Concentration Fluctuations and Variability at Local and Regional Scales: Use of a Lagrangian Two-Particle Dispersion Model Coupled with LES Fields

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Abstract A Lagrangian two-particle dispersion model (L2PDM) driven by velocity fields from large-eddy simulations (LESs) is used to compute the mean and fluctuating concentrations in a highly convective boundary layer. The model results agree with data from two convection tank experiments.

Keywords Concentration fluctuations, Lagrangian two-particle modeling, LES

1. Introduction

A striking feature of atmospheric dispersion is its large variability. This is especially true in the convective boundary layer (CBL) where the plume from an elevated source meanders due to the large convective eddies, producing high fluctuations in surface concentrations. The concentration peaks are caused by intermittent transport of plume segments to the surface by CBL downdrafts, where the plume spread about the local centerline is due to small-scale turbulence (Gifford, 1959). The concentration fluctuations are characterized by their root-mean-square (rms) value σ_c or the fluctuation intensity σ_c/C, where C is the ensemble-mean concentration. Measurements show that surface σ_c/C can be large ranging from 1 to 10 for short averaging times (< 5 min) and downstream distances (< 5 km).

In this work, we extend Thomson's (1990) Lagrangian two-particle dispersion model (L2PDM) for concentration fluctuations in homogeneous turbulence to the inhomogeneous conditions of the CBL by coupling it with velocity fields from large-eddy simulations (LES) (e.g., Moeng and Sulllivan, 1994). Thomson's model handles the two-particle motion due to the ``unresolved" or LES subfilter-scale (SFS) velocities, whereas the LES ``resolved" velocities address particle displacements due to the larger-scale motion.

2. Models

In an L2PDM, one tracks the simultaneous motion of two particles that start from a small separation and spread due to inertial-subrange turbulence leading to ``relative dispersion" about the plume centerline (Batchelor, 1950). Thomson (1990) used stochastic equations to follow the evolution of the six-dimensional position and velocity arrays defining the two-particle system. He produced a relative dispersion (σ_r) with $\sigma_r \propto t^{3/2}$ at short times (t) and $\sigma_r \propto t^{1/2}$ at long times, consistent with Batchelor's (1950) theory, and σ_c results in agreement with wind-tunnel data.

In using LES fields to drive the particles, we decompose the total or Lagrangian velocity ($\boldsymbol{u}_{Lk}$) of particle k (= 1, 2) as $\boldsymbol{u}_{Lk} = \boldsymbol{u}_{Rk}\ (\boldsymbol{x}_{pk},t) + \boldsymbol{u}_{Sk}\ (\boldsymbol{x}_{pk};\ \boldsymbol{x}_{pj},\ t)$, where the resolved and SFS velocities (subscripts $\boldsymbol{R}$ and $\boldsymbol{S}$) of a particle (subscript p) are superposed as in the 1-particle LPDM (Weil et al., 2004); a bold-faced symbol denotes a vector. The SFS velocity depends on the positions of both particles (k and j) due to the two-point velocity correlation built into the SFS model (Thomson's); the resolved velocity correlation is implicitly included in the computed LES fields.

For a continuous point source (CPS), a one-particle LPDM can be used to find the mean concentration from the probability density function (PDF), p_1, of particle position $\boldsymbol{x}_p$ (Weil et al., 2004). For the two-particle releases, the plume concentration c also is computed from a p_1 but one using both particle positions, which accounts for the relative dispersion. Such dispersion leads to a narrower plume and higher local concentrations c than for the mean dispersion. The C and σ_c fields are obtained from an ensemble of N widely-spaced sources at height z_s in a horizontal plane, creating N ``independent" realizations of the c field (see Weil et al, 2012).

The Moeng and Sullivan (1994) LES model was adopted for the 1-particle LPDM (Weil et al., 2004) and served as a reference case. The LES was run for a 5 $\times$ 5 $\times$ 2 km^3 domain, 96^3 grid points, a surface heat flux of 0.24 K ms^{-1}, a mean CBL height z_i of 1 km, a convective velocity scale w_* of 2 ms^{-1}, and a mean wind speed U over the CBL of 3 ms^{-1}; thus, $U/w_* = 1.5$. For the two-particle model, the EULAG (EUlerian/semi-LAGrangian) model (Prusa et al., 2008) was adopted and run for the same setup, domain size, and variables as in Weil et al. (2004).

3. Results

We performed L2PDM simulations for four release heights: z_s/z_i = 0.07, 0.25, 0.49, and 0.8; the first three matched those in the Willis and Deardorff (WD) (1976, 1978, 1981) experiments and all were close to or the same as in Hibberd (2000). The simulations were driven by LES fields input sequentially from 210 data volumes stored at 10-s intervals. The C and σ_c fields were obtained with N = 25 CPS releases, each with 2.1×10^5 particles, whereas the laboratory experiments used an instantaneous line source (ILS). For sufficiently high U/w_* ($\geq$1.5), WD

(1976) argued that the C fields for the CPS and ILS were equal upon replacing t by x/U in the ILS results; i.e., rms longitudinal velocity fluctuations σ_u would not significantly affect the CPS results. However, no data were given for the σ_c fields.

Figure 1 presents L2PDM results of the mean dimensionless crosswind-integrated concentration (CWIC), C^yUz_i/Q at the surface versus the dimensionless downwind distance $X = w_*x/(Uz_i$, the ratio of travel time (x/U) to the eddy turnover time (z_i/w_*). For the lowest source, the L2PDM results agree well with the earlier 1-particle LPDM and the WD (1976) data, establishing consistency between the 1- and 2-particle LPDMs. However, the Hibberd (2000) data has a much lower peak CWIC, which is probably due to the long ILS setup time (t_s =$0.4z_i/w_*$) with emissions distributed over t for $t \leq t_s$. The L2PDM generally agrees with the lab data for the other sources showing a systematic variation with z_s and X, although the Hibberd data has a reduced and delayed peak for $z_s/z_i =$ 0.25, likely due to the t_s.

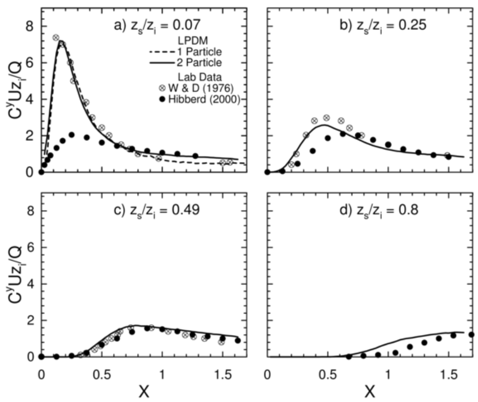

Fig. 1. Dimensionless CWIC at surface versus *X* for 1-and 2-particle LPDMs and comparison to the convection tank experiments of Willis and Deardorff (1976 1978, 1981) and Hibberd (2000); Weil et al. (2004) only provided the 1-particle LPDM results for z_s/z_i = 0.07.

Figure 2 shows the CWIC fluctuation intensity, $\sigma_C{}^y/C^y$, versus X at the surface. The CPS results (solid line) and lab data are consistent at short range, where the $\sigma_C{}^y/C^y$ is dominated by plume vertical meandering; the large initial drop in $\sigma_C{}^y/C^y$ is due to the increase of σ_r relative to the rms meander. However, once the decrease in $\sigma_C{}^y/C^y$ subsides, the CPS results tend to higher values than the data. We believe that this is due to the CBL longitudinal variance $\sigma_u{}^2$ generating plume c fluctuations in low winds: U/w_* (~1.5) or equivalently σ_u/U ~ 0.4. Thus, we modeled the release as an ILS (no σ_u effects), and this result (dashed line) agrees much better with the data. More study is required of the $\sigma_C{}^y/C^y$ *(X)* variation with U/w_*.

Overall, these results support the L2PDM-LES approach for modeling mean and fluctuating concentrations due to sources in the CBL, and our contention that the CBL longitudinal variance $\sigma_u{}^2$ affects the rms concentration (σ_c) more than the mean (C) at low values of U/w_*. This contention requires further investigation.

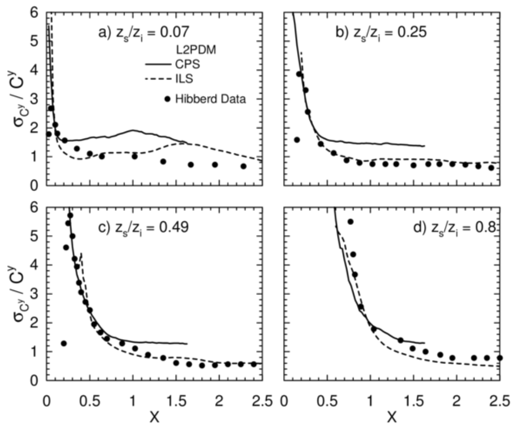

Fig. 2. Fluctuation intensity of surface CWIC versus *X* compared to Hibberd (2000) data.

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4. References

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Question and Answer

Q: Peter Viaene: Why do you limit to 2 particles?

A: Jeffrey Weil: We restrict the model to 2 particles because it is sufficient to determine both the mean **and** rms concentrations and it has lower computational demands than models for higher numbers (n) of particles. In principle one needs multi-particle spatial correlations to compute the n–particle relative motions, and these are not readily available; the 2-particle velocity correlations exist and are used in Thomson's (1990) model. Models do exist for tetrads (n = 4) (e.g., Toschi, F., and E. Bodenschatz, 2009: Lagrangian properties of particles in turbulence. *Ann. Rev. Fluid Mech.*, **41**, 375—404) and clusters of n = 6 particles (Sawford, B.L., S.B. Pope, and P.K. Yeung, 2013: Gaussian Lagrangian stochastic models for multi-particle dispersion. *Phys. Fluids*, **25**, 055101-1—055101-19). However, in the latter case (n = 6), the model is constrained by the n = 2 spatial correlations, and the higher-n spatial correlations are neglected.

Q: Enrico Ferrero: 1) Is there any limitation due to the fact that the two-particle model is valid only for homogeneous isotropic turbulence? 2) Which kind of PDF do you use in the Lagrangian model?

A: Jeffrey Weil: 1) Thomson's (1990) 2-particle stochastic model is only used for the subgrid-scale or subfilter-scale treatment, and we believe that the homogeneous isotropic assumption is adequate at this scale and consistent with the LES. The larger-scale inhomogeneous and anisotropic motion of the CBL flow is handled by the LES resolved velocities, which evolve in a natural way in the computed flow field. 2) For Thomson's 2-particle model, the PDF of the random velocity forcing is assumed to be joint normal.