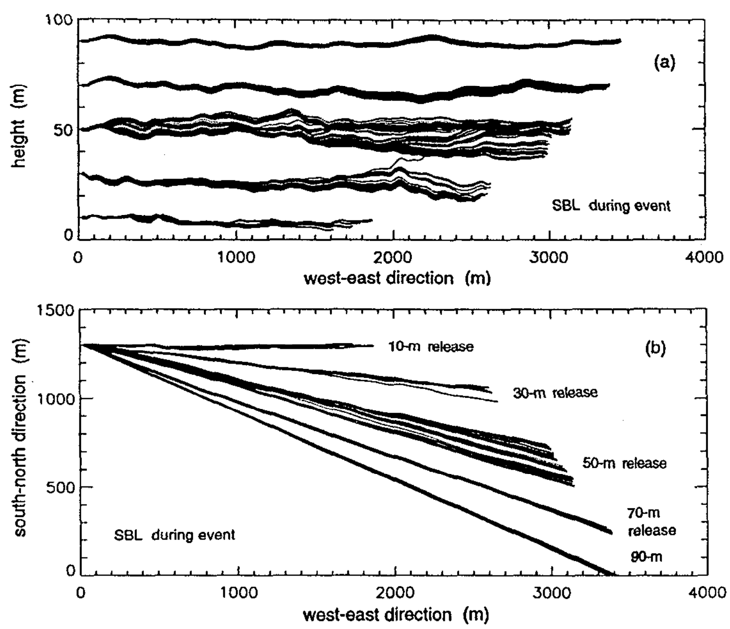

Figure 6. Location of marker particles for 5-minute release during SBL event in (a) x-z plane, and (b) x-y plane.

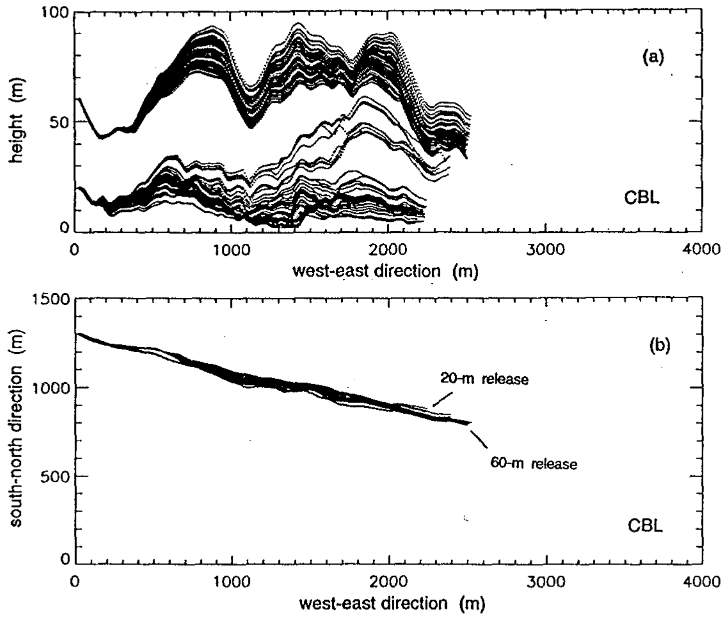

Figure 7. Location of marker particles for 5-minute release into CBL in (a) x-z plane, and (b) x-y plane.

understanding of turbulence in stably-stratified conditions is incomplete. LES can be used in 'numerical' experiments to increase our understanding. In addition, LES results can allow us to study transport and dispersion in the SBL, and evaluate the performance of simpler dispersion models in situations where field data are not available.

The study presented here shows the ability of LES, with advanced SGS turbulence models that include energy backscatter, to capture the unsteady and intermittent behavior of turbulence in the SBL. The strong wind shear in the SBL is demonstrated to have a significant, height-dependent effect on the speed and direction of transport. The enhanced periods of turbulence have a further effect on the dispersion of material, as illustrated by the location of marker particles. The enhanced dispersion leads to differential transport, especially for material dispersed to different heights. The resulting differences in concentrations of airborne material have important implications for health assessments of hazardous materials released to the atmosphere.

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