

# Large-eddy simulations based on transported subgrid-scale energy

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## Abstract

In large-eddy simulations (LES) the large or grid scales (GS) which are responsible for the most important transfers of mass, momentum and heat are explicitly calculated while the effect of the small scales is modelled by a subgrid-scale (SGS) model. In many flow simulations the small scales of motion are statistically close to isotropic, carry a relatively small amount of the total kinetic energy, and adjust almost immediately to the dynamics of the large scales. However, in many engineering and Natural flows the isotropic assumption of the small scale motions is not observed, even at very high Reynolds numbers, particularly for the passive scalar field [1]. Furthermore, in many LES the SGS motions do possess a significant part of the total kinetic energy [2]. Moreover, for high Reynolds numbers and/or coarse meshes the SGS motions need a non-negligible time to adjust to local unsteadiness from the large scales *i.e.* the *local equilibrium assumption* between the large and small scales of motion - which is used in the great majority of SGS models - is not observed [3, 4].

One way to overcome these limitations, by discarding the *local equilibrium assumption*, consists in developing SGS models based on the transport equation of the SGS kinetic energy [5, 6, 7, 8, 9, 10]. The use of a transport equation for the SGS kinetic energy is interesting also to many hybrid RANS/LES and URANS/LES modelling strategies [11, 12, 13]. Similarly, in LES involving a passive or active scalar field several new unclosed terms arise, and one way to deal with these unknown terms is to solve an additional SGS scalar variance transport equation. For example, in LES of reacting flows the variance of the mixture fraction is very important and therefore some combustion models use an additional transport equation for the variance of the SGS mixture fraction [14].

The study of transport equations for the SGS kinetic energy and SGS scalar variance is thus of great relevance since in LES most of the terms from these equations are unknown and have to be modelled. This presentation focusses in the development of SGS models

based on modeled transport equations for the SGS kinetic energy and SGS scalar variance, by addressing three (3) topics.

We start by analyzing the physical mechanisms associated with the dynamics of the SGS kinetic energy. The most intense kinetic energy exchanges between GS and SGS occur near the large flow structures and not randomly in space (Fig. 1). The GS kinetic energy is dominated by GS advection and GS pressure/velocity interactions, while the GS/SGS diffusion plays an important role to the local dynamics of both GS and SGS kinetic energy. The so-called *local equilibrium assumption* holds globally but not locally as most viscous dissipation of SGS kinetic energy takes place within the vortex cores whereas forward and backward GS/SGS transfer occurs at quite different locations (Fig. 2). Finally, it is shown that SGS kinetic energy advection may be locally large as compared to the other terms of the SGS kinetic energy transport equation [3, 4].

Next we address the effect of the existing SGS models on the vortices obtained from classical SGS models. One way to assess this issue, consists in analyzing the transport equation for the resolved enstrophy. Special emphasis is placed on the *enstrophy SGS dissipation term*, which represents the effect of the SGS models on the vortices computed from LES. When the filter is placed in the inertial range region the evolution of the vorticity norm is governed by the enstrophy production and enstrophy SGS dissipation, which represents, in the mean, a sink of resolved enstrophy. Thus the coherent vortices obtained from LES are subjected to an additional (nonviscous) dissipation mechanism. Extensive tests are conducted using several SGS models in order to analyze their ability to represent the enstrophy SGS dissipation. The models analyzed are the Smagorinsky, structure function, filtered structure function, dynamic smagorinsky, gradient, scale similarity, and mixed. It is shown, using both DNS and LES that the Smagorinsky, structure function, and mixed models cause excessive vorticity dissipation compared to the other models. An estimation of the "vorticity error" and its wave number dependence is given, for each SGS model. Both DNS and LES show that the dynamic Smagorinsky and filtered structure function models seem to be the best suited to a correct prediction of the resolved vorticity field (Fig. 3) [15, 16].

Finally, we discuss SGS models based on transport equations for the SGS kinetic energy and SGS scalar variance. In particular we analyze the modeling of the diffusion and dissipation terms. In virtually all models using these equations, the diffusion terms are lumped together, and their joint effect is modeled using a "gradient-diffusion" model. It is shown that provided the implicit grid filter from the LES is in the dissipative range the diffusion terms pertaining to the SGS kinetic energy and SGS scalar variance transport equations are well represented by a gradient-diffusion model. However, this situation changes dramatically for both equations when considering inertial range filter sizes and high Reynolds numbers. The reason for this lies in part in a loss of local balance between the SGS turbulent diffusion and diffusion caused by GS/SGS interactions, which arises at inertial range filter sizes. Moreover, due to the deficient modeling of the diffusion by SGS pressure-velocity interactions, the diffusion terms in the SGS kinetic energy equation

are particularly difficult to reconcile with the gradient-diffusion assumption. In order to improve this situation, a new model, inspired by Clark's SGS model, is developed for this term. The new model shows very good agreement with the exact SGS pressure-velocity term in a priori tests and better results than the classical model in a posteriori LES tests [17].

By far the greatest challenge for modelling in the transport equations for the SGS kinetic energy and SGS scalar variance comes from the *viscous and the molecular SGS dissipation* terms that represent the final (dissipation) stages of the "energy cascade mechanism" whereby the SGS kinetic energy and SGS scalar variance are dissipated through the action of the molecular viscosity and diffusivity, respectively. We analyze the topology and spatial localisation of the viscous and the molecular SGS dissipation terms, and assess three models currently used for these terms. The models analysed here are the classical model used by *e.g.* Schumann [5] and Yoshizawa [6], the model used in hybrid RANS/LES by Paterson and Peltier [18], and by Hanjalic [19], and the model for the molecular SGS dissipation of SGS scalar variance from Jiménez *et al.* [14]. The classical models for the molecular SGS dissipation give very good results. Moreover, the model constants approach asymptotically the theoretical values as the Reynolds number and filter sizes increases, which supports the use of a constant value in engineering and geophysical applications, instead of using a dynamic procedure for their computation as in Ghosal *et al.* [8]. For the molecular SGS dissipation of SGS scalar variance the model from Jiménez *et al.* [14] performs even better than the classical model and should be the preferred model for this term when the Schmidt number is close to 1.0. Finally, all the tests showed that the models used in hybrid RANS/LES tested here give very poor. The reason behind this is connected with the deficient spectral representation of the exact molecular SGS dissipation term (Fig. 4) [20].

**Keywords:** large eddy simulation (LES), grid/subgrid-scale interactions, LES based on transport equations for the SGS kinetic energy and SGS scalar variance, diffusion and dissipation terms.

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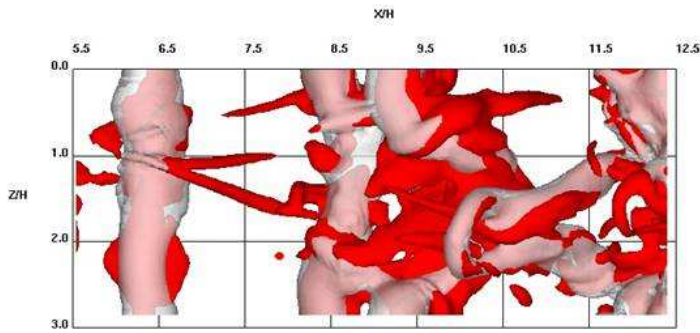


Figure 1: *Illustration of the influence of the flow coherent vortices (grey) on the evolution of the SGS kinetic energy (red) in the far field of a plane jet*

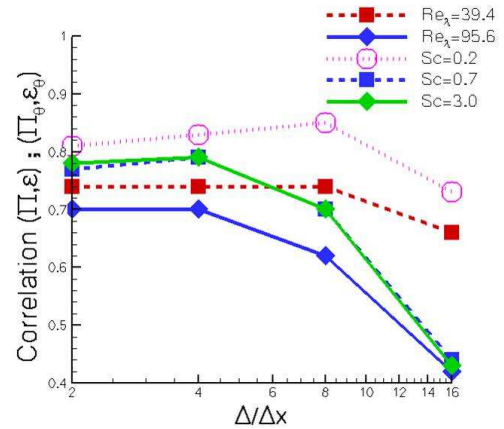


Figure 2: *The failure of the local equilibrium assumption between the kinetic energy transfer into the small scales of motion  $\Pi$  and the viscous dissipation  $\epsilon$ .*

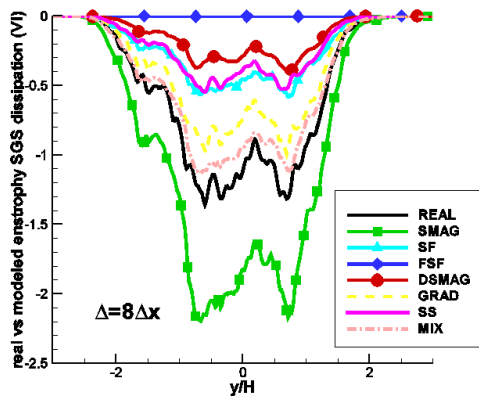


Figure 3: *Comparison between the real and modeled anisotropy SGS dissipation in classical a-priori tests.*

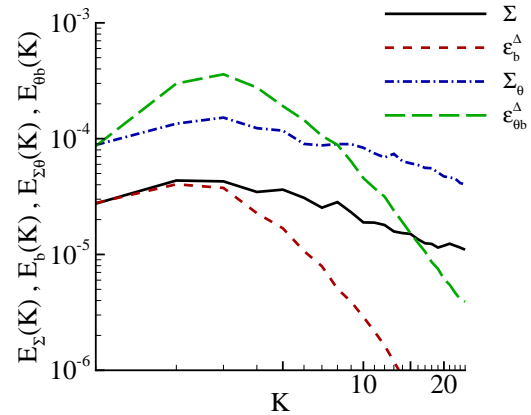


Figure 4: *Comparison of spectra of the exact -  $\Sigma$  and  $\Sigma_\theta$  - and modeled -  $\epsilon_b^\Delta$  and  $\epsilon_{\theta b}^\Delta$  - viscous and molecular SGS dissipation terms using the hybrid RANS/LES model.*