SUBGRID-SCALE MODELING OF VELOCITY AND PASSIVE SCALAR FOR THE LARGE-EDDY SIMULATION OF NON-HOMOGENEOUS TURBULENT FLOWS

Y. Favre¹, H. Touil², G. Balarac¹ and E. Léveque²

¹ Grenoble-INP / CNRS / UJF-Grenoble 1, LEGI UMR 5519, Grenoble, F-38041, France
² Laboratory of Physics, Ecole normale supérieure de Lyon / CNRS / University of Lyon
46 Allée d’Italie, 69364 Lyon cedex 7, France.
E-mail: guillaume.balarac@grenoble-inp.fr, emmanuel.leveque@ens-lyon.fr

Abstract. Subgrid-scale modeling that relies on the separation between the mean and the fluctuating part of a turbulent field is introduced in the context of large-eddy simulations of non-homogeneous turbulent flows. Subgrid-scale models are proposed explicitly for both the velocity and passive scalar fields. Performances are examined, and comparisons are made with the classic and dynamic Smagorinsky models for the simulation of a temporal turbulent jet.

1. Introduction

In the large-eddy simulation (LES) of a turbulent flow, the mesh resolution is dramatically depreciated so that only the large-scale motions are resolved numerically. This is physically justifiable since large-sized eddies contain most of the kinetic energy, and their strength make them the efficient carriers of momentum, heat, mass, etc. On the contrary, small-sized eddies are mainly responsible for dissipation and contribute little to transport. Avoiding the numerical integration of small-scale motions is therefore desirable in most situations. The actual large-scale motions are solutions of the flow equations, e.g. the Navier-Stokes equations, supplemented by an unknown term accounting for the stress exerted by the unresolved subgrid-scale (SGS) excitations on the simulated flow. A common thread to it consider that this stress is essentially responsible for diffusion at grid scale, which in turn calls for the modeling of an additional SGS viscosity and, possibly, SGS diffusivities for the fields of temperature, concentration of species, etc. Unlike the constant-property molecular diffusion coefficients, the SGS viscosity and diffusivities are here space-and-time-dependent quantity that are closely related to the nature of turbulent motions. In the context of engineering flows, which may experience unsteady events such as shear-layer mixing, vortex shedding or external disturbances (e.g., a blade in a turbine), the modeling of these quantities is recognized to be a difficult problem.
2. Subgrid-scale modeling

Our approach is rooted in the idea that the SGS modeling of a turbulent field, e.g. the velocity field or a passive-scalar field, should distinguish between the mean (in the statistical sense) and fluctuations. Such splitting, which is, to some extent, reminiscent of the Reynolds decomposition, has already been examined in the past, mainly on the basis of phenomenological arguments (Schumann, 1975). Recently, we have managed to connect it analytically to the scale-by-scale energy budget of locally homogeneous shear flows (Lévéque et al., 2007), therefore removing some empiricism in the SGS modeling. For the velocity field, these developments have lead to a shear-improved Smagorinsky model (SISM), which has already been validated in various flow configurations (Toschi et al., 2006; Saha & Biswas, 2010; Caluzac et al., 2010). In the SISM, the SGS viscosity expresses as

\[ \nu_{sgs}(x, t) = (C_s \Delta)^2 \left( |\mathbf{s}(x, t)| - |\langle \mathbf{s}(x, t) \rangle| \right), \]

where \( C_s \) is the Smagorinsky constant for homogeneous and isotropic turbulence, \( \Delta \) is the local grid resolution and \( \mathbf{s}(x, t) \) is the resolved rate-of-strain tensor. Importantly, the correcting term to the Smagorinsky viscosity, \( |\langle \mathbf{s}(x, t) \rangle| \), is the norm of the rate-of-strain tensor of the mean flow.

The SISM accommodates to the effects pertaining to the presence of strong shear by reducing significantly the value of the Smagorinsky viscosity in that situation, whereas the standard Smagorinsky model is recovered in the bulk. Interestingly, the SISM does not call for any adjustable parameter besides \( C_s = 0.18 \), which is fixed for all flows. There is no need for \textit{ad hoc} damping function. The SISM does not use any kind of dynamic adjustment either. The simplicity and the manageability of the original Smagorinsky model are therefore preserved; this is a valuable quality of the shear-improved Smagorinsky model.

It is now our motivation to extend this approach to a turbulent passive-scalar field, e.g. the temperature field, \( \theta(x, t) \). The scale-by-scale scalar-variance budget implies that the mean flux (of scalar-variance) across scale \( \Delta \) should behave as

\[ F_{\theta}(\Delta, x, t) \sim \Delta^2 \left( |\nabla \theta'(x, t)|^2 \cdot |\mathbf{s}(x, t)| \right), \]

where \( \theta'(x, t) \) denotes the fluctuations of the scalar field at scale \( \Delta \): \( \theta'(x, t) = \langle \theta(x, t) \rangle + \theta'(x, t) \). By definition, the SGS diffusivity associated with the scalar field, \( \chi_{sgs}(x, t) \), satisfies

\[ F_{\theta}(\Delta, x, t) \sim \left\langle \chi_{sgs}(x, t) |\nabla \theta(x, t)|^2 \right\rangle. \]

This yields

\[ \chi_{sgs}(x, t) = (C_\theta \Delta)^2 |\mathbf{s}(x, t)| \cdot \frac{|\nabla \theta'(x, t)|^2}{|\nabla \theta(x, t)|^2}, \]

where \( C_\theta \) is a constant. This latter expression resembles the Smagorinsky SGS diffusivity, except for the ratio \( |\nabla \theta'(x, t)|^2/|\nabla \theta(x, t)|^2 \). In regions of homogeneous and isotropic turbulence, \( \chi_{sgs}(x, t) \) reduces consistently to the Smagorinsky model, \( \chi_{sgs}(x, t) = (C_\theta \Delta)^2 |\mathbf{s}(x, t)| \), since \( |\nabla \theta'(x, t)|/|\nabla \theta(x, t)| \approx 1 \). On the contrary, in regions of strong mean scalar gradients, the Smagorinsky prediction is significantly decreased since \( |\nabla \theta'(x, t)|/|\nabla \theta(x, t)| \ll 1 \). Assuming that \( \nu_{sgs}/\chi_{sgs} = 0.6 \) in homogeneous and isotropic turbulence (Métais & Lesieur, 1992), \( C_\theta \) is fixed at \( C_s/0.6 \approx 0.3 \).
Figure 1. DNS results: (a) isosurfaces of positive $Q$ colored by the tangential vorticity to illustrate the development of Kelvin-Helmholtz vortices in the first stage of the transition; (b) isosurfaces of positive $Q$ colored by the axial vorticity to illustrate the development of streamwise vortices at the end of the potential core; (c) spectra of the scalar variance in the middle of the shear layer for $Sc = 5$ (solid line), $Sc = 0.75$ (dashed line) and $Sc = 0.1$ (dotted line). The turbulent kinetic energy spectrum is also shown (bold line).

3. Large-eddy simulation of a temporal jet

The proposed SGS models are now compared with the standard Smagorinsky model (SSM) and the dynamic Smagorinsky model (DSM) (Germano et al., 1991; Moin et al., 1991). For this purpose, simulations of a temporal planar jet are performed by using a pseudo-spectral code. The computational domain is cubic and periodic in the three directions, and its size is four times the initial jet width, $h$. The initial field is generated by super-imposing divergence-free random fluctuations to a mean “hyperbolic tangent” velocity profile. A passive-scalar is seeded in the jet with the same “hyperbolic tangent” profile to investigate the SGS modeling of the mixing: $\theta = 1$ in the jet and 0 elsewhere. The Reynolds number is $Re_h = Uh/\nu_{mol} = 3200$ and three different Schmidt numbers are considered: $Sc = \nu_{mol}/\chi_{mol} = 0.1, 0.75$ and 5. The mean values entering in the modeling of $\nu_{sgs}(x,t)$ and $\chi_{sgs}(x,t)$ are estimated by averaging spatially over homogeneous directions (perpendicular to the jet axis).

Figures 1 (a) and (b) show the evolution of the coherent vortices at two distinct instants of the turbulent jet transition. The coherent vortices are shown by isosurfaces of positive $Q$. We recall that $Q$ is the second invariant of the velocity gradient tensor and it is recognized as a good indicator of coherent vortices in the flow (Dubief & Delcayre, 2000). The beginning of the transition towards a fully turbulent state is first characterized by the emergence of Kelvin-Helmholtz vortices, both at the upper and lower shear layers (Fig. 1 (a)), and is followed by the appearance of pairs of streamwise vortices connecting each two consecutive pairs of Kelvin-Helmholtz rollers (Fig. 1 (b)). These transition mechanisms are well described in previous studies (da Silva & Pereira, 2004). Figure 2 shows contours of the scalar values for different Schmidt number values to illustrate the mixing process. In the early transition stage, the mixing process is dominated by molecular diffusion. Later, the turbulent mixing process combines radial pulsations caused by the Kelvin-Helmholtz vortices and fluid ejection caused by the counter-rotating streamwise vortice. Note that the range of excited scalar scales depends on the molecular diffusivity value. Figure 1 (c) shows the scalar variance spectra for different Schmidt numbers. Thus, for a very diffusive scalar (small Schmidt number), the small scales
fluctuations are damped, which limits the development of high-scalar gradient. Conversely, for high Schmidt numbers, scalar scales can be smaller than the velocity scales. The scalar SGS modeling should be able to account for these effects related to value of the Schmidt number (Brun et al., 2008).

### 3.1. A priori computation of the subgrid-scale viscosity and diffusivity

A priori tests are first carried out, i.e. $\nu_{sgs}(x,t)$ and $\chi_{sgs}(x,t)$ are evaluated from the filtered DNS data (with resolution $256^3$). The mean values of these SGS predictions are compared directly with

$$
\langle \nu_{sgs} \rangle = -\frac{1}{2} \frac{\langle \tau_{ij} S_{ij} \rangle}{\langle S_{ij} S_{ij} \rangle} \quad \text{and} \quad \langle \chi_{sgs} \rangle = -\frac{\langle T \frac{\partial \theta}{\partial x_i} \frac{\partial \theta}{\partial x_j} \rangle}{\langle \frac{\partial \theta}{\partial x_i} \frac{\partial \theta}{\partial x_j} \rangle}
$$

obtained from DNS. Comparisons are shown at the end of the potential core in Figure 3. The filter width $\Delta$ is equal to $4 \cdot \Delta_{DNS}$ (the cut-off wave number is $k_c \approx 50$). Note that, in this region and for this filter width, the SGS viscosity is of the order of the molecular viscosity, indicating that the SGS modeling is truly effective. As expected, SSM is too dissipative with an over-prediction of the SGS viscosity and diffusivity. DSM and SISM largely limit this over-prediction.
for the SGS viscosity, whereas the improvement is more moderate for the SGS diffusivity. For all models (including DSM), the over-prediction of the SGS diffusivity increases with the Schmidt number.

3.2. A posteriori tests: DNS for the velocity field and LES for the scalar field

A posteriori tests are now performed. At first, only the scalar field is solved by LES. The velocity field is solved by DNS, filtered and used to integrate the LES scalar-transport equation. This allows us to examine the performance of the SGS scalar-flux modeling without taking into account the modeling of the SGS Reynolds stress tensor. Figure 4 compares the resolved scalar variance with the filtered scalar variance extracted from the DNS. As expected from previous a priori tests, SSM underestimates the scalar variance due to an over-estimation of the SGS diffusivity. DSM and SISM limit this under-prediction but significant differences appear with DNS as the Schmidt number increases, i.e. when the SGS modeling becomes predominant in the scalar dynamics.

3.3. A posteriori tests: LES for the velocity and scalar fields

Finally, full LES (for velocity and scalar fields) are performed. First, Figure 5 (a) compares the resolved turbulent kinetic energy profiles computed with each model with the filtered turbulent kinetic energy extracted from the DNS. SSM strongly under-predicts the resolved turbulent kinetic energy, whereas DSM and SISM lead to a much better prediction. Figure 6 illustrates the coherent vortices by isosurfaces of positive $Q$ for the different LES. The result is compared with coherent vortices given by the filtered DNS. The over-prediction of the dissipation provided by SSM limits the coherent vortices development. Conversely, DSM and SISM allow for a correct development of the coherent vortices.

Concerning the scalar dynamics, Figure 5 (b)-(d) displays the scalar variance profiles for different Schmidt numbers. The results are very comparable to those described in 3.2.1, indicating that the velocity field is suitably resolved in the LES. Indeed, a strong under-prediction of the scalar variance is found for SSM, whereas DSM and SISM yields a correct behavior of the scalar variance. Note that significant differences appear with DNS results as the Schmidt number increases. This is also shown by scalar variance spectrum (Fig. 7). Indeed, SSM leads to a large under-prediction of the scalar “energy” for the smallest resolved scales, whereas DSM and SISM limit this excessive scalar dissipation. However, discrepancies with the DNS scalar
Figure 5. Resolved turbulent kinetic energy (a) and scalar variance profiles for $Sc = 0.1$ (b), $Sc = 0.75$ (c) and $Sc = 5$ (d) computed from LES results for both velocity and scalar fields: filtered DNS (symbol); SSM (dotted line); DSM (dashed line); SISM (solid line).

Figure 6. Isosurface of positive $Q$ colored by the axial vorticity at the end of the potential core: filtered DNS (a); SSM (b); DSM (c); SISM (d).
Figure 7. Scalar variance spectrum for $Sc = 0.1$ (a), $Sc = 0.75$ (b) and $Sc = 5$ (c) computed from LES results for both velocity and scalar fields: DNS (bold line); SSM (dotted line); DSM (dashed line); SISM (solid line).

Table 1. Cost in CPU time of each simulation relying on different SGS modeling; SSM is taken as the reference.

| Schmidt number: $Sc$ | SSM | DSM | SISM | DNS |
|----------------------|-----|-----|------|-----|
| 0.1                  | 1   | 1.6 | 1.1  | 130 |
| 0.75                 | 1   | 1.7 | 1.15 | 129 |
| 5                    | 1   | 1.7 | 1.1  | 129 |

The variance spectrum is more important for higher values of the Schmidt number.

All these comparisons indicate that DSM and SISM behave roughly similarly in terms of accuracy. However, Table 1 compares the cost in CPU time of each simulation and shows some differences. Considering that SISM is about 30% faster than DSM (in our computations), this former appears as an interesting alternative to DSM in terms of computational cost.

4. Conclusion

New variants of the Smagorinsky model are introduced to close the velocity and scalar filtered transport equations. These variants appear to be interesting alternatives to the classic dynamic procedure in terms of accuracy and computational cost. The regime of high Schmidt numbers definitively requires further improvements in the SGS modeling.

Acknowledgments

YF and GB are supported by the Agence Nationale pour la Recherche (ANR) under Contract No. ANR-2010-JCJC-091601. Most computations have been performed by using the local computing facilities (PSMN) at Ens-Lyon under grant CPER-CIRA (2007-2013).

References

Schumann, U.: Subgrid scale model for finite difference simulations of turbulent flows in plane channels and annuli J. Comput. Phys. 18:376-404, 1975.

Lévêque, E., Toschi, F., Shao, L. and Bertoglio, J.-P.: Shear-improved Smagorinsky model for large-eddy simulation of wall-bounded turbulent flows J. Fluid Mech. 570:491, 2007.
Toschi, F., Kobayashi, H., Piomelli, U. and Iaccarino, G.: Backward-facing step calculations using the shear-improved smagorinsky model *Proceedings of the Summer Program 2006* 570:491, CTR, Standford, USA.

Saha P. and Biswas G.: Assessment of a shear-improved subgrid stress closure for turbulent channel flows *Int. J. Heat and Mass Transfer* 53(21-22):4789, 2010.

Cahuzac, A., Boudet, J., Borgnat, P. and Lévêque, E.: Smoothing algorithms for mean-flow extraction in large-eddy simulation of complex turbulent flows *Phys. Fluids* 22:125104, 2010.

Métais, O. and Lesieur, M.: Spectral large-eddy simulation of isotropic and stably stratified turbulence *J. Fluid Mech.* 239:157, 1992

Germano, M., Piomelli, U., Moin, P. and Cabot, W. H.: A dynamic subgrid-scale eddy viscosity model *Phys. Fluids A* 3:1760-1765, 1991

Moin, P., Squires, K., Cabot, W. and Lee, S.: A dynamic subgrid-scale model for compressible turbulence and scalar transport *Phys. Fluids A* 3:2746-2757, 1991

Dubief, Y. and Delcayre, F.: On coherent-vortex identification in turbulence *J. Turbulence* 1, 2000

da Silva, C. B. and Pereira, J.C.F.: The effect of subgrid-scale models on the vortices obtained from large-eddy simulations *Phys. Fluids* 16:4506, 2004.

Brun, C., Balarac, G., da Silva, C. B. and Métais, O.: Effects of molecular diffusion on the subgrid-scale modelling of passive scalars *Phys. Fluids* 20:025102, 2008.