

**Modelling of subgrid-scale stress and passive
scalar flux in large eddy simulations of wall
bounded turbulent flows**

by

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Modelling of subgrid-scale stress and passive scalar flux in large eddy simulations of wall bounded turbulent flows

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Abstract

The aim of the thesis is to develop and validate subgrid-scale models that are relevant for large eddy simulations of complex flows including scalar mixing. A stochastic Smagorinsky model with adjustable variance and time scale is developed by adding a stochastic component to the Smagorinsky constant. The stochastic model is shown to provide for backscatter of both kinetic energy and scalar variance without causing numerical instabilities. In addition, new models for the subgrid-scale stress and passive scalar flux are derived from modelled subgrid scale transport equations. These models properly account for the anisotropy of the subgrid scales and have potentials wall bounded flows. The proposed models are validated in wall bounded flows with and without rotation and show potential or significantly improve predictions for such cases.

Descriptors: Turbulence, large-eddy simulation, subgrid-scale model.

Preface

This thesis contains the following papers:

Paper 1. Linus Marstorp, Geert Brethouwer & Arne V. Johansson. A stochastic subgrid model with application to turbulent flow and scalar mixing. *Phys. Fluids* **19**, 035107.

Paper 2. Linus Marstorp, Geert Brethouwer & Arne V. Johansson. Explicit algebraic subgrid stress models with application to rotating channel flow. *Submitted to J. Fluid Mech.*

Paper 3. Linus Marstorp, Geert Brethouwer & Arne V. Johansson. An explicit algebraic model for the subgrid-scale passive scalar flux. *Submitted to Phys. Fluids*

Paper 4. Linus Marstorp, Qiang Li, Philipp Schlatter, Geert Brethouwer & Arne V. Johansson. *Validation of SGS models in LES of turbulent zero pressure gradient boundary layer*. Technical report

Division of work between authors

The project was initiated and defined by Arne Johansson and Geert Brethouwer. The work was performed by Linus Marstorp under the supervision of Arne Johansson and Geert Brethouwer. The large eddy simulations in papers 1-3 were performed by Marstorp. The stochastic model that we present in paper 1 was originally proposed by Krister Alvelius. The papers 1-3 were written by Linus Marstorp and reviewed by Arne Johansson and Geert Brethouwer. Paper 4 is a result of a collaboration with Philipp Schlatter and Qiang Li. Qiang Li performed most of the simulations and Linus Marstorp wrote most of the report.

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CHAPTER 1

Introduction

The nature of turbulent flows is chaotic and three-dimensional with a wide range of the scales of motion. Predictions of (Newtonian) turbulent flows require numerical solution of the Navier-Stokes equations. Unfortunately, direct numerical simulations, DNS, whereby the Navier-Stokes equations are directly solved without resorting to models demand very high resolution because all scales of motion, even the smallest turbulent eddies, have to be resolved in order to capture the correct physics of the flow. DNS of flows of engineering interest is not feasible because the range of the scales of motion is usually very wide. A less computationally expensive approach is to solve the Navier-Stokes equations in the mean sense. This is usually referred to as a Reynolds averaged Navier-Stokes, RANS, approach. The RANS approach provides for mean statistics, such as the mean velocity profile and the mean turbulence kinetic energy, but all turbulent motions have to be modelled. Thus, RANS cannot capture the dynamics of a flow. The subject for this study is a third approach; Large Eddy Simulation, LES, which captures the dynamics of the largest turbulence length scales and only requires modelling of the smallest scales of motion. LES is more computationally demanding than RANS but is less expensive than DNS, because only the largest scales of motion have to be resolved. Today, LES is used in the industry as a tool for numerical simulation of turbulent flows. As an example, figure 1.1 shows the flow over an airfoil. We can see that the LES is able to capture the large scale motions of the flow.

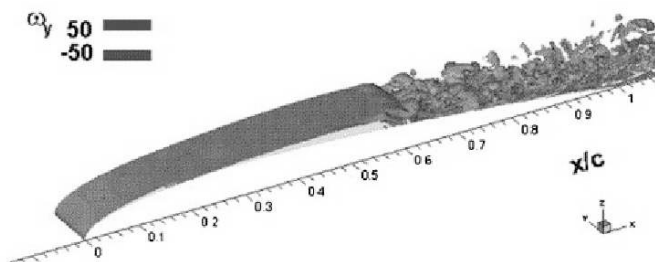


FIGURE 1.1. LES of the flow around an airfoil showing the isosurfaces of vorticity. Liu (2006).

LES is a promising tool to predict mixing of scalars in turbulent flows. A passive scalar can represent, for example, small temperature fluctuations or a pollutant carried by the flow. One interesting application is the prediction of mixing of pollutants in urban areas. Figure 1.2 shows results from a LES of the spread of a pollutant in an urban area. The turbulent eddies transport the pollutant to the surroundings. Knowledge of passive scalar mixing is also a first step towards the understanding of reactive flows, where the mixing of species plays an important role.

The aim of this thesis is to apply new approaches to develop subgrid models for the stress and passive scalar flux. These models are relevant for LES of complex flows including scalar mixing.

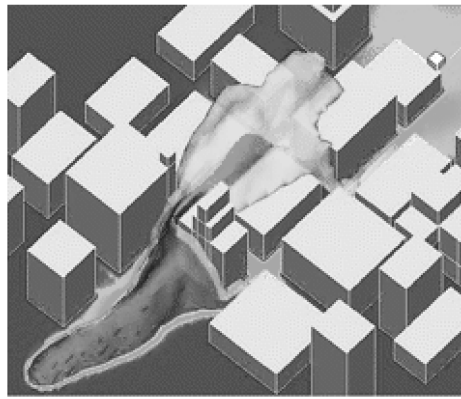


FIGURE 1.2. LES of mixing of a pollutant in an urban area.
Tseng et al. (2006).

CHAPTER 2

Large eddy simulations

A Large Eddy Simulation (LES) is a numerical simulation of the Navier-Stokes equations in which only the large length and time scales are resolved, and in which the influence of the non-resolved scales has to be modelled. LES was originally a tool for numerical simulation of the large scale dynamics of meteorological flows in two dimensions. Smagorinsky (1962) was among the pioneers. He studied the dynamics of the atmospheric circulation using a subgrid model based on the local strain rate to account for the action of the scales smaller than the grid spacing. The model accounted for a large portion of the eddy transfer. Today the Smagorinsky model is still the most widely used subgrid scale, SGS, model in LES. Deardorff (1970) applied what he called the meteorological approach to three dimensional turbulence in plane Poiseuille flow using 6720 grid points. The simulation did not have the proper no-slip conditions at the solid walls, but nevertheless the LES was able to capture some of the large scale structures in turbulent channel flow. Moin and Kim (1982) were the first to perform a well resolved LES of turbulent channel flow with proper boundary conditions using 0.5 million grid points. As an SGS model they used a Smagorinsky type of eddy viscosity model with wall damping of the model constant. The LES results were in good agreement with turbulence statistics obtained from experiments.

Efforts were made to improve the SGS modelling over existing eddy viscosity models. Mixed models, where the Smagorinsky model is combined with a second model term, were proposed. Clark et al. (1979) proposed a mixed non-linear model where the second term is a tensor eddy diffusivity type of term. Bardina et al. (1983) proposed the mixed scale similarity model where the second term is an estimate of the SGS stress computed from the resolved velocity field and an explicit test filter. The dynamic Smagorinsky model due to Germano et al. (1991) was a major step towards improved SGS modelling. With the dynamic determination of the model constant there was no need for ad hoc wall damping functions, and it enabled LES of flows involving both laminar and turbulent regions. Variations of the dynamic approach have been applied to a wide range of SGS models. It is also well known that the performance of an SGS model can be improved by removing large scale information from the

model. The SGS model used by Schumann (1975) might be considered as the first high pass filtered model. He proposed a version of the Smagorinsky model where the mean velocity gradient is removed before the rate of strain tensor is computed. More recent examples of such high pass filtered SGS models are the filtered structure function model proposed by Ducros et al. (1996) and the high pass filtered Smagorinsky model proposed by Stolz et al. (2005). These types of models have particular potential for LES of transitional flows.

2.1. Governing equations

The incompressible Navier-Stokes equations and the passive scalar equation considered here read

$$\begin{aligned}\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \nabla^2 u_i \\ \frac{\partial u_i}{\partial x_i} &= 0 \\ \frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} &= \frac{\nu}{Pr} \nabla^2 \theta\end{aligned}\tag{2.1}$$

where u_i and θ denote the velocity and passive scalar respectively, p is the pressure, ν is the viscosity, and Pr is the Prandtl number. To remove the scales smaller than a prescribed filter scale Δ , a low pass filtering operation is applied to the Navier-Stokes equation. The filter can be represented by a convolution

$$\tilde{u}(\mathbf{x}, t) = \int G(\mathbf{x} - \mathbf{y}) u(\mathbf{y}, t) d\mathbf{y}.\tag{2.2}$$

The filter kernel $G(\mathbf{x} - \mathbf{y})$ is homogeneous, which implies that the filter commutes with the differential operator. Applying the filter operation to the incompressible Navier-Stokes equations and the passive scalar equation leads to

$$\begin{aligned}\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + \nu \nabla^2 \tilde{u}_i - \frac{\partial \tau_{ij}}{\partial x_j} \\ \frac{\partial \tilde{u}_i}{\partial x_i} &= 0 \\ \frac{\partial \tilde{\theta}}{\partial t} + \tilde{u}_j \frac{\partial \tilde{\theta}}{\partial x_j} &= \frac{\nu}{Pr} \nabla^2 \tilde{\theta} - \frac{\partial q_j}{\partial x_j}\end{aligned}\tag{2.3}$$

In the filtered equations τ_{ij} is the subgrid scale, SGS, stress which is given by

$$\tau_{ij} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j\tag{2.4}$$

The SGS scalar flux q_i in the filtered passive scalar flux equation is given by

$$q_i = \widetilde{u_i \theta} - \tilde{u}_i \tilde{\theta}\tag{2.5}$$

The SGS stress τ_{ij} and the SGS flux q_i represent the effect of the small unresolved scales on the large resolved scales, see Pope (2000). Both τ_{ij} and q_i

have to be modelled in order to close the system of equations.

2.2. Some important SGS stress models

2.2.1. The Smagorinsky model

The widely known Smagorinsky (1962) model is an eddy viscosity model which reads

$$\tau_{ij} = -2\nu_T \tilde{S}_{ij} \quad (2.6)$$

where $\tilde{S}_{ij}$ is the resolved rate of strain. The eddy viscosity, ν_T , is constructed from the filter length scale Δ and a velocity scale $\Delta|\tilde{S}_{ij}|$, according to

$$\nu_T = (C_s \Delta)^2 |\tilde{S}_{ij}| \quad (2.7)$$

where $|\tilde{S}_{ij}| = (2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}$ and $C_s > 0$ is a model constant. The model is stable and computationally inexpensive. Moreover, a constant Smagorinsky constant, C_s , is consistent with the Kolmogorov theory for the energy cascade in isotropic turbulent flows Pope (2000). However, the Smagorinsky model has several known deficiencies. One example is that with $C_s > 0$ the SGS-dissipation is strictly positive, i.e. there is no backscatter of SGS kinetic energy. Another example is that the model constant has to be damped in near wall regions. The latter problem is also associated with eddy viscosity models for RANS.

The corresponding SGS model for the passive scalar is the eddy diffusion model

$$q_i = -\frac{\nu_T}{Pr_T} \frac{\partial \tilde{\theta}}{\partial x_i}. \quad (2.8)$$

Like the Smagorinsky model, the eddy diffusion model does not provide for backscatter. Another deficiency is its inability to predict the anisotropy of the scalar variance SGS dissipation, as pointed out by Kang and Meneveau (2001).

2.2.2. Dynamic Smagorinsky model

In the dynamic Smagorinsky model developed by Germano et al. (1991), information about the resolved scales is used to estimate the Smagorinsky constant. According to the Germano identity the difference between the SGS stress evaluated at two different filter scales is

$$\tau_{ij}^{\hat{\Delta}} - \widehat{\tau_{ij}^{\Delta}} = \widehat{\tilde{u}_i \tilde{u}_j} - \hat{\tilde{u}}_i \hat{\tilde{u}}_j \quad (2.9)$$

where the hat operator denotes an explicit test filter at larger filter width, $\hat{\Delta} > \Delta$. By replacing the real SGS stress by the modelled stress and by assuming scale invariance of the Smagorinsky constant the following relation is obtained

$$-2C_s^2 \left(\hat{\Delta}^2 |\hat{\tilde{S}}| \hat{\tilde{S}}_{ij} - \Delta^2 |\tilde{S}| \tilde{S}_{ij} \right) = \widehat{\tilde{u}_i \tilde{u}_j} - \hat{\tilde{u}}_i \hat{\tilde{u}}_j \quad (2.10)$$

Germano originally proposed to compute the model constant as

$$\begin{aligned}
C_s^2 &= \frac{\langle L_{ij} \tilde{S}_{ij} \rangle}{\langle M_{ij} \tilde{S}_{ij} \rangle} \\
L_{ij} &= \widehat{\tilde{u}_i \tilde{u}_j} - \hat{u}_i \hat{u}_j \\
M_{ij} &= -2(\hat{\Delta}^2 |\hat{S}| \hat{\tilde{S}}_{ij} - \Delta^2 |\tilde{S}| \tilde{S}_{ij})
\end{aligned} \tag{2.11}$$

where the brackets $\langle \rangle$ denote averaging in homogeneous directions. Lilly (1992) proposed the more widely used procedure, $C_s^2 = \langle L_{ij} M_{ij} \rangle / \langle M_{ij} M_{ij} \rangle$, which is a least-square solution to (2.10) minimising the error $\langle L_{ij} - C_s^2 M_{ij} \rangle$.

Averaging in homogeneous directions according to (2.10) is not possible in complex geometries that lack such directions. In that case, time averaging is an option, but it is not consistent with Galilean invariance unless it is implemented in a Lagrangian frame of reference. Meneveau et al. (1996) developed such a Lagrangian dynamic model with averaging along path lines. Without the averaging the dynamic model provides for backscatter but the model constant yields excessively large fluctuations and it can easily become unstable.

With the dynamic approach, the Smagorinsky constant is adjusted to the local flow conditions. The model provides for a correct near wall scaling, and it can be applied to flows containing both laminar and turbulent regions. Variations of the dynamic approach have been applied to a wide range of SGS models. A recent example is the three coefficient nonlinear dynamic model developed by Wang and Bergstrom (2005).

2.2.3. Scale similarity model

In the scale similarity model developed by Bardina et al. (1983), the SGS stress is assumed to be similar to the one constructed by the resolved velocity field and an explicit test filter with equal or larger filter scale

$$\tau_{ij} = \widehat{\tilde{u}_i \tilde{u}_j} - \hat{u}_i \hat{u}_j. \tag{2.12}$$

In (2.12) the hat-operator denotes the test filter with, $\hat{\Delta} \geq \Delta$. The correlation coefficient with the real SGS stress is higher for the scale similarity model than for the Smagorinsky model (Liu et al. (1994)), and the model provides for physical backscatter of turbulent energy. However, the scale similarity model does not provide for enough dissipation. Therefore, it is usually used in an ad hoc combination with a Smagorinsky term, which provides for additional dissipation and stabilises the simulations. An example of such a mixed model is the dynamic mixed model proposed by Zang et al. (1993).

It is a straightforward process to extend the scale similarity model to the SGS

passive scalar flux

$$q_i = \widehat{\tilde{u}_i \tilde{\theta}} - \hat{\tilde{u}}_i \hat{\tilde{\theta}}. \quad (2.13)$$

For instance, Calmet and Magnaudet (1997) applied the dynamic mixed model proposed by Zang et al. (1993) to LES of mass transfer in a turbulent channel.

2.2.4. Approximate deconvolution model

The approximate deconvolution model, ADM, by Stolz and Adams (1999) belongs to the group of velocity estimation models. In the ADM, the full unfiltered velocity is estimated by an approximate defiltering operation

$$u_i \approx u_i^* = Q_N \star \tilde{u}_i$$

$$Q_N = \sum_{\nu=0}^N (I - G)^\nu \approx G^{-1} \quad (2.14)$$

where the star operator denotes a convolution and Q_N is an N -order approximation of the inverse filter kernel G^{-1} . The SGS stress is then computed from the approximation $\tau_{ij} = \widetilde{u_i^* u_j^*} - \widetilde{u_i^*} \widetilde{u_j^*}$. With $N = 0$, the ADM corresponds to the scale-similarity model.

Like the scale similarity model, the ADM does not dissipate an adequate amount of energy. In order to model the energy transfer from resolved scales to the SGS an additional relaxation term $-\chi(I - Q_N \star G) \star \tilde{u}$ is added to the right hand side of equation (2.3). This is equivalent to an explicit filtering of the resolved velocity field at each time step. The model coefficient, χ , can be determined by a dynamic approach. LES of turbulent channel flow has shown a significant improvement over results obtained with the dynamic Smagorinsky model.

2.2.5. Removing the largest scales from SGS modelling

It is well known that the performance of an SGS model can be improved by removing some of the low wave number contents from the SGS model. Ducros et al. (1996) showed that the structure function model is able to predict transition phenomena if a high pass filter is applied before calculating the second order structure function. The high pass filtering approach was extended to the Smagorinsky model by Sagaut et al. (2000).

A method similar to high-pass filtering is the variational multiscale method due to Hughes et al. (2001a). In the multiscale method the resolved scales are separated into different ranges. In the simplest version modelling is only applied to the equation governing the smallest resolved scales. Hughes et al. applied their approach on the Smagorinsky model and found that the method outperformed the standard Smagorinsky model in LES of isotropic turbulence. Good results were also obtained in turbulent channel flow, see Hughes et al.

(2001b).

Recently, Stolz et al. (2005) developed high pass filtered eddy viscosity models for LES based on the high pass filtered strain rate

$$\tilde{S}_{ij}(H * \tilde{u}) = \frac{1}{2} \left(\frac{\partial H * \tilde{u}_i}{\partial x_j} + \frac{\partial H * \tilde{u}_j}{\partial x_i} \right), \quad (2.15)$$

where H is a suitable high-pass filter and $*$ denotes a convolution in physical space. These Smagorinsky type of models have been successfully applied to LES of transitional and turbulent flows. The high pass filtered Smagorinsky model provides for backscatter even if $C_s > 0$.

2.2.6. Stochastic models

The SGS models described so far depend on the resolved quantities in a deterministic way. However, the nature of the smallest turbulent scales appears as partly random to the resolved scales. The real sub-grid scale stress tensor contains stochastic noise that cannot be modelled by any deterministic sub-grid-scale model.

Stochastic sub-grid modelling has been treated by several authors. Leith (1990) supplemented the Smagorinsky model by random SGS stresses calculated as the rotation of a stochastic potential. Schumann (1995) also modelled the stochastic behaviour of the SGS scales by adding random SGS stresses to the Smagorinsky model. Alvelius and Johansson (1999) proposed a stochastic model consisting of a modified Smagorinsky constant

$$C_s'^2 = C_s^2(1 + X) \quad (2.16)$$

where X is a stochastic process with prescribed variance and timescale. Stochastic modelling enables control of the magnitude and the time scale of the backscatter that could otherwise lead to numerical instabilities.

2.2.7. Transport equation models

Models based on transport equations of the Reynolds stress are frequently used in RANS. They account for history effects and are able to accurately predict complex flows of interest in engineering applications. The same approach can be adopted to LES. In analogy with Reynolds decomposition, the full unfiltered velocity can be decomposed as

$$u_i = \tilde{u}_i + u_i' \quad (2.17)$$

where u'_i is the fluctuating SGS velocity. If (2.17) is inserted into the definition of the SGS stress we have

$$\begin{aligned}\tau_{ij} &= L_{ij} + C_{ij} + R_{ij} \\ L_{ij} &= \widetilde{\tilde{u}_i \tilde{u}_j} - \tilde{u}_i \tilde{u}_j \\ C_{ij} &= \widetilde{\tilde{u}_i u'_j} + \widetilde{\tilde{u}_j u'_i} \\ R_{ij} &= \widetilde{u'_i u'_j}\end{aligned}\tag{2.18}$$

where L_{ij} is the Leonard stress, C_{ij} is the cross stress, and R_{ij} is the SGS Reynolds stress. Transport equations can be derived for either the complete SGS stress, or for some of the component parts. Germano (1992) derived the transport equation for τ_{ij} using a homogeneous filter

$$\begin{aligned}\frac{\partial \tau_{ij}}{\partial t} + \tilde{u}_k \frac{\tau_{ij}}{\partial x_k} &= -\tau_{ik} \frac{\partial \tilde{u}_j}{\partial x_k} - \tau_{jk} \frac{\partial \tilde{u}_i}{\partial x_k} + \frac{2}{\rho} \left(\widetilde{p S_{ij}} - \tilde{p} \tilde{S}_{ij} \right) \\ &- 2\nu \left(\widetilde{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k}} - \frac{\partial \tilde{u}_i}{\partial x_k} \frac{\partial \tilde{u}_j}{\partial x_k} \right) - \frac{\partial D_{ijk}}{\partial x_k}.\end{aligned}\tag{2.19}$$

Here D_{ijk} is a diffusion term including both turbulent and molecular diffusion and $\tilde{S}_{ij}$ is the resolved strain rate tensor. Equation (2.19) has strong similarities with the Reynolds stress transport equation. The first two terms on the right hand side are production terms, the third term is the pressure strain 'correlation' and the fourth term is the viscous dissipation. The transport equation for the Reynolds stress tensor is easily obtained by replacing the filter operator $\sim$ by an ensemble average, and by using the Reynolds decomposition $u = \tilde{u} + u'$ and the rule $\widetilde{\tilde{u} u'} = 0$. The latter rule is not valid in LES, i.e. $\widetilde{\tilde{u} u'} \neq 0$. The similarities between the SGS stress and Reynolds stress transport equations make it possible to adapt some of the concepts of Reynolds stress modelling to SGS stress modelling for LES. For example, Chaouat and Schiestel (2005) developed a three-equation SGS model based on the transport equations of the SGS Reynolds stress, the SGS kinetic energy, and the dissipation rate of the SGS Reynolds stress. Their model accurately describes the anisotropy of the turbulence field and it captures transition phenomena.

CHAPTER 3

Subgrid scale modelling for large eddy simulations

The subgrid scale models proposed in this thesis are developed by applying two different approaches. The first approach is stochastic subgrid modelling. The idea behind stochastic subgrid modelling is to model the random interactions between the resolved scales and the subgrid scales in terms of stochastic processes with the aim to improve the description of the smallest resolved scales in LES. The second approach is explicit algebraic subgrid scale modelling based on modelled transport equations for the SGS stress and the SGS flux. The main ideas in explicit algebraic subgrid modelling are to obtain a realistic description of the individual SGS stresses and scalar fluxes and to account for system rotation in a proper way.

3.1. Stochastic SGS modelling

The subgrid scales appear as partly random to the resolved scales and there is a random interaction between the resolved scales and the subgrid scales. This random interaction cannot be described by models that depend on the resolved field in a deterministic way. The stochastic model considered here (Marstorp et al. 2007) was originally proposed by Alvelius and Johansson (1999). It is based on the Smagorinsky model in which the eddy viscosity is constructed from the filter scale Δ and a velocity scale $\Delta|\tilde{S}_{ij}|$. We let $X(x, t)$ represent a random fluctuation in the velocity scale $\Delta(1 + X)|\tilde{S}_{ij}|$ induced by the interactions with the subgrid scales. As a result we obtain a partly stochastic eddy viscosity

$$\nu_T = C_s^2(1 + X(x, t))\Delta^2|\tilde{S}_{ij}| \quad (3.20)$$

where C_s is the Smagorinsky constant, Δ is the filter scale, and X is a stochastic process with zero mean $\langle X \rangle$ and a controllable variance. The part corresponding to the Smagorinsky model can generate the right amount of mean dissipation whereas the stochastic part provides for backscatter and creates realistic SGS fluctuations.

The controllable variance and time scale of X enables significant backscatter without leading to numerical instabilities, because the backscatter has a short correlation time scale and it is very local in space. Figure 3.1 shows the PDF of the SGS dissipation of kinetic energy and scalar variance from LES of homogeneous shear flow. About 40% of the transfer is backscatter. The stochastic

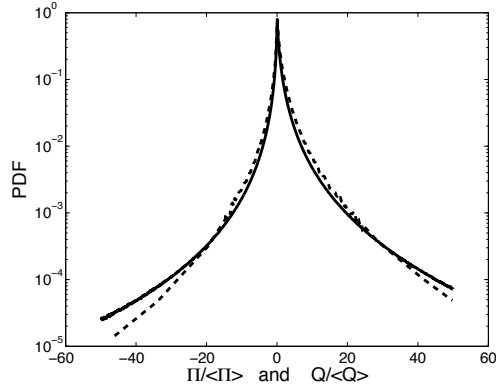


FIGURE 3.1. *PDF of the energy SGS dissipation and the scalar variance SGS dissipation according to the stochastic Smagorinsky model. Energy SGS dissipation, dashed line; scalar variance SGS dissipation, solid line.*

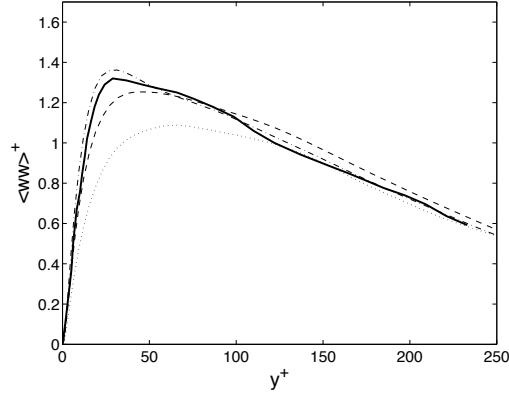


FIGURE 3.2. Resolved spanwise Reynolds stress component in turbulent channel flow. Stochastic model, dashed line; Smagorinsky model, dotted line; dynamic Smagorinsky model, dash-dotted line; filtered DNS, thick solid line.

contribution to the eddy viscosity improves the resolved velocity statistics in LES of turbulent channel flow. As an example figure 3.2 shows the spanwise velocity fluctuations. The stochastic model increases the spanwise fluctuations near the wall resulting in a significantly better description of $\langle \tilde{w}\tilde{w} \rangle$ compared to the standard Smagorinsky model. The stochastic interaction between the resolved and subgrid scales seems to be an important part of the dynamics in LES of wall bounded flows.

3.2. Explicit algebraic subgrid scale models

3.2.1. Explicit algebraic SGS stress models

The main ideas in explicit algebraic subgrid stress models is to obtain a realistic description of the individual SGS stresses and to account for system rotation. The subgrid scale stress model presented in Marstorp et al. (2008a) is derived using the same methodology as the explicit algebraic Reynolds stress model, EARSM, by Wallin and Johansson (2000). It is based on a modelled transport equation and consists of three terms

$$\tau_{ij} = K_{SGS} \left(\frac{2}{3} \delta_{ij} + \beta_1 \tau_{SGS} \tilde{S}_{ij} + \beta_4 \tau_{SGS}^2 (\tilde{S}_{ik} \tilde{\Omega}_{kj} - \tilde{\Omega}_{ik} \tilde{S}_{kj}) \right) \quad (3.21)$$

where $\tilde{\Omega}_{ij}$ and $\tilde{S}_{ij}$ are the resolved strain rate and rotation rate tensors respectively and τ_{SGS} is the time scale of the SGS velocity field. The first term on the right hand side is the isotropic part, the second term is an eddy viscosity part, and the third term is a nonlinear tensor that creates a realistic anisotropy of the SGS stress. β_1 and β_4 are coefficients that depend on the resolved velocity gradients and the model parameters. The SGS kinetic energy, K_{SGS} , is modelled using the Smagorinsky velocity scale, i.e

$$K_{SGS} = c \Delta^2 |\tilde{S}_{ij}|^2 ,$$

where the model parameter c can be either determined dynamically or expressed (non-dynamically) in terms of β_1 . The SGS timescale is modelled using the inverse shear. The system rotation enters explicitly in the transport equation for τ_{ij} and is accounted for by simply replacing $\tilde{\Omega}_{ij}$ by $\tilde{\Omega}_{ij}^R$ where

$$\tilde{\Omega}_{ij}^R = \tilde{\Omega}_{ij} + \frac{13}{4} \epsilon_{ikj} \Omega_k . \quad (3.22)$$

The new explicit algebraic model for the SGS stress benefits from the ability to account for rotation. Figure 3.3 shows the mean bulk velocity in rotating turbulent channel flow. The mean bulk velocity is defined as

$$U_b^+ = \frac{1}{2\delta u_\tau} \int_{-\delta}^{\delta} \langle u \rangle dy \quad (3.23)$$

and depends strongly on the rotation number, $Ro_b = 2\Omega\delta/U_b$. Here Ω is the spanwise rotation rate and δ is half the channel width. The explicit model using the non-dynamic determination of K_{SGS} captures the behaviour of U_b^+ fairly well because it can handle the laminarisation imposed by the system rotation, whereas the standard Smagorinsky model with wall damping of C_s fails. Especially, at high rotation rates the explicit model benefits from the asymptotic behaviour $\beta_1, \beta_4 \rightarrow 0$ as $Ro_b \rightarrow \infty$.

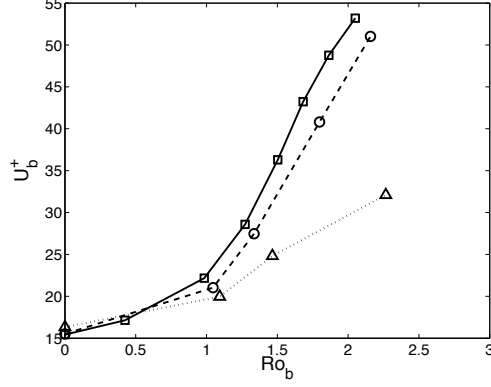


FIGURE 3.3. Mean bulk velocity at various rotation numbers. DNS, solid line; explicit model, dashed line; Smagorinsky model, dotted line.

3.2.2. An explicit algebraic model for the SGS scalar flux

The anisotropy of a passive scalar field is known to persist down to very small scales. Therefore, it can be justified to develop SGS scalar flux models that can account for the passive scalar anisotropy persisting at the SGS level. The idea behind the explicit algebraic SGS scalar flux model presented in Marstorp et al. (2008b) is to obtain a model with a realistic description of the individual SGS fluxes. The explicit model is based on a modelled transport equation for q_i and is derived in the same manner as the EASFM of Wikström et al. (2000). The solution to the modelled transport equation can be expressed explicitly as

$$q_i = -\tau^{SGS} c_{amp} A_{ij}^{-1} \tau_{jk} \frac{\partial \tilde{\theta}}{\partial x_k}, \quad (3.24)$$

where A_{ij}^{-1} is a function of the resolved velocity gradients and the model parameters, τ^{SGS} is the time scale of the SGS velocity field, and c_{amp} is a model constant. The model provides for a more complete description of the SGS scalar flux compared to the eddy diffusivity model. It can be rewritten as a mixed model

$$q_i = -\tau^{sgs} c_{amp} \frac{A_{kj}^{-1} \tau_{jk}}{3} \frac{\partial \tilde{\theta}}{\partial x_i} - \tau^{sgs} c_{amp} \left(A_{ij}^{-1} \tau_{jk} - \delta_{ik} \frac{A_{lj}^{-1} \tau_{jl}}{3} \right) \frac{\partial \tilde{\theta}}{\partial x_k} \quad (3.25)$$

The first term is an eddy diffusion term that provides for scalar SGS dissipation and the second part is a tensor eddy diffusivity type of term that improves the description of the individual SGS scalar fluxes. The model depends explicitly on the SGS stresses and for that reason it is appropriate to use the explicit SGS flux model together with the explicit algebraic SGS stress model described above. System rotation can be accounted for because it explicitly enters the

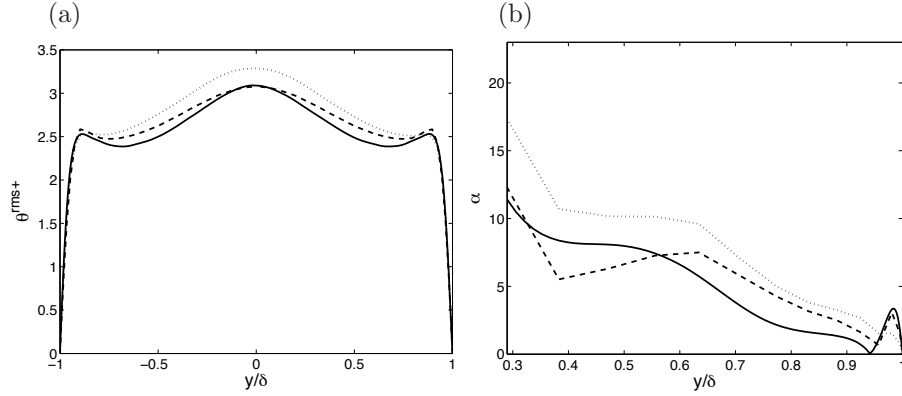


FIGURE 3.4. (a): Resolved scalar fluctuations from LES of in non-rotating channel flow. (b): Near wall behaviour of α in rotating channel flow. DNS data, solid line; new explicit model, dashed line; eddy diffusivity model, dotted line.

transport equation for q_i .

Figure 3.4a shows the root-mean-square of the scalar fluctuations in LES of turbulent channel flow using the explicit algebraic SGS flux model. The explicit model provides for a good description of the scalar fluctuations showing that the eddy diffusivity part of the model produces a realistic amount of mean SGS scalar dissipation. The explicit model has potential for rotation flows. Figure 3.4b shows the direction of the scalar fluxes, $\alpha = \text{atan}(\langle v\theta \rangle / \langle u\theta \rangle)$ where $\langle u\theta \rangle$ and $\langle v\theta \rangle$ are the streamwise and wall normal scalar fluxes, at the destabilised side of spanwise rotating channel flow. We have added the SGS scalar fluxes to the resolved turbulence fluxes to enable comparison between LES and DNS. The figure shows that the explicit model provides for a slightly better description of α compared to the eddy diffusivity model with a constant $Pr_T = 0.4$.

3.2.3. Validation in $Re_\tau = 950$ turbulent channel flow

One advantage of a realistic description of the individual stresses is that the sum of the resolved stresses and the modelled SGS stresses can be compared with non-filtered DNS data. The grid-scale dependence of the predictions using the dynamic version of the explicit algebraic model and the dynamic Smagorinsky model is investigated in LES of turbulent channel flow at $Re_\tau = 950$. Three different resolutions were tested. In wall units these correspond to $\Delta x^+ = 187, 124, 93$, $\Delta z^+ = 93, 62, 47$ and on average $\langle \Delta y^+ \rangle = 20, 20, 14$ respectively, i.e. the resolution is rather coarse. Figure 3.5 shows the streamwise Reynolds stress component. The explicit algebraic model using dynamic

determination of K_{SGS} provides for a fairly good and filter scale independent description of $\langle \tilde{u}\tilde{u} \rangle + \langle \tau_{11} \rangle$, indicating that the improved description of τ_{11} results in a realistic description of the resolved streamwise fluctuation, $\langle \tilde{u}\tilde{u} \rangle$. The dynamic Smagorinsky model predicts a too large near wall peak in $\langle \tilde{u}\tilde{u} \rangle$ and shows a quite strong sensitivity to the grid resolution.

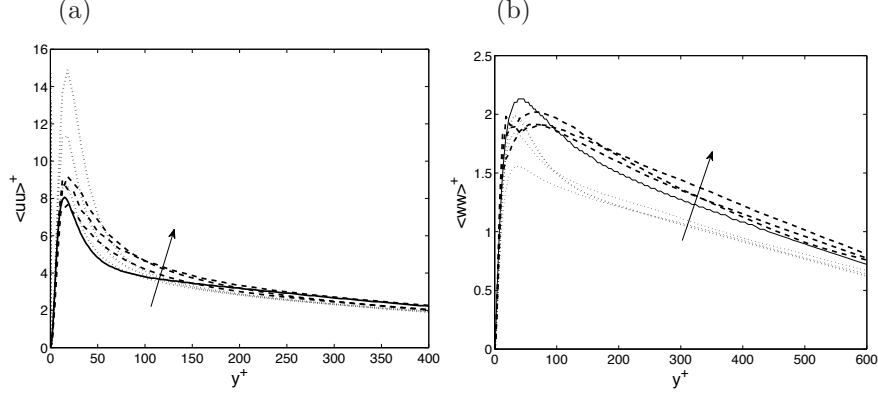


FIGURE 3.5. The sum of the resolved and SGS stress in the streamwise direction (a) and spanwise direction (b) in turbulent channel flow at $Re_\tau = 950$. DNS, solid line; explicit algebraic model, dashed lines; resolved data using the dynamic Smagorinsky model, dotted lines. The arrow points in the direction of increased filter width.

In the same manner, the realistic description of the individual SGS fluxes provided by the explicit SGS scalar flux model enables meaningful comparison with non-filtered DNS data. The sum of the resolved streamwise scalar flux and the SGS streamwise flux are shown in figure 3.6 at the three different resolutions in channel flow at $Re_\tau = 950$. The new explicit model provides for a less filter scale dependent description of the near wall peak in the streamwise turbulence scalar flux than the eddy diffusivity model, at the three different resolutions tested here. It seems as the improved description of the individual SGS fluxes provided by the new explicit model also improves the description of the mean turbulence scalar fluxes.

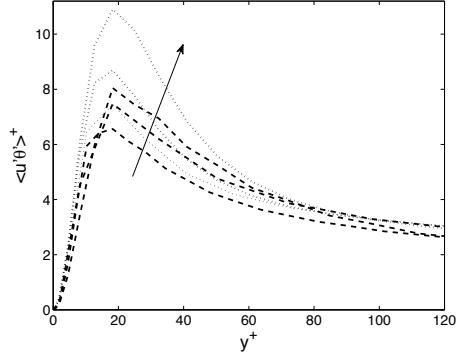


FIGURE 3.6. Streamwise scalar flux at various resolutions in channel flow at $Re_\tau = 950$. Non-filtered DNS data, solid line; new explicit model, dashed lines; eddy diffusivity model, dotted lines. The arrow points in the direction of increased filter width.

3.3. Validation of of the explicit algebraic SGS stress model in zero pressure gradient boundary layer

Zero pressure gradient boundary layer flow is an interesting test case for validation of SGS models because it involves the complexity of two inhomogeneous directions. It is a more demanding than turbulent channel flow which is the most frequently used test case for LES.

In Marstorp et al. (2008c) we compare LES with the new explicit algebraic model (3.21), the dynamic Smagorinsky model (Germano 1991), and the high pass filtered dynamic Smagorinsky model proposed by Schlatter et al. (2006) to the DNS data by Li (2007). Figure 3.7a shows the mean velocity profile normalised with the wall friction velocity, u_τ , at $Re_\theta = 780$. The dynamic Smagorinsky model and the explicit model overpredict the mean velocity profile in the outer region whereas the high pass filtered dynamic Smagorinsky model underpredict the mean velocity profile. A distinguishing characteristic for the high pass filtered model is the increased level of the wall normal and spanwise fluctuations near the wall, whereas the dynamic Smagorinsky model and the explicit model predict significantly lower level of fluctuations (figure 3.7 b). Again, the sum of the mean resolved stresses and the mean SGS stresses predicted by the explicit algebraic model is in good agreement with the non-filtered DNS data.

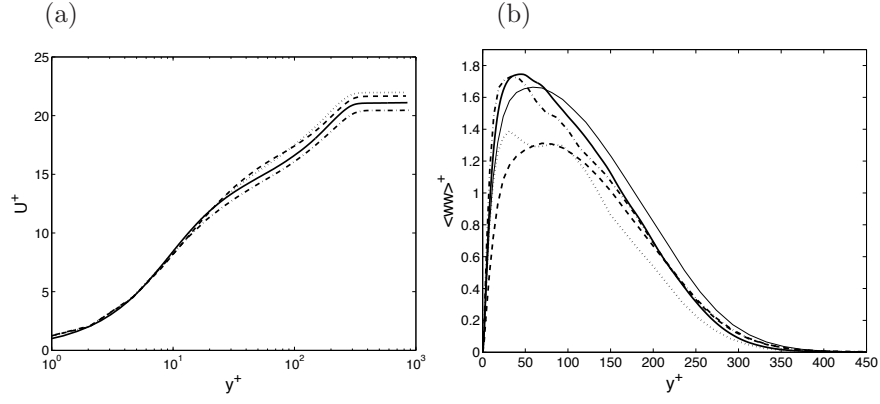


FIGURE 3.7. Turbulence statistics at $Re_\theta = 780$. (a): Mean velocity profile in wall units. (b): $\langle ww \rangle$ in wall units. Non-filtered DNS data, thick solid line; new explicit model, dashed lines; dynamic smagorinsky model, dotted line; sum of $\langle \tau_{33} \rangle$ and $\langle \tilde{w}\tilde{w} \rangle$ using the explicit model, thin solid line.

CHAPTER 4

Outlook

The proposed stochastic SGS model provides for an improved description of the smallest resolved scales in LES with scalar mixing. In the future we wish to investigate the implications for reacting flows where the small scale scalar statistics are important, see Pitsch (2006). The stochastic model may here offer interesting possibilities to this challenging area for LES-computations, because it offers an approach to properly incorporate small-scale effects of scalar mixing and dissipation.

The proposed explicit algebraic SGS stress and flux models have strong similarities with the corresponding RANS models (EARSIM Wallin and Johansson (2000) and EASFM Wikström et al. (2000)). Therefore, it might be interesting to use explicit SGS modelling in hybrid RANS-LES methods, where it might be convenient to use the same type of model in the inner and outer domains. It is also of interest to combine stochastic and explicit algebraic SGS modelling because they complement each other. A combination would provide for an improved small scale dynamics as well as a realistic anisotropy of the SGS stress and scalar flux. Such a combination might be appropriate in LES of combustion near solid walls.

Further validation of the proposed explicit algebraic SGS stress and flux models will be performed in zero pressure gradient boundary layer. The future aim is to further increase the Reynolds number in order to investigate if these models are able to reproduce high Reynolds number effects of in LES of turbulent boundary layer flow.

References

- Ahlman D, Brethouwer G, Johansson A. 2006. Implementation of a method for simulation of compressible wall-bounded mixing flows. Tech. Rep.. Dept. of Mechanics, Royal Institute of Technology.
- Alvelius K, Johansson A V. 1999. Stochastic modelling in LES of a turbulent channel flow with and without system rotation. *In Doctoral Thesis*, Department of Mechanics KTH Sweden.
- Bardina J Ferziger J.H Reynolds, W.C. 1983. Improved turbulence models based on large eddy simulation of homogeneous incompressible flows. Technical report No. **TF-19** Stanford University
- Brethouwer G, Matsuo Y. 2005. DNS of rotating homogeneous shear flow and scalar mixing. Proc. 4th Int. Symp. on Turbulence and Shear Flow Phenomena (TSFP4), Williamsburg, USA. Editors: J A C Humphrey et al.
- Calmet I, Magnaudet J. 1997. Large-eddy simulations of high-Schmidt number mass transfer in a turbulent channel flow. *Phys. Fluids* **9**, 438-455.
- Cerutti S. , Meneveau, C. 1998. Intermittency and relative scaling of subgrid scale energy dissipation in isotropic turbulence. *Phys. Fluids* **10** , 928-937.
- Chaouat B, Schiestel R, (2005) A new partially integrated transport equation model for subgrid-scale stresses and dissipation rate for turbulent developing flows. *Phys. Fluids* **17**, 035106.
- Clark RA, Ferziger JF, Reynolds WC. 1979. Evaluation of subgrid-scale models using an accurately simulated turbulent flow. *J. Fluid Mech.* **91**, 1-16.
- Deardorff J.W. 1970. A numerical study of three-dimensional turbulent channel flow at large Reynolds numbers. *J. Fluid Mech.* **41** , 453-480.
- Ducros F, Comte P, Lesieur M. Large-eddy simulation of transition to turbulence in a boundary layer developing spatially over a flat plate. *J. Fluid Mech.* **326**, 1-36.
- Germano M, Piomelli U, Moin P, Cabot W. 1991. A dynamic subgrid-scale eddy viscosity model. *Phys. Fluids A* **3**, 1760-1765.
- Germano M. 1992. Turbulence: the filtering approach. *J. Fluid Mech.* **238** , p. 325
- Hughes TJR, Mazzei L, Oberai AA. 2001. The multiscale formulation of large eddy simulations: Decay of homogeneous isotropic turbulence. *Phys. Fluids*, **13**, 505-512.

- Hughes TJR, Mazzei L, Oberai AA. 2001. Large eddy simulation of turbulent channel flows by the variational multiscale method. *Phys. Fluids*, **13**, 1784-1799.
- Kang H S, Meneveau C. 2001. Passive scalar anisotropy in a heated turbulent wake, new observations and implications for large eddy simulations. *J. Fluid Mech.* **442**, 161-170.
- Leith C E. 1990. Stochastic backscatter in a subgrid-scale model: Plane shear mixing layer. *Phys. Fluids A* **2**, 297-299.
- Li Q. 2007. Direct numerical simulation of a turbulent boundary layer with passive scalar transport. *Technical report*
- Lilly S. 1992. A proposed modification of the Germano subgrid scale closure method. *Phys. Fluids A* **4**, 633-635.
- Liu S, Meneveau C, Katz J, 1994. On the properties of similarity subgrid-scale models as deduced from measurements in a turbulent jet. *J. Fluid Mech.* **275**, 83-119.
- Liu C. High performance computation for DNS/LES. *Applied Math. Modelling* **30**, 1143-1165.
- Marstorp L, Brethouwer G, Johansson A. 2007. A stochastic subgrid model with application to turbulent flow and scalar mixing. *Phys. Fluids* **19**, 035107.
- Marstorp L, Brethouwer G, Johansson A. 2008. Explicit algebraic subgrid stress models with application to rotating channel flow. *Submitted to J. Fluid Mech.*
- Marstorp L, Brethouwer G, Johansson A. 2008. An explicit algebraic model for the subgrid-scale passive scalar flux. *Submitted to Phys. Fluids*
- Marstorp L, , Qiang Li, Philipp Schlatter, Brethouwer G, Johansson A. 2008. Validation of SGS models in LES of turbulent zero pressure gradient boundary layer. *Technical report*
- Meneveau C, Lund T, Cabot W. 1996. A Lagrangian dynamic sub-grid scale model of turbulence. *J. Fluid Mech.* **319**, 353-385.
- Moin P, Kim J. 1982. Numerical investigation of turbulent channel flow. *J. Fluid Mech.* **118**, 341-377.
- Piomelli U, Cabot W, Moin P, Lee S. 1991. Subgrid-scale backscatter in turbulent and transitional flows. *Phys. Fluids A* **3**, 1766-1771.
- Pitsch H. 2006 Large-Eddy Simulation of turbulent combustion. *Annual rev. of Fluid Mech.* **38**, 453-482
- Pope S. 2000. Turbulent flows. Cambridge University Press, Cambridge, UK.
- Sagaut P, Comte P, Ducros F. Filtered subgrid-scale models. *Phys. Fluids*, **12**, 233-236.
- Schlatter P, Brandt L, Bruhn T, Henningson DS. 2006. Dynamic high-pass filtered eddy-viscosity models for LES of turbulent boundary layers *Bulletin American Physical Society*, **51**, 213.
- Schumann U. 1975. Subgrid scale model for finite difference simulation of turbulent flows in plane channels and annuli. *J. Comp. Phys.* **18**, 376-404.
- Schumann U. 1995. Stochastic backscatter of turbulence energies and scalar variance by random subgrid-scale fluxes. *Proceedings of the Royal Society of London, Series A, Phys.* **451**, 293-318.
- Smagorinsky J S. 1962. General circulation experiments with the primitive equations: I. The basic experiments. *Mon. Weather Rev.* **91**, 99.

- Stolz S, Adams N. 1999. An approximate deconvolution procedure for large-eddy simulation. *Phys. Fluids* **11**, 1699-1701.
- Stolz S, Schlatter P, Kleiser L.(2005) High-pass filtered eddy-viscosity models for large-eddy simulations of transitional and turbulent flow. *Phys. Fluids* **17**, 065103.
- Tseng YH, Meneveau C, Parlange MB. 2006. Modeling flow around bluff bodies and predicting urban dispersion using large eddy simulation. *Environ. Sci. Technol.* **40**, 2653-2662.
- Wallin S, Johansson AV. 2000. An explicit algebraic Reynolds stress model for incompressible and compressible turbulent flows. *J. Fluid Mech.* **403** , p. 89
- Wang B, Bergstrom D (2005) A dynamic nonlinear subgrid-scale stress model. *Phys. Fluids*, **17**, 035109.
- Wikström P M, Wallin S, Johansson A V. 2000. Derivation and investigation of a new algebraic model for the passive scalar flux. *Phys. Fluids* **12**, 688-702.
- Zang Y, Street R, Koseff J. 1993. A dynamic subgrid-scale model and its application to turbulent recirculating flows. *Phys. Fluids A* **5**, 3186-3196.

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