

# A Framework for the Assessment and Creation of Subgrid-Scale Models for Large-Eddy Simulation

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Received: October 25, 2016. Revised: December 23, 2016. Accepted: December 23, 2016.

Published online: June 27, 2017.

The following book chapter appeared in *Progress in Turbulence VII: Proceedings of the iTi Conference in Turbulence 2016*. Ed. by Örlü, R., Talamelli, A., Oberlack, M., Peinke, J. Springer International Publishing, pp. 133–139 and can be found at [http://dx.doi.org/10.1007/978-3-319-57934-4\\_19](http://dx.doi.org/10.1007/978-3-319-57934-4_19).

**Abstract** We focus on subgrid-scale modeling for large-eddy simulation of incompressible turbulent flows. In particular, we follow a systematic approach that is based on the idea that subgrid-scale models should preserve fundamental properties of the Navier–Stokes equations and turbulent stresses. To that end, we discuss the symmetries and conservation laws of the Navier–Stokes equations, as well as the near-wall scaling, realizability and dissipation behavior of the turbulent stresses. Regarding each of these properties as a model constraint, we obtain a framework that can be used to assess existing and create new subgrid-scale models. We show that several commonly used velocity-gradient-based subgrid-scale models do not exhibit all the desired properties. Although this can partly be explained by incompatibilities between model constraints, we believe there is room for improvement in the properties of subgrid-scale models. As an example, we provide a new eddy viscosity model, based on the vortex stretching magnitude, that is successfully tested in large-eddy simulations of turbulent plane-channel flow.

## 1 Introduction

The Navier–Stokes equations form a very accurate model for fluid flows. This model, however, does not form a tractable model, because in general not enough computational power is available to predict the behavior of practical turbulent flows with it. We therefore focus on large-eddy simulation, which aims at predicting the large-scale behavior of turbulent flows. In large-eddy simulation, the large scales of motion in a flow are explicitly computed, whereas small-scale motions are modeled.

In the current work, we address the question of how to construct subgrid-scale models for these small-scale motions in turbulent flows. To answer this question, we follow a systematic approach based on the idea that it is desirable that subgrid-scale models are consistent with the physical and mathematical properties of the Navier–Stokes equations and the turbulent stresses. These properties can therefore be seen as requirements for subgrid-scale modeling and we will use them to assess existing and construct new subgrid-scale models.

The structure of this paper is as follows. In Section 2 we describe several properties of the Navier–Stokes equations and turbulent stresses, and we discuss their importance. This leads to a framework of model requirements that, in Section 3, is used to analyze the properties of existing subgrid-scale models. Finally, in Section 4 we give an example of a new eddy viscosity model that

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can be derived from the model constraints and we test it in large-eddy simulations of turbulent plane-channel flow.

## 2 Model Constraints for Large-Eddy Simulation

In large-eddy simulation, the large-scale behavior of incompressible turbulent flows is described by the filtered incompressible Navier–Stokes equations [15],

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} \tau_{ij}, \quad \frac{\partial \bar{u}_i}{\partial x_i} = 0. \quad (1)$$

The turbulent stresses,  $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ , are not solely expressed in terms of the filtered velocity field and therefore have to be modeled. In what follows we will discuss a number of fundamental properties of the Navier–Stokes equations and the turbulent stresses that lead to constraints for this modeling process. More detailed information about these properties and the resulting constraints for subgrid-scale models can be found in previous work [16].

**Symmetries of the Incompressible Navier–Stokes Equations** The incompressible Navier–Stokes equations are form invariant under several coordinate transformations [11, 12]. Such transformations, or symmetries, play an important role because they ensure that the description of fluids is the same in all inertial frames of reference. They also relate to conservation and scaling laws [13]. Speziale [18], Oberlack [11, 12] and Razafindralandy et al. [13] therefore argue that it is desirable that these symmetries are preserved by subgrid-scale models. We distinguish invariance under the time (S1) and pressure (S2) translations, the generalized Galilean transformation (S3), rotations and reflections (S4), scaling transformations (S5), two-dimensional material frame-indifference (S6) and time reversal (S7) [11, 12].

**Conservation Laws** Even though the incompressible Navier–Stokes equations are inherently dissipative, they obey several conservation laws. In particular, we have conservation of generalized linear momentum (C1), conservation of angular momentum (C2) and conservation of an infinite hierarchy of vorticity-related quantities (C3) [3]. Conservation laws should not be violated by subgrid-scale models.

**Near-Wall Scaling of the Turbulent Stresses** Using numerical simulations, Chapman and Kuhn [2] have revealed the near-wall scaling of the time-averaged turbulent stresses. Focusing on wall-resolved large-eddy simulations, we would like to make sure that modeled stresses exhibit the same near-wall scaling behavior (N). In particular, the desired scaling of an eddy viscosity is  $\nu_e = \mathcal{O}(x_2^3)$ , where  $x_2$  represents the wall-normal coordinate. This ensures that dissipative effects due to the model fall off quickly enough near solid boundaries.

**Realizability of the Turbulent Stresses** Vreman et al. [23] showed that, for positive spatial filters, the turbulent stress tensor,  $\tau_{ij}$ , is realizable, i.e., it has no negative eigenvalues. As these eigenvalues can be interpreted as (partial) energies, it seems desirable that subgrid-scale models exhibit realizability (R) as well.

**Production of Subgrid-Scale Kinetic Energy** Subgrid-scale models generally increase the dissipation of large-scale kinetic energy, i.e., the transport of energy from large to small scales of motion. We now focus on this process, which is also referred to as the production of subgrid-scale kinetic energy.

**Vreman’s Requirements** Vreman [22] showed that the production of subgrid-scale kinetic energy due to the true turbulent stresses is zero for certain (laminar) flows. He therefore argues that the production due to subgrid-scale models should also be zero for these flows (P1a). On the other hand, subgrid-scale models should not turn off in regions of flows where turbulence occurs (P1b). This ensures that subgrid-scale models are neither overly nor underly dissipative.

**Nicoud et al. Requirements** On the basis of physical grounds, Nicoud et al. [9] reason that certain flows cannot be maintained if energy is transported to subgrid scales. They therefore see it as a desirable property that the modeled production of subgrid-scale kinetic energy vanishes for these flows. In particular, they require that a model’s production of subgrid-scale kinetic energy vanishes for all two-component flows (P2a) and for the pure axisymmetric strain (P2b). Note that requirement P2a is not compatible with P1b, because the latter requires that certain two-component flows have a nonzero production of subgrid-scale kinetic energy [16].

**The Second Law of Thermodynamics** In turbulent flows, energy can be transported from large to small scales (forward scatter) and vice versa (backscatter). The second law of thermodynamics requires that the net transport is of the former type (P3) [13].

**Verstappen’s Requirements** Verstappen [20] argues that large-eddy simulation is ultimately aimed at predicting large-scale flow dynamics, independent of small-scale motions. Therefore, subgrid-scale models have to cause scale separation. This can be achieved by ensuring that subgrid-scale models are sufficiently dissipative, such that they counterbalance the convective production of small-scale kinetic energy and dissipate any kinetic energy (initially) contained in small scales of motion (P4). Requirements P4 and P2b cannot be satisfied at the same time, because the former requires a nonzero dissipation for the axisymmetric strain [16].

### 3 Analysis of Existing Subgrid-Scale Models

With the list of fundamental properties of Section 2, we obtain a framework that can be used to assess the behavior of subgrid-scale models. Table 1 provides a summary of the analysis of some commonly used velocity-gradient-based subgrid-scale models.

Velocity-gradient-based subgrid-scale models automatically preserve certain symmetries (S1–S4). Scaling invariance (S5), however, is usually violated because of the use of the local grid size as characteristic length scale [11, 13]. The dynamic procedure [5] may restore scaling invariance [1, 11, 13]. The importance of two-dimensional material frame-indifference (S6) is disputed [12], while time reversal invariance (S7) is generally not regarded as a desirable property of subgrid-scale models [1]. The three conservation laws (C1–C3) are trivially preserved for symmetric subgrid-scale models appearing in the form  $\partial/\partial x_j \tau_{ij}^{\text{mod}}$ . Realizability (R) does not pertain to traceless subgrid-scale models, including the eddy viscosity models studied here.

The general view that we obtain from Table 1 is that existing subgrid-scale models do not satisfy all the desired properties. This can partly be understood from incompatibilities between model constraints, especially the different dissipation requirements, and from difficulties with satisfying scale invariance. We do, however, believe that there is room for improvement in the properties of subgrid-scale models that are based on the velocity gradient.

Table 1: Summary of the properties of several subgrid-scale models. The properties considered are S1–4: time, pressure, generalized Galilean, and rotation and reflection invariance; S5: scaling invariance; S6: two-dimensional material frame-indifference; S7: time reversal invariance; C1: conservation of generalized linear momentum; C2: conservation of angular momentum; C3: conservation of vorticity-related quantities; N: the proper near-wall scaling behavior; R: realizability; P1a: zero subgrid dissipation for laminar flow types; P1b: nonzero subgrid dissipation for nonlaminar flow types; P2a: zero subgrid dissipation for two-component flows; P2b: zero subgrid dissipation for the pure axisymmetric strain; P3: consistency with the second law of thermodynamics; P4: sufficient subgrid dissipation for scale separation. The horizontal rule separates eddy viscosity models from models that contain tensor terms that are nonlinear in the velocity gradient

	S1–4	S5 <sup>a</sup>	S6	S7 <sup>a</sup>	C1	C2	C3	N <sup>a</sup>	R	P1a	P1b	P2a	P2b	P3	P4
Smagorinsky [17]	Y	N	Y	N	Y	Y	Y	N		N	Y	N	N	Y	Y
WALE [10]	Y	N	N	N	Y	Y	Y	Y		N	Y	N	N	Y	Y
Vreman [22]	Y	N	N	N	Y	Y	Y	N		N	Y	N	N	Y	Y
$\sigma$ [9]	Y	N	Y	N	Y	Y	Y	Y		Y	N	Y	Y	Y	N
QR [20]	Y	N	Y	N	Y	Y	Y	N		Y	N	Y	N	Y	N
S3PQR [19]	Y	N	Y <sup>b</sup>	N <sup>b</sup>	Y	Y	Y	Y		Y <sup>b</sup>	Y <sup>b</sup>	Y <sup>b</sup>	N	Y <sup>b</sup>	Y <sup>b</sup>
AMD [14]	Y	N	Y	N	Y	Y	Y	N		Y	N	Y	N	Y	Y
Vortex stretching	Y	N	Y	N	Y	Y	Y	Y		Y	N	Y	Y	Y	N
Gradient [4, 6]	Y	N	N	Y	Y	Y	Y	N	Y	Y	N	Y	N	N	
EASSM [7]	Y	N	N	N	Y	Y	Y	N	Y	N	Y	N	N	Y	

<sup>a</sup>The dynamic procedure [5] may restore these properties [1, 11, 13].

<sup>b</sup>Depending on the value of the model parameter and/or the implementation.

## 4 Example of a New Subgrid-Scale Model

The framework of model constraints can also be used to create new subgrid-scale models. For example, we previously derived the vortex-stretching-based (VS) eddy viscosity model [16],

$$\tau_{ij}^{\text{mod,dev}} = -2(C_{\text{VS}}\delta)^2 \sqrt{2 \text{tr}(\bar{S}^2)} \left( \frac{\text{tr}(\bar{S}^2 \bar{\Omega}^2) - \frac{1}{2} \text{tr}(\bar{S}^2) \text{tr}(\bar{\Omega}^2)}{-\text{tr}(\bar{S}^2) \text{tr}(\bar{\Omega}^2)} \right)^{3/2} \bar{S}_{ij}. \quad (2)$$

Here,  $C_{\text{VS}}$  is a model constant, whereas  $\delta$  denotes the characteristic length scale of the large-eddy simulation.  $\bar{S}$  and  $\bar{\Omega}$  represent the rate-of-strain and rate-of-rotation tensors, i.e., the symmetric and asymmetric parts of the velocity gradient,  $\partial \bar{u}_i / \partial x_j$ . The quantity  $4(\text{tr}(\bar{S}^2 \bar{\Omega}^2) - \frac{1}{2} \text{tr}(\bar{S}^2) \text{tr}(\bar{\Omega}^2))$  is the (squared) vortex stretching magnitude [19], which corrects for the dissipation behavior and the near-wall scaling of the Smagorinsky model.

Figure 1 shows results of large-eddy simulations of turbulent plane-channel flow obtained using the vortex-stretching-based eddy viscosity model. These simulations were performed using an incompressible Navier–Stokes solver that employs a symmetry-preserving finite-volume discretization on a staggered grid [21]. A  $64^3$  grid was used that was stretched in the wall-normal direction. The value of the model constant,  $C_{\text{VS}} \approx 0.58$ , was obtained by matching the average model dissipation with that of the Smagorinsky model [9, 19]. The mean velocity in the near-wall region is predicted remarkably well for this  $C_{\text{VS}}$ . Also the location of the peaks in the Reynolds stresses and the behavior of the stresses in the center of the channel is predicted well. The underpredicted center line velocity and the over- and undershoots in the Reynolds stresses seem to be common deficiencies of eddy viscosity models. All in all, these encouraging results show how new subgrid-scale models with built-in desirable properties can be constructed.

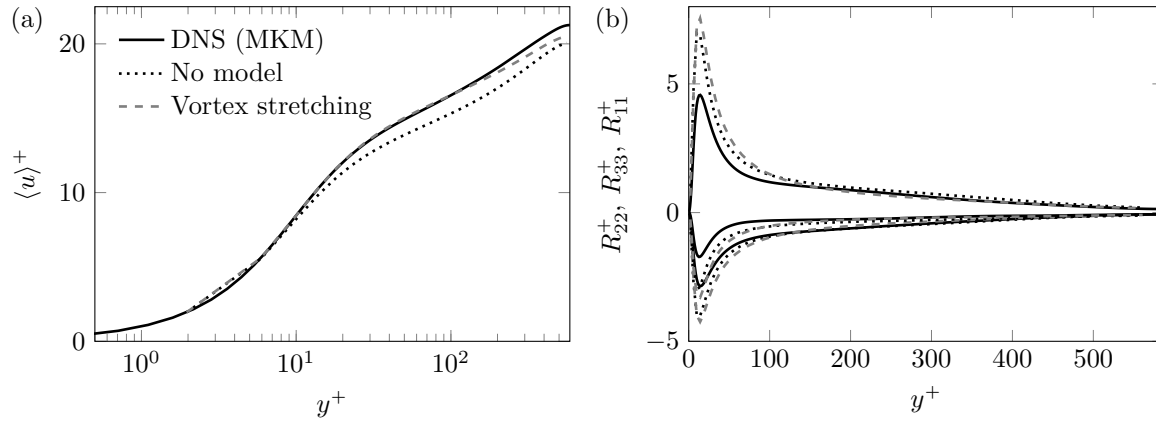


Figure 1: (a) Mean velocity profile and (b) diagonal deviatoric Reynolds stresses compensated by the average model contribution, as obtained from large-eddy simulations of turbulent plane-channel flow at  $Re_\tau \approx 590$  on a  $64^3$  grid. Simulations were performed without a subgrid-scale model (*dotted line*) and with the vortex-stretching-based eddy viscosity model (*dashed line*) of Eq. (2) with  $C_{VS} \approx 0.58$ . Results from direct numerical simulations (DNS) [8] are shown as reference (*solid line*). All quantities are shown in wall units

**Acknowledgements** The authors thankfully acknowledge Professor Martin Oberlack for stimulating discussions during several stages of this project. Professor Michel Deville is kindly acknowledged for sharing his insights relating to nonlinear subgrid-scale models and realizability. This work is part of the research programme Free Competition in the Physical Sciences with project number 613.001.212, which is financed by the Netherlands Organisation for Scientific Research (NWO).

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