A SUBGRID LAGRANGIAN STOCHASTIC MODEL FOR TURBULENT SCALAR DISPERSION

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ABSTRACT

A large eddy simulation (LES) with the dynamic Smagorinsky-Germano subgrid-scale (SGS) model is used to study passive scalar dispersion in a turbulent boundary layer. Instead of resolving the passive scalar transport equation, fluid particles containing scalar are tracked in a Lagrangian way. The Lagrangian velocity of each fluid particle is considered to have a large-scale part (directly computed by the LES) and a small-scale part. The movement of fluid elements containing scalar at a subgrid level is given by a three-dimensional Langevin model. The stochastic model is written in terms of SGS statistics at a mesh level. The results of the LES are compared with the wind-tunnel experiments of Fackrell and Robins (1982 *J. Fluid Mech.* **117** 1-26) and with the LES results of Sykes and Henn (1992 *Atmos. Environment* **26A** 3127-3144), who used a completely Eulerian approach with a non dynamic SGS model. Our simulations predict the quantitative features of the experiments of Fackrell and Robins (1982 *J. Fluid Mech.* **117** 1-26). Moreover, by using the Lagrangian approach, scalar fluxes are computed with no additional modeling assumptions and show good agreement with the experimental data.

INTRODUCTION

Owing to an increasing interest in environmental problems, considerable attention has been focused on the prediction of concentration levels downwind of polluting sources in turbulent boundary layers. Since the pioneering work of Deardorff (1970), LES has become a well established tool for the study of turbulent flows (Meneveau and Katz, 2000), the transport of passive scalars (Sykes and Henn, 1992; Kemp and Thomson, 1996) as well as the dispersion of reactive plumes (Sykes et al., 1992; Meeder and Nieuwstadt, 2000). Current LES of scalar fields are increasingly applied to the study of atmospheric dispersion of pollutants, to the evaluation of mixing and segregation rates (Meeder and Nieuwstadt, 2000) or concentration peaks (Xie et al., 2004). However, these Eulerian approaches are less employed when it comes to computing the concentration variance or the SGS characteristics of the scalar field. In this study, a Lagrangian stochastic model is coupled with a LES with the dynamic Smagorinsky-Germano SGS model (Germano et al., 1991), in order to obtain concentration field fluctuations and scalar fluxes.

In order to model the velocity field that advects the fluid elements at a subgrid level, the three-dimensional Langevin equation model (Thomson, 1987), is written in terms of the local SGS characteristics. This way, the Lagrangian stochastic model is entirely given by the quantities directly computed by the LES with the dynamic Smagorinsky-Germano SGS model, Germano et al. (1991).

The results of the computations are compared with the wind-tunnel dispersion results of Fackrell and Robins (1982) and with the LES of Sykes and Henn (1992), who used an Eulerian approach with a non dynamic SGS model.

LARGE-EDDY SIMULATION

A turbulent boundary layer flow is computed using the LES code ARPS 4.5.2. The continuity and momentum equations obtained by grid filtering the Navier-Stokes equations are:

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0$$
$$\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \tau_{ij}^r\right) + \tilde{B}_i \quad (1)$$

where u_i is the fluid velocity, p is the total pressure, ν the molecular kinematic viscosity, ρ the density and $i = 1, 2, 3$ refers to the x (streamwise), y (spanwise), and z (normal) directions respectively. B_i includes the gravity and the Coriolis force. The tilde denotes application of the filtering operation:

$$\tilde{u}_i(\vec{x}, t) = \int_V u_i(\vec{x} - \vec{r}, t) G(\vec{r})\, d\vec{r} \quad (2)$$

where the grid filter is given by:

$$G(\vec{r}) = \begin{cases} 1/\tilde{\Delta} & \text{if } |\vec{x} - \vec{r}| < \tilde{\Delta}/2 \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

The filter width $\tilde{\Delta}$ is defined as $\tilde{\Delta} = \left(\tilde{\Delta}_x \tilde{\Delta}_y \tilde{\Delta}_z\right)^{1/3}$, where

$\tilde{\Delta}_x$, $\tilde{\Delta}_y$, $\tilde{\Delta}_z$ are the grid spacings in the x, y and z directions, respectively.

The effect of the sub-grid scales on the resolved eddies in equation 1 is presented by the SGS stress, $\tau^r_{ij} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$.

The pressure equation is obtained by taking material derivative of the equation of state and replacing the time derivative of density by the velocity divergence using the mass continuity equation:

$$\frac{\partial \widetilde{\Delta p}}{\partial t} + \tilde{u}_j \frac{\partial \widetilde{\Delta p}}{\partial x_j} = \frac{\rho}{c^2} \left(\frac{1}{\tilde{\theta}} \frac{\partial \tilde{\theta}}{\partial t} - \frac{\partial \tilde{u}_i}{\partial x_i} \right) \tag{4}$$

where Δp is the pressure deviation from an undisturbed dry, hydrostatic base state, c is the speed of sound and θ the potential temperature. The flow studied here is a neutral turbulent boundary layer. The potential temperature variations are therefore negligible.

The determination of the SGS stress, τ^r_{ij}, is parameterized using an eddy viscosity hypothesis:

$$\tau^r_{ij} - \frac{1}{3}\delta_{ij}\tau^r_{kk} = -2K_m \tilde{S}_{ij} \tag{5}$$

where the turbulent eddy viscosity K_m is:

$$K_m = C\tilde{\Delta}^2 |\tilde{S}|, \tag{6}$$

the resolved-scale strain tensor is defined as

$$\tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \tag{7}$$

and $|\tilde{S}| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$ is the magnitude of $\tilde{S}_{ij}$. The model coefficient C in equation 6 is determined locally and instantaneously with the dynamic SGS closure developed by Germano et al. (1991) and modified by Lilly (1992).

The dimensions of the computational domain in the streamwise, spanwise and wall-normal directions are, respectively, $l_x = 6H$, $l_y = 3H$ and $l_z = 2H$, H being the boundary layer depth. The Reynolds number based on the friction velocity and the boundary layer depth is $Re = 15040$. The grid is uniform in the xy-planes and stretched in the z-direction by a hyperbolic tangent function. The grid spacings are $\Delta_x = 0.083H$, $\Delta_y = 0.083H$ and $0.0025H < \Delta_z < 0.083H$.

The no-slip boundary condition is applied at the wall. On the top of the domain and in the spanwise direction the mirror free-slip and the periodic boundary conditions are applied, respectively. In the streamwise direction, at the end of the domain the wave-radiation open boundary condition is used (Klemp and Wilhelmson, 1978) in order to allow waves in the interior of the domain to pass out freely through the boundary with minimal reflection. At the beginning of the domain, in the streamwise direction forcing is applied. The data set is obtained from the experimental results of Fackrell and Robins (1982).

The motion of fluid particles is computed by solving the following equation:

$$\frac{dx_i}{dt} = v_i \tag{8}$$

x_i is the position and v_i is the Lagrangian velocity of the fluid particle, given by:

$$v_i(t) = \tilde{u}_i(\vec{x}(t)) + v'_i(t) \tag{9}$$

This velocity is considered to have an Eulerian large-scale part $\tilde{u}_i(\vec{x}(t))$ (which is known) and a fluctuating SGS contribution $v'_i(t)$, which is not known and will be modeled by the stochastic model described in the following section. The Lagrangian large-scale velocities are obtained by an interpolation procedure. We used a tri-linear quadratic Lagrange interpolation method with 27 nodes. The time-integration of equation 8 is performed using a second-order Runge-Kutta method. At the boundaries, in the x-direction, particles that move out of the domain are re-introduced at the source, in the y-direction they are re-introduced using the periodic boundary conditions. Particles that reach the ground rebound respecting symmetric conditions.

SUBGRID LAGRANGIAN STOCHASTIC MODEL

The movement of fluid elements containing a scalar at a subgrid level is given by a three-dimensional Langevin model:

$$\begin{cases} dv_i = \left(\gamma_i(\vec{x},\vec{v},t) + \alpha_{ij}(\vec{x},t)\left(v_j - \tilde{u}_j\right)\right)dt + \beta_{ij}(\vec{x},t)d\eta_j(t) \\ dx_i = v_i dt \end{cases} \tag{10}$$

where $d\eta_j$ is the increment of a vector-valued Wiener process with zero mean, $\langle d\eta_j \rangle = 0$, and variance dt, $\langle d\eta_i d\eta_j \rangle = dt\delta_{ij}$. The fluid particle velocity is given by a deterministic part $\gamma_i + \alpha_{ij}v'_j$ and by a completely random part $\beta_{ij}d\eta_j$. Within the deterministic term, γ_i stands for the large-scale velocity contribution, while $\alpha_{ij}v'_j$ stands for the fluctuating SGS velocity of the fluid particle. The coefficients α_{ij}, β_{ij} and γ_i are determined by the following analysis. Their expressions are given by the equations 17, 18 and 19.

Since $\vec{v}(t)$ is Markovian, the Lagrangian subgrid PDF of the fluid velocity $\mathcal{P}_{\mathcal{L}}(\vec{v},t)$ satisfies a Fokker-Planck equation:

$$\begin{aligned} \frac{\partial \mathcal{P}_{\mathcal{L}}(\vec{v},t)}{\partial t} &= -\frac{\partial}{\partial v_l}\left[\left(\gamma_l + \alpha_{lm}(v_m - \tilde{u}_m)\right)\mathcal{P}_{\mathcal{L}}(\vec{v},t)\right] \\ &+ \frac{1}{2}\frac{\partial^2}{\partial v_l \partial v_m}\left(\beta_{lk}\beta_{mk}\mathcal{P}_{\mathcal{L}}(\vec{v},t)\right) \end{aligned} \tag{11}$$

By integrating this equation all the subgrid statistical moments of $\vec{v}(t)$ can be obtained. The local Lagrangian mean and variance write as:

$$\frac{d\bar{v}_i}{dt} = \delta_{il}\gamma_l + \delta_{il}\alpha_{lm}(\bar{v}_m - \tilde{u}_m) \tag{12}$$

$$\frac{d\overline{v_i^2}}{dt} = 2\gamma_i\bar{v}_i + 2\alpha_{im}(\overline{v_m v}_i - \bar{v}_m\tilde{u}_i) + \beta^2_{ik} \tag{13}$$

The coefficients of the stochastic model, α_{ij}, β_{ij} and γ_i, are determined by relating the subgrid statistical moments of $\vec{v}(t)$ to the filtered Eulerian moments of the fluid velocity. Here, we proceed by analogy with van Dop et al. (1986) who developed this approach in the case of a classic Reynolds averaged decomposition. By introducing a subgrid Eulerian PDF $\mathcal{P}_{\mathcal{E}}(\vec{u},t)$

$$\bar{u}_i(\vec{x},t) = \int_{-\infty}^{+\infty} u_i(\vec{x},t)\mathcal{P}_{\mathcal{E}}(\vec{u};t)du_i \tag{14}$$

and by assuming that at a mesh level $\mathcal{P}_{\mathcal{L}}(\vec{v},t)$ and $\mathcal{P}_{\mathcal{E}}(\vec{u},t)$ are equivalent, the subgrid Lagrangian mean fluid velocity, at a given position and at a given time is supposed equal to the filtered Eulerian fluid velocity given by the filtered Navier-Stokes equations:

$$\overline{v^n}_i(t_o) = \widetilde{u^n}_i(\vec{x}_o) \tag{15}$$

and

$$\left(\frac{d\overline{v^n}_i}{dt}\right)_{t=t_o} = \left(\frac{d\widetilde{u^n}_i}{dt}\right)_{\vec{x}=\vec{x}_o} \tag{16}$$

Finally, knowing that the subgrid turbulence is homogeneous and isotropic (basic assumption of the LES), the coefficients of the stochastic model are given by:

$$\alpha_{im} = \frac{3}{2\tilde{k}}\left(\frac{1}{3}\frac{d\tilde{k}}{dt} - \frac{C_0\tilde{\varepsilon}}{2}\right)\delta_{im} \tag{17}$$

$$\beta_{ik} = \sqrt{C_0\tilde{\varepsilon}}\delta_{ik} \tag{18}$$

$$\gamma_i = \frac{\partial\tilde{u}_i}{\partial t} + \frac{\partial(\tilde{u}_i\tilde{u}_j)}{\partial x_j} + \frac{\partial\tau^r_{ij}}{\partial x_j} \tag{19}$$

where $\tilde{k}$ is the subgrid turbulent kinetic energy, $\tilde{\varepsilon}$ is the subgrid turbulent dissipation rate and C_0 is the Lagrangian constant. The fluid velocity given by the modified Langevin model writes as:

$$\begin{aligned} dv_i &= \left[\frac{\partial\tilde{u}_i}{\partial t} + \frac{\partial(\tilde{u}_i\tilde{u}_j)}{\partial x_j} + \frac{\partial\tau^r_{ij}}{\partial x_j}\right. \\ &+ \left.\frac{3}{2}\frac{v_i - \tilde{u}_i}{\tilde{k}}\left(\frac{1}{3}\frac{d\tilde{k}}{dt} - \frac{C_0\tilde{\varepsilon}}{2}\right)\right] dt \\ &+ \sqrt{C_0\tilde{\varepsilon}}\,\eta(t)dt \end{aligned} \tag{20}$$

The large-scale velocity of the fluid particle is directly computed by the LES with the dynamic Smagorinsky-Germano SGS model. In order to determine the SGS contribution (α_{ij} and β_{ik}) we need to resolve an additional transport equation for $\tilde{k}$. This equation is deduced from Deardorff (1980).

$$\frac{\partial\tilde{k}}{\partial t} + \tilde{u}_j\frac{\partial\tilde{k}}{\partial x_j} = \frac{K_m}{3}\frac{g}{\theta_0}\frac{\partial\tilde{\theta}}{\partial z} + 2K_m\tilde{S}^2_{ij} + 2\frac{\partial}{\partial x_j}\left(K_m\frac{\partial\tilde{k}}{\partial x_j}\right) + \tilde{\varepsilon} \tag{21}$$

where $\tilde{\varepsilon} = C_\varepsilon\tilde{k}^{3/2}/\tilde{\Delta}$. The terms on the right-hand side of equation 21 correspond to the production by buoyancy, the production by shear, the diffusion of $\tilde{k}$ and the dissipation. Since we are interested in neutral flows the potential temperature variation is neglected. The turbulent eddy viscosity K_m is computed by a dynamic procedure as described in the previous section.

THE DIFFUSION MODEL

In order to take diffusion into account a deterministic, continuous in time pairing particle exchange model is used. A full description of this model can be found in Michelot (1996) or in Simoëns et al. (1997). We will resume here only the main aspects.

The domain is divided in boxes that are small compared to the length scale of the flow (Pope, 1985). In each box, at each time step, particles are randomly selected by pairs. For each pair (m, n), the particle concentrations $c_m(t)$ and $c_n(t)$ will evolve according to:

$$\begin{cases} \dfrac{dc_m(t)}{dt} = \psi\left(c_n(t) - c_m(t)\right) \\ \dfrac{dc_n(t)}{dt} = \psi\left(c_m(t) - c_n(t)\right) \end{cases} \tag{22}$$

ψ is a relaxation coefficient. From a theoretical analysis ψ is chosen so that the PDF p_c of the concentration tends to a Gaussian function in isotropic turbulence. As suggested by Spalding (1971), ψ can be expressed as $\psi = \xi/T_{diff}$, where ξ is a random number between -1 and 1, and the diffusion time T_{diff} can be written as $T_{diff} = T/C_{diff}$, with C_{diff} a constant and T the time scale of the velocity fluctuations defined as $T = k/\varepsilon$. Pope (1985) explained that C_{diff} has to be adjusted with the relaxation of the standard deviation of the concentration level σ_c. Even though Pope (1985) suggested a value of 2, Michelot (1996) proposed a value of 2.25 as more appropriate.

MODEL PREDICTIONS AND DISCUSSION

Description of the simulated experiment

A full description of the experimental facility and results can be found in Fackrell and Robins (1982). Here, the main characteristics of the experiment necessary for understanding the simulations are given.

A turbulent boundary layer over a rough wall is generated in an open-circuit wind tunnel. A plume from a point source at $z_s/H = 0.19$ is studied. The elevated source has a 8.5mm diameter and it emits at the average velocity of the flow over its height. The source gas consists only of a neutrally buoyant mixture of propane and helium. The former is used as a trace gas for concentration measurements. Fackrell and Robins (1982) measured the mean concentration, the concentration fluctuations and the fluxes in the passive scalar plume.

Velocity field

The height H of the turbulent boundary layer is 1.2m and the roughness length is $z_0/H = 2.4\times10^{-4}$. The mean velocity at the boundary layer edge U_e is 4m/s and the friction velocity $u_*/U_e = 0.047$. Figures 1 and 2 show predicted profiles of mean velocity and turbulent kinetic energy compared with the experimental data of Fackrell and Robins (1982) and the LES of Sykes and Henn (1992). In order to obtain the correct mean velocity and turbulence levels, Sykes and Henn (1992) used the roughness length as an adjustable parameter. For the profiles presented here they set the roughness length, z_0, to $2\times10^{-3}H$. The mean values are obtained by averaging the fluctuating field over the horizontal extent of the domain and also over a time period sufficiently long to obtain stable statistics. The LES resulted in a fairly accurate prediction of the mean velocity.

For the turbulent kinetic energy the SGS part, the resolved part and the total of the calculated field are separated. The SGS contribution $\tilde{k}$ is obtained from equation 21. We note that the SGS part is small compared to the total turbulent kinetic energy, except near the wall. Most of the turbulent kinetic energy has been resolved by the LES. The agreement between the numerical results and the measurements is quite good, however, the LES shows discrepancies near the wall, where the fluctuations are mostly parameterized.The parameterization of the small-scale statistics gives an overestimation of the turbulent kinetic energy and the velocity fluctuation variances at the wall compared to the results of Sykes and Henn (1992). Probably, the increasing anisotropy near the wall is not correctly represented by our correction. In this study, we only consider elevated releases, at $z = 0.19H$, where the simulated turbulence is largely resolved and in close agreement with the observations.

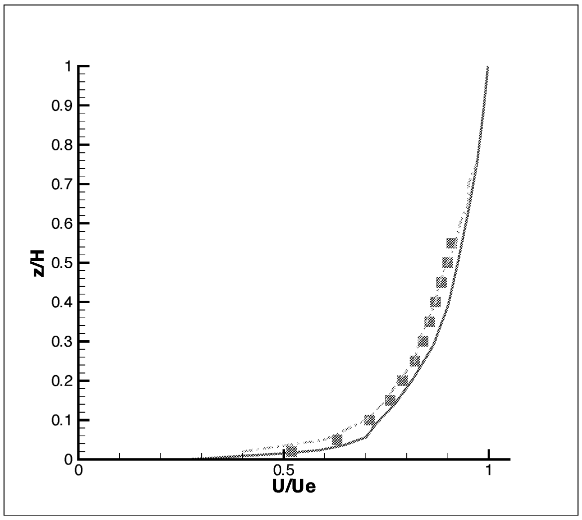

Figure 1: Vertical profile of streamwise mean velocity. Line - LES; Dashed-dotted - LES of Sykes and Henn (1992); Squares - measurements of Fackrell and Robins (1982).

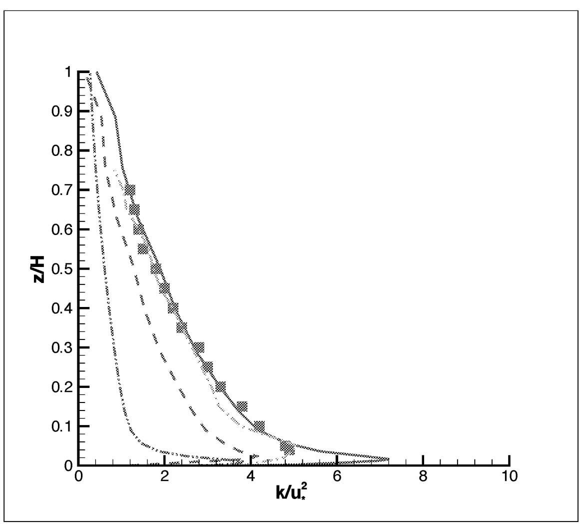

Figure 2: Vertical profile of turbulent kinetic energy. Lines LES: Broken line - resolved; Chain - sub-grid; Full line - total; Dashed-dotted - total of Sykes and Henn (1992); Squares - measurements of Fackrell and Robins (1982).

Mean concentration field

The vertical profile of mean concentration at $z/H = 2.88$ from the source is shown on figure 3. The computed concentration profile is in good agreement with the experimental results, except near the wall. This is probably due to the unresolved nature of the turbulence near the wall.

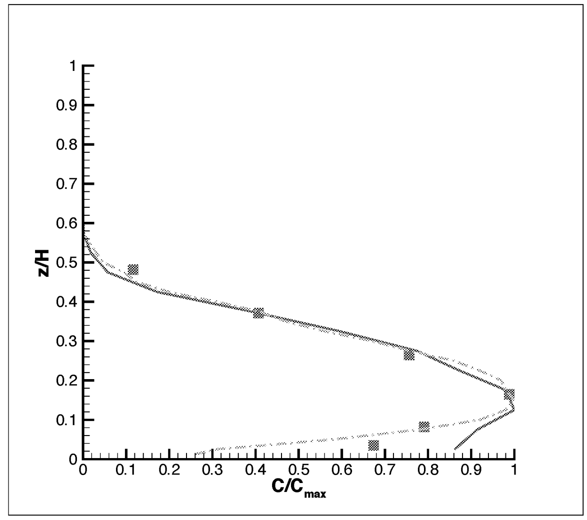

Figure 3: Vertical profiles of mean concentration at $x = 2.88H$. Line - LES; Dashed-dotted - total of Sykes and Henn (1992); Squares - measurements of Fackrell and Robins (1982).

Concentration fluctuations

The vertical profile of the concentration fluctuation variance, $\overline{c^2}$, normalized by its maximum value is illustrated in figure 4, showing close agreement with the experimental data. However, for the same reason as for the mean concentration profile, the concentration fluctuation is overestimated at the ground.

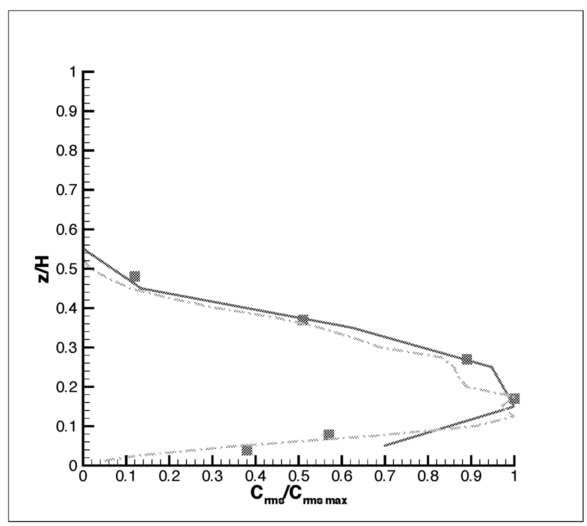

Figure 4: Vertical profiles of mean-square concentration at $x = 2.88H$. Line - LES; Dashed-dotted - total of Sykes and Henn (1992); Squares - measurements of Fackrell and Robins (1982).

Skewness and kurtosis

In figure 5 the flatness coefficient of the concentration PDF is plotted against the skewness coefficient. The collapse of the data for five different downstream distances from the source is remarkable. The profiles have a parabolic form as clearly seen with the best fit quadratic curve. This fact was previously supported by Mole and Clark (1995) and Chatwin and Sullivan (1990) for scalar dispersion in turbulent shear flows. They reported that for all probability distributions, the skewness coefficient S and the flatness coefficient K should verify the relation $K \geq S^2 + 1$, the equality being verified only in the case when the sample space consists of exactly two discrete values i.e. without any molecular diffusion. The numerical results are slightly greater than $K = S^2 + 1$ because diffusion is taken into account in our modeling.

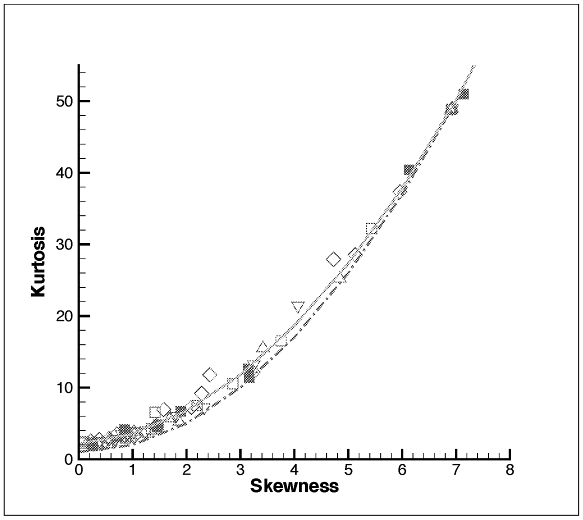

Figure 5: Profiles of the flatness coefficient K of concentration as a function of skewness coefficient S. Symbols: LES; Full square - $x/H = 0.96$; Triangle - $x/H = 1.92$; Triangle (down) - $x/H = 2.88$; Square - $x/H = 3.83$; Diamond - $x/H = 4.79$. Line - best fitted quadratic curve. Dashed-dotted - $S^2 + 1$

Concentration fluxes

Figure 6 shows the mass flux profile, $\overline{wc}$, at $x = 2.88H$. In the figure C_{max} is the local maximum concentration for each profile. The evolution of the profile shapes is in good agreement with the experimental data. The flux profiles develop from being antisymmetric about the source height near the source, toward a ground-level source profile.

CONCLUSION

A LES coupled with a Lagrangian stochastic model has been applied to the study of passive scalar dispersion downwind of a localized source of contaminant. Fluid particles are tracked in a Lagrangian way. The Lagrangian velocity of each fluid particle is considered to have a large-scale part and a small-scale part at a subgrid level. The subgrid movement of fluid elements containing scalar is given by a three-dimensional Langevin model using the filtered SGS statistics in inhomogeneous turbulence. The results of the computations are compared with the wind-tunnel experiments of Fackrell and Robins (1982) and with the LES of Sykes and Henn (1992) who used an Eulerian approach with a non dynamic SGS model. Discrepancies near the lower wall are due to the fact that turbulence in this region is modeled rather than resolved.

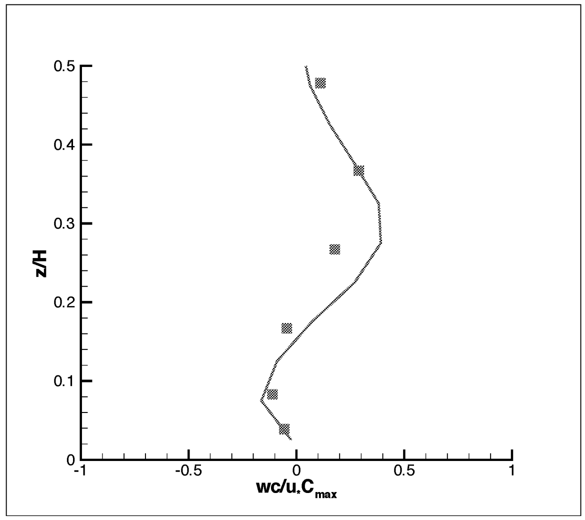

Figure 6: Vertical profiles of vertical scalar flux, $\overline{wc}$ at $x = 2.88H$. Line - LES; Dashed-dotted - total of Sykes and Henn (1992); Squares - measurements of Fackrell and Robins (1982).

The LES coupled with the Lagrangian stochastic model provides good description of the plumes from elevated sources. Vertical profiles of mean concentration, concentration fluctuation variances and scalar fluxes match well with the experimental profiles.

Chemical reactions can be easily included without additional scalar equations and only by attributing initially different scalar species to each fluid particle. Improvement of the LES would noticeably improve the concentration levels at the wall. Further developments will include the anisotropy of the flow near the surface in the stochastic model.

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