Anisotropy-resolving subgrid-scale modelling
using explicit algebraic closures
for large eddy simulation

by

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Anisotropy-resolving subgrid-scale modelling using explicit algebraic closures for large eddy simulation
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Abstract
The present thesis deals with the development and performance analysis of anisotropy-resolving models for the small, unresolved scales ("sub-grid scales", SGS) in large eddy simulation (LES). The models are characterised by a description of anisotropy by use of explicit algebraic models for both the subgrid-scale (SGS) stress tensor (EASSM) and SGS scalar flux vector (EASSFM). Extensive analysis of the performance of the explicit algebraic SGS stress model (EASSM) has been performed and comparisons made with the conventional isotropic dynamic eddy viscosity model (DEVM). The studies include LES of plane channel flow at relatively high Reynolds numbers and a wide range of resolutions and LES of separated flow in a channel with streamwise periodic hill-shaped constrictions (periodic hill flow) at coarse resolutions. The former simulations were carried out with a pseudo-spectral Navier–Stokes solver, while the latter simulations were computed with a second-order, finite-volume based solver for unstructured grids. The LESs of channel flow demonstrate that the EASSM gives a good description of the SGS anisotropy, which in turn gives a high degree of resolution independence, contrary to the behaviour of LES predictions using the DEVM. LESs of periodic hill flow showed that the EASSM also for this case gives significantly better flow predictions than the DEV. In particular, the reattachment point was much better predicted with the EASSM and reasonably well predicted even at very coarse resolutions, where the DEV is unable to predict a proper flow separation.

The explicit algebraic SGS scalar flux model (EASSFM) is developed to improve LES predictions of complex anisotropic flows with turbulent heat or mass transfer, and can be described as a nonlinear tensor eddy diffusivity model. It was tested in combination with the EASSM for the SGS stresses, and its performance was compared to the conventional dynamic eddy diffusivity model (DEDM) in channel flow with and without system rotation in the wall-normal direction. EASSM and EASSFM gave predictions of high accuracy for mean velocity and mean scalar fields, as well as stresses and scalar flux components.

An extension of the EASSM and EASSFM, based on stochastic differential equations of Langevin type, gave further improvements. In contrast to conventional models, these extended models are able to describe intermittent transfer of energy from the small, unresolved scales, to the resolved large ones.

The present study shows that the EASSM/EASSFM gives a clear improvement of LES of wall-bounded flows in simple, as well as in complex geometries in comparison with simpler SGS models. This is also shown to hold for a wide range of resolutions and is particularly accentuated for coarse resolution. The
advantages are also demonstrated both for high-order numerical schemes and
for solvers using low-order finite volume methods. The models therefore have
a clear potential for more applied computational fluid mechanics.

Descriptors: Turbulence, large eddy simulation, explicit algebraic subgrid-
scale model, passive scalar, stochastic modelling, periodic hill flow.
Explicita algebraiska modeller för anisotropi-beskrivande sub-grid-skaletmodellering i storvirvelsimulering ("LES")

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Sammanfattning


Den explicita algebraiska skalärfuxmodellen (EASSFM) är utvecklad för att förbättra LES-prediktioner av komplexa, anisotropa strömningar och kan beskrivas som en ickelinjär virvelviskositetsmodell i tensorform. Den testades i kombination med en EASSM för SGS-spänningsarna och jämfördes med en konventionell dynamisk virvelviskositetsmodell (DEDM) i kanaströmning med och utan rotation kring den väggnormala riktningen. EASSM och EASSFM gav LES-prediktioner av hög noggrannhet för medelhastigheter och medelskalär såväl som för spännings och skalärfuxkomponenter.

En utvidgning av SGS-modellerna, EASSM och EASSFM, baserad på stokastiska differentialekvationer av Langevintyp, gav ytterligare förbättring. Till skillnad från konventionella modeller kan dessa utvidgade modeller också beskriva intermittent överföring från de små, modellerade skalorna, till de upplösta stora virvlarna.
Den föreliggande studien visar att EASSM/EASSFM ger en klar förbättring av LES av väggnära strömningar i enkla såväl som mer komplexa geometrier (med relativt grov nätupplösning) i jämförelse med enklare modeller, både med beräkningskoder med högre och lägre ordnings noggrannhet. Modellen har därför en tydlig potentiell för mer tillämpade strömningsberäkningar.

Deskriptorer: Turbulens, storvirvelsimulering, explicita algebraiska subgridskalemodeller, passiv skalär, stokastisk modellering.
Preface

The present thesis deals with the development and performance analysis of the anisotropy resolving explicit algebraic subgrid-scale (SGS) models for large eddy simulation (LES). The first part introduces the basics of turbulence, LES and SGS modelling. The concept of nonlinear SGS stress modelling and, especially, the explicit algebraic SGS stress model are discussed. The tensor eddy diffusivity modelling and, specifically, the explicit algebraic SGS scalar flux model are also introduced. The performance of the explicit algebraic SGS models is demonstrated in LES of plane channel flow with and without system rotation and channel flow with periodic hill-shaped constrictions. An approach for a stochastic extension of the explicit algebraic SGS models is also discussed. The second part contains the following papers.


Paper II. A. Rasam, S. Wallin, G. Brethouwer and A. V. Johansson, 2014
Large eddy simulation of channel flow with and without periodic constrictions using the explicit algebraic subgrid-scale model, Submitted to J. Turbulence.

A comparison between isotropic and anisotropy-resolving closures in large eddy simulation of separated flow, Internal report.


Paper V. A. Rasam, G. Brethouwer and A. V. Johansson, 2014
A stochastic extension of the explicit algebraic subgrid-scale models, Under revision for publication in Phys. Fluids.
Division of work between authors
The main advisor of the project is Prof. Arne V. Johansson (AJ) and the co-
advisor is Dr. Geert Brethouwer (GB).

Paper I
Numerical simulations and writing of the article are carried out by Amin Rasam
(AR). AJ and GB provided supervision and also comments on the article. Dr.
Philipp Schlatter and Dr. Qiang Li have contributed to some of the discussions
and have commented on the manuscript.

Paper II
Implementation of the model in the code as well as performing the simulations
and writing the manuscript have been carried out by AR. AJ and GB have pro-
vided supervision and comments on the manuscript. Dr. Stefan Wallin (SW)
has contributed to the discussions and has commented on the manuscript.

Paper III
Implementation of the model in the code as well as writing the manuscript
and performing the simulations have been carried out by AR. AJ and GB have
provided supervision and comments on the manuscript. SW has contributed
to the discussions and has commented on the manuscript.

Paper IV
Development and implementation of the model as well as writing the manu-
script and performing the simulations have been carried out by AR. AJ and
GB have provided supervision and comments on the manuscript.

Paper V
Development and implementation of the model as well as writing the manu-
script and performing the simulations have been carried out by AR. AJ and
GB have provided supervision and comments on the manuscript.
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Part I

Introduction
Turbulence

Turbulence occurs in many engineering and environmental flows. It is characterised by random and chaotic motions and it is a phenomenon involving three-dimensional vortex stretching. These characteristics of turbulence are best observed in flow visualisations. Figure 1.2 shows vortical structures in a turbulent channel flow at a moderate Reynolds number using the $\lambda_2$ criterion for vortex identification (Jeong & Hussain 1995). Random and chaotic vorticity is readily observable in the whole flow field. Turbulence occurs at high Reynolds numbers and enhances mixing and heat transfer. Turbulent flows also consist of a broad range of spatial and temporal scales. Some of these characteristics of turbulence can be observed in figure 1.1 where snapshots of the instantaneous temperature field of a turbulent channel flow are shown.

It is important to quantify the relation between the various scales of turbulence to understand the mechanism of turbulence energy production, transfer and dissipation. One of the basic ideas in turbulence which discusses this connection is the energy cascade concept (Richardson 1922). It states that turbulent flows can be imagined to consist of eddies of different sizes. The large energy containing eddies are unstable and break down and transfer energy into smaller eddies. This process goes on till the smallest eddies where the energy is transformed into heat by viscous effects. This idea is stated in Richardson’s famous poem:

\begin{quote}
Big whorls have little whorls
That feed on their velocity
And little whorls have lesser whorls
And so on to viscosity (in the molecular sense).
\end{quote}

The size of the largest scales, where the turbulent energy is produced, is typically set by the flow domain, e.g. channel height in case of the channel flow in figures 1.1 and 1.2 and their time scale is found from their length scale and the large-scale velocity, see e.g. Tennekes & Lumley (1972). The size and time scale of the smallest scales are deduced from Kolmogorov’s first hypothesis (Kolmogorov 1941). It states that at sufficiently high Reynolds number, the statistics of the small scales are universal and are determined solely by the viscosity $\nu$ and energy dissipation rate $\varepsilon$. Hence, their length $\eta$, time $t_\eta$ and velocity $v_\eta$ scales, called Kolmogorov scales, are found from
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Figure 1.1. Contour plots of instantaneous temperature field of channel flow at $Re = 590$ and $Pr = 0.71$, reproduced from DNS data from [Rasam et al.] (2013). The upper (hot) and lower (cold) walls are at constant but different temperatures.

dimensional analysis as

$$
\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}, \quad t_\eta = \left(\frac{\nu}{\varepsilon}\right)^{1/2}, \quad \nu_\eta = (\nu\varepsilon)^{1/4}.
(1.1)
$$

Another important hypothesis in the study of turbulence, describing the idea of the scale invariance and quantifying the energy cascade, is Kolmogorov’s second hypothesis. It states that at sufficiently high Reynolds number the statistics of the scales sufficiently larger than $\eta$ and much smaller than the largest energetic scales are solely described by $\varepsilon$. The range of scales at which this hypothesis refers to is termed the inertial range and the energy spectrum in this range is given by

$$
E(k) = C_k \varepsilon^{2/3} k^{-5/3},
(1.2)
$$

where $k$ is the magnitude of the wave number and $C_k \approx 1.5$ (Sreenivasan 1995) is the Kolmogorov constant. This equation implies the scale invariance of energy (Meneveau & Katz 2000). As it will be briefly shown in the proceeding chapters (see also e.g. Meneveau & Katz 2000; Sagaut 2010), various scale invariance assumptions are used in the subgrid-scale models in large eddy simulation. Equation (1.2) is also used in developing and assessing subgrid-scale model coefficients, such as the constant in the eddy viscosity model in simulations of isotropic turbulence (see e.g. Davidson 2003).

The governing equations of turbulent flows are the Navier–Stokes and continuity equations, which in the incompressible and non-dimensional form are expressed as

$$
\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \quad \frac{\partial u_i}{\partial x_i} = 0,
(1.3)
$$

where $Re$ is the characteristic Reynolds number of the flow, $u_i$ are the velocity components, $p$ is the pressure and the summation convention over the repeated indices is used. The transport of a passive scalar $\theta$ in a turbulent flow is
expressed as

$$\frac{\partial \theta}{\partial t} + \frac{\partial u_j \theta}{\partial x_j} = \frac{1}{RePr} \frac{\partial^2 \theta}{\partial x_j \partial x_j}, \quad (1.4)$$

where $Pr$ is the Prandtl number. There are a number of approaches for the numerical solution of the Navier–Stokes and passive scalar transport equations for turbulent flows. A direct numerical simulation (DNS), which solves the Navier–Stokes equations without making any assumptions, resolves all the scales from the large integral scales down to the Kolmogorov scales. It provides the most detailed information about the flow at various scales. The computational cost of DNS scales with the Reynolds number as $\sim Re^{37/14}$ (Choi & Moin 2012), hence it is not affordable for high Reynolds number engineering type of flows. However, simple canonical flows, i.e. channel, pipe and boundary layer flows, have been studied using DNS. The first DNS of fully developed incompressible channel flow was performed by Kim et al. (1987) at Reynolds number $Re_T = 180$, based on the friction velocity and channel half height. Many DNSs of canonical flows at higher Reynolds numbers have been performed since this pioneering work, see e.g. the review by Kim (2012).

The Reynolds averaged Navier–Stokes (RANS) modelling approach starts with the Reynolds decomposition (Reynolds 1895)

$$u_i = \overline{u_i} + u'_i, \quad \theta = \overline{\theta} + \theta'$$

where the overbar denotes an ensemble averaged quantity and $u'_i$ and $\theta'$ are the velocity and scalar fluctuations, respectively. Introducing the Reynolds decomposition into the incompressible Navier–Stokes equations (1.3) and passive scalar transport (1.4) and taking the ensemble average yields the basic RANS equations

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial \overline{u_i} \overline{u_j}}{\partial x_j} = \frac{1}{Re} \frac{\partial \overline{\rho}}{\partial x_i} - \frac{\partial \overline{u'_i u'_j}}{\partial x_j} + \frac{\partial^2 \overline{u_i}}{\partial x_j \partial x_j}, \quad \frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{u_i} \theta}{\partial x_i} = \frac{1}{RePr} \frac{\partial^2 \overline{\theta}}{\partial x_j \partial x_j} - \frac{\partial \overline{u'_i \theta'}}{\partial x_j},$$

(1.6) (1.7)

where all the turbulent effects are contained in the Reynolds stress tensor $\overline{u'_i u'_j}$, and scalar flux vector $\overline{u'_i \theta'}$. Hence, it provides only approximate information about the ensemble averaged quantities. The closure problem arises from the $\overline{u'_i u'_j}$ and $\overline{u'_i \theta'}$ terms which are not known and need to be modelled to close the equations.

The first approximation for $\overline{u'_i u'_j}$ based on the mixing-length theory was proposed by Boussinesq in 1877. In a general form it can be written as the following eddy viscosity model

$$\overline{u'_i u'_j} - \frac{2}{3} K \delta_{ij} = -2 \nu_T \overline{S_{ij}}, \quad \overline{S_{ij}} = \frac{1}{2} \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right),$$

(1.8)
where $K = \overline{u'_i u'_i}/2$ is the mean turbulence kinetic energy, $\mathbf{S}_{ij}$ is the mean strain-rate tensor, the symmetric part of the mean velocity gradient tensor, $\nu_T$ is the eddy viscosity which needs to be modelled using a proper length $L$ and velocity scale $V$. Different levels of approximation are used to model $\nu_T$. Algebraic models (also called zero equation models) relate $L$ and $V$ to the mean velocity gradients and the flow geometry. In one-equation models, a transport equation is solved for the turbulence kinetic energy or a similar quantity and an auxiliary turbulent quantity such as the turbulent length scale is computed via an algebraic relation. Examples of one-equation models are the models by Baldwin & Barth (1990) and Spalart & Allmaras (1992). One can also solve two transport equations for two turbulent quantities such as turbulence kinetic energy $K$ and dissipation $\varepsilon$. These models are hence called two-equation models. The $K-\varepsilon$ model by Launder et al. (1975) is an example of these models.

Another alternative for modelling the Reynolds stress tensor is to solve transport equations for each of its components derived from the modelled Navier–Stokes equations, see e.g. Pope (2000) for a discussion about these models. This approach incorporates more physics but is computationally more expensive and complicated than the other approaches. These differential Reynolds stress models may be further simplified by introducing the weak equilibrium assumption by Rodi (1972). It states that in certain flow conditions the advection and diffusion of the Reynolds stress anisotropy can be neglected in its transport equation. This leads to a considerable simplification of the equations and allows for an algebraic formulation of the Reynolds stresses (Rodi 1972). The algebraic relation is, however, implicit in the Reynolds stresses but explicit solutions can be found (Pope 1975; Gatski & Speziale 1993; Wallin & Johansson 2000), resulting in the so called explicit algebraic Reynolds stress models (EARSM). These models are able to capture the anisotropy of the turbulence with a limited overhead in the computational efforts, as compared to eddy-viscosity-based two-equation models. The principle objective of this thesis work is to utilise this modelling approach also for large eddy simulations.

The mixing-length theory (Taylor 1915) was first used to formulate the eddy diffusivity model (EDM) for the mean turbulent scalar flux $\overline{u'_i \theta'}$ which is expressed as

$$
\overline{u'_i \theta'} = -D_T \frac{\partial \overline{\theta}}{\partial x_i}, \quad D_T = \frac{\nu_T}{P_{r_T}},
$$

(1.9)

where $D_T$ is the eddy diffusivity coefficient and $P_{r_T}$ is the turbulent Prandtl number. The simplest formulation for the eddy diffusivity is obtained using a constant value or an empirical correlation (e.g. Reynolds 1975) for $P_{r_T}$ in (1.9). In analogy with the eddy viscosity, two-equation models have also been proposed for computing $D_T$. The model by Nagano & Kim (1988), for example, solves transport equations for half the mean scalar variance $K_\theta = \overline{\theta'^2}/2$ and its dissipation rate $\varepsilon_\theta$. The corresponding $K_\theta - \varepsilon_\theta$ model is used to construct the time scale $\tau_\theta = K_\theta/\varepsilon_\theta$ which is then used to compute $D_T \sim K_\tau$. 
Since the eddy diffusivity assumes an alignment between $u'\theta'$ and the mean scalar gradient it cannot correctly predict all the individual components of the scalar flux. A better representation can be obtained by introducing a tensor eddy diffusivity (Batchelor 1949) so that the EDM is expressed as

$$u'\theta' = -D_{ij} \frac{\partial \theta}{\partial x_j}, \quad (1.10)$$

where $D_{ij}$ is the tensor eddy diffusivity. An example of a tensor EDM is the model by Daly & Harlow (1970)

$$u'\theta' = -C_{\theta} \tau_{\theta} u'_i \frac{\partial \theta}{\partial x_i}, \quad (1.11)$$

where $\tau_{\theta}$ is a suitable time scale of turbulence and $C_{\theta}$ is the model coefficient.

An alternative approach to the EDM is to solve for modelled transport equations for $u'\theta'$, see e.g. Launder (1978), in a similar manner as for the Reynolds stress transport equations. This approach is computationally much more expensive than the EDM but also more accurate. Similar to the EARS, explicit algebraic scalar flux models (EASFM) can be derived from the modelled transport equations of the normalised $u'\theta'$ using the weak equilibrium assumption (Wikström et al. 2000; Girimaji & Balachandar 1998). The final expression for the EASFM of Wikström et al. (2000) is a tensor EDM. The model by Daly & Harlow (1970) can be obtained again by some further simplifications. In this thesis, the approach by Wikström et al. (2000) is applied to large eddy simulation of scalar transport.

Large eddy simulation (LES) is one of the more recent tools for computing turbulent flows. The aim of LES is to resolve the relevant large-scales of the turbulent flow while modelling the influence of the remaining unresolved smaller scales, called subgrid-scales (SGS), on the resolved ones. The separation of scales into the resolved and unresolved scales is usually done by the grid. Due to a more universal behaviour of the turbulence at small scales at high Reynolds numbers, one hopes that simple models, commonly adapted from the RANS approach, can accurately represent the effects of the unresolved scales on the resolved ones. Unlike the RANS approach, LES provides a detailed description of the structure of turbulence. It is computationally much more expensive than RANS simulations but less expensive than DNS, since the small scales, which need fine resolutions for a proper representation, are not resolved in LES. The computational cost of a wall-resolved LES using traditional SGS models scales with Reynolds number as $\sim Re^{26/14}$ (Choi & Moin 2012) which, although much lower than the cost of DNS, is not yet affordable for simulation of many high Reynolds number engineering flows. Nevertheless, the emergence of more powerful computational resources in the past decades, have led to many advances in the field of LES and many steps toward its application to complex flows have been taken, see e.g. the reviews by Moin (2002) and Pitsch (2006).

To show the qualitative differences between LES and DNS, vortical structures in a turbulent channel flow visualised using the $\lambda_2$ criterion are shown in figure 1.2.
It is clear from the figure that the DNS resolves more fine structures than the LES and the difference becomes larger as the LES resolution becomes coarser. A brief introduction to the basics of LES is given in the next chapter. In the following, a short history of LES is given.

LES was first formulated by Smagorinsky (Smagorinsky 1963) for meteorological applications using an eddy viscosity in the SGS model. His work was extended to LES of channel flow by Deardorff (1970) who used wall-functions. Since then, there have been many studies on the prescription of the Smagorinsky model coefficient and its behaviour, see the more recent paper by Meyers & Sagaut (2006). One of the important milestones in the development of LES was the introduction of the dynamic procedure proposed by Germano et al. (1991). The dynamic procedure allowed for the computation of the Smagorinsky coefficient during the simulations instead of a priori prescription and gives a correct asymptotic near-wall behaviour of the computed eddy viscosity. It also switches off the model in laminar areas allowing for a better prediction of transitional flows. The Germano identity that is used in the dynamic procedure is extensively applied in different areas of LES, see Meneveau (2012).

It is generally accepted that a necessary condition for LES to correctly predict different mean flow statistics is that the SGS model provides a reasonably correct amount of energy dissipation in an average sense (Meneveau 1993). Isotropic eddy viscosity SGS models (EVM) with a dynamically determined coefficient satisfy this criterion (Jiménez 1995). However, the SGS stress tensor predicted by this model has little correlation with the real SGS stress tensor, i.e. the correlation coefficient is less than 0.25 (Clark et al. 1979; Liu et al. 1994). This deficiency is due to the imposed alignment between the eigenvectors of the modelled SGS stress and strain-rate tensors in these models, which is not the case for the real SGS stress tensor (Borue & Orszag 1998; Tao et al. 2002; Horinić 2003; Wang & Bergstrom 2005; Rasam et al. 2014a). Therefore, the eddy viscosity models can predict a quantitatively correct mean SGS dissipation but are unable to correctly mimic the SGS dissipation dynamics. Also, the SGS anisotropy cannot be correctly represented by these models, which is a problem at coarse resolutions and near the walls where the SGS dynamics is highly anisotropic (Rasam et al. 2011). Baggett et al. (1997) argued that in LES of wall-bounded flows close to the walls the number of anisotropic non-Kolmogorov-type of modes, i.e. those that depend on more parameters than just the energy dissipation and viscosity, will be of the order of $Re_{\tau}^{2}$ ($Re_{\tau}$ is the Reynolds number based on the friction velocity). This implies that isotropic SGS models, which are unable to model the SGS anisotropy properly, cannot provide reliable LES predictions unless those anisotropic scales are resolved by the grid. This implies that the cost of LES of a wall-bounded flow increases considerably with the Reynolds number.

Subgrid-scale models have been proposed to improve the geometrical description of the modelled SGS stress tensor and resolve the SGS anisotropy. The scale similarity model (Bardina et al. 1980) which has a high correlation with
Figure 1.2. Vortical structures in turbulent channel flow at \( Re_x = 590 \) (Rasam et al. 2013) visualized by isosurfaces of \( \lambda_2 \), colored by the velocity magnitude. DNS data with grid resolution in the streamwise, spanwise and wall-normal directions \( \Delta^+_{x} = 9.6, \Delta^+_{z} = 4.8 \) and \( \Delta^+_{y} = 0.04 \sim 7.2 \), respectively (a). LES data, using the explicit algebraic SGS stress model with grid resolution \( \Delta^+_{x} = 38.3, \Delta^+_{z} = 19.2 \) and \( \Delta^+_{y} = 0.31 \sim 19.2 \) (b) and with grid resolution \( \Delta^+_{x} = 58.1, \Delta^+_{z} = 29.0 \) and \( \Delta^+_{y} = 0.71 \sim 28.9 \) (c).
the real SGS stress (as high as 0.8), nonlinear models (Lund & Novikov 1992; Wong 1992; Kosovic 1997; Wang & Bergstrom 2005; Marstorp et al. 2009) and mixed models based on combination of the scale similarity and EVM (see e.g. Zang et al. 1993), are examples of such models. They give a better description of the SGS stresses than the EVM. The nonlinear models are introduced in the next chapter. In particular, the explicit algebraic SGS stress model (EASSM) by Marstorp et al. (2009), a nonlinear mixed model, will be discussed in detail. Its performance is the subject of investigation in this thesis.

Subgrid-scale models are often tested in LES of simple canonical flows. The reason is the availability of accurate numerical methods for the simulations and DNS or experimental data. However, the ultimate goal of LES is to simulate turbulent flows in complex geometries, with relevance to industrial applications, with a reasonable accuracy. In more complex flows, low-order numerical methods are usually employed since they are robust and flexible. But they have inherent numerical dissipation due to discretisation errors which can be of the order of the SGS dissipation (Chow & Moin 2003). There is no doubt that the performance of an SGS model is significantly affected by the presence of numerical dissipation. Therefore, LES practitioners often tend to increase the number of grid points to decrease the numerical errors and parameterisation errors of the SGS models. In papers II and III, we perform LESs of channel flow with streamwise-periodic constrictions using the EASSM and the dynamic EVM (DEVM) at various resolutions. In these studies we demonstrate the advantages of the EASSM over DEV in LES with a low-order numerical method with inherent numerical dissipation. It was found that the DEV was too dissipative and predicted a too short separation bubble, especially at coarse resolutions. It was also not able to predict a correct SGS shear stress in areas where it has the same sign as the strain-rate tensor which clearly affects the development of the separated shear layer. By contrast, the EASSM was found to provide for lower SGS dissipation in the presence of numerical dissipation. It gave a reasonable prediction of the separation bubble at all resolutions and the shear stress was reasonably well predicted in the whole domain.

Another important topic in LES is the modelling of scalar fields since it has numerous applications from the calculation of heat transfer and dispersion of pollutants in the atmosphere to turbulent combustion. Basic and yet valuable knowledge about mixing can be gained by investigating the passive scalar dynamics in LES. The eddy diffusivity model (EDM) is often used in LES of passive scalar transport. It assumes an alignment between the SGS scalar flux and the resolved scalar gradient vector. However, this is not true in many cases such as shear induced SGS scalar flux close to the walls, e.g. in turbulent channel flow with heat transfer, or the SGS scalar flux induced by rotation, see Rasam et al. (2013). In these examples the SGS scalar flux exists not due to a mean resolved scalar gradient but due to other reasons. Therefore, the EDM cannot predict the correct SGS flux in these cases. Scale similarity and gradient SGS scalar flux models have been proposed to improve SGS predictions...
but they are not dissipative enough and therefore are often combined with an eddy diffusivity term [Salvetti & Banerjee, 1995; Porté-agel et al., 2001; Higgins et al., 2004]. A recent example of a mixed nonlinear SGS scalar flux model is the dynamic tensor EDM by Wang et al. (2008). It consists of a standard eddy diffusivity part and a tensor eddy diffusivity part which is a quadratic tensor function of the resolved strain-rate tensor. Recent studies (Chumakov, 2008) show that the direction of SGS scalar flux vector is more connected with the eigenvectors and eigenvalues of the SGS stress tensor than the resolved scalar gradient vector. In Rasam et al. (2013) (paper IV) we propose an explicit algebraic SGS scalar flux model (EASSFM) for the passive scalar. It is a dynamic nonlinear tensor eddy diffusivity model that improves LES predictions over the EDM, is more consistent with the findings of Chumakov (2008), is more accurate at coarse resolutions than the EDM and is suitable for LES of rotating flows.

It is well known that the instantaneous energy transfer between the resolved and unresolved scales can be both downscale and upscale. The reverse energy cascade (backscatter) is of physical importance to the dynamics of turbulent wall-bounded flows both for the velocity and scalar fields [Leslie & Quarini, 1979; Piomelli et al., 1991; Hartel et al., 1994; Domaradzki et al., 1993, 1994; Dunn & Morrison, 2003; Cimarelli & De Angelis, 2012], but most SGS models do not provide backscatter. It is possible to introduce backscatter in the SGS model predictions via stochastic processes which has been the subject of many investigations [Leith, 1990; Mason & Thompson, 1992; Schumann, 1995]. Inclusion of backscatter and randomness through the introduction of stochastic extensions of the SGS stresses not only improves characteristics of the SGS dissipation such as its variance and length scale but also improves the predictions of the resolved quantities. A stochastic extension of the EASSM and EASSFM is the subject of paper V.
Large eddy simulation

2.1. Separation of scales through the filtering operation

In contrast to direct numerical simulation (DNS), where all the flow scales down to the Kolmogorov ones are resolved, large eddy simulation (LES) is based on a separation of scales. This separation is commonly introduced by a filtering operation which decomposes the velocity and scalar fields into a resolved part, represented by the grid, and an unresolved part. The effect of the unresolved part on the resolved one is modelled. The filtering operation on a function $\phi(x,t)$, as defined by Leonard (1975), is a convolution of a kernel $G_\Delta$ and this function

$$\tilde{\phi}(x,t) = \int_D \phi(\xi,t)G_\Delta(x-\xi)d\xi,$$

where integration is carried out over the whole domain $D$. Commonly used filter kernels are the spectral cutoff, box and Gaussian filters. Only the spectral cutoff filter provides for a clear separation of scales in the spectral space, but it does not have spatial localisation properties and the resulting stress tensor violates the realisability conditions (Vreman et al. 1994) and the filtered scalar can attain physically incorrect values (Meneveau & Katz 2000). A thorough discussion of different filters and their characteristics can be found in Pope (2000) and Sagaut (2010).

2.2. Governing equations and the closure problem

The governing equations of LES including passive scalar transport are obtained by filtering the Navier–Stokes, continuity and the scalar transport equations. Following the Leonard’s decomposition (Leonard 1975) for the nonlinear terms these equations become

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\tilde{u}_i\tilde{u}_j) = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial \tilde{u}_i}{\partial x_i} = 0,$$

(2.2)

$$\frac{\partial \tilde{\theta}}{\partial t} + \frac{\partial}{\partial x_i}(\tilde{u}_i\tilde{\theta}) = \frac{1}{RePr} \frac{\partial^2 \tilde{\theta}}{\partial x_i \partial x_i} - \frac{\partial q_i}{\partial x_i} - \frac{\partial \tilde{q}_i}{\partial x_i} = 0,$$

(2.3)

where the SGS stress tensor $\tau_{ij}$ and scalar flux vector $q_i$ include terms that are not directly expressed in terms of $\tilde{u}_i$ and $\tilde{\theta}$

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{\theta}, \quad q_i = L_{i\theta} + C_{i\theta} + R_{i\theta} = \tilde{u}_i \tilde{\theta} - \tilde{u}_i \tilde{\theta},$$

(2.4)
2.3. EDDY VISCOSITY AND DIFFUSIVITY MODELS

where

\[ L_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j, \quad L_{i\theta} = \tilde{u}_i \tilde{\theta} - \tilde{u}_i \tilde{\theta} \]  (2.5)

\[ C_{ij} = \tilde{u}_i u'_j + \tilde{u}_j u'_i, \quad C_{i\theta} = \tilde{u}'_i \tilde{\theta} + \tilde{u}_i \tilde{\theta}' \]  (2.6)

\[ R_{ij} = u'_i u'_j, \quad R_{i\theta} = u'_i \tilde{\theta}' \]  (2.7)

where \( u'_i = u_i - \tilde{u}_i \). In the Leonard decomposition (2.5), (2.6) and (2.7), \( R_{ij} \) is the Reynolds subgrid tensor representing the interactions between subgrid-scales, \( C_{ij} \) is the cross-stress tensor accounting for large and small scale interactions and \( L_{ij} \) is the Leonard tensor reflecting the interactions among the large scales. The SGS fluxes \( L_{i\theta}, C_{i\theta} \) and \( R_{i\theta} \) are analogous to the Leonard stress, the cross stress and the SGS Reynolds stress tensors, respectively.

\( \tau_{ij} \) and \( q_i \) impose a closure problem and need to be modelled. Since the scales larger than the cutoff are directly computed in LES, \( \tau_{ij} \) and \( q_i \) can be modelled in terms of the resolved quantities. In the proceeding sections the commonly used eddy diffusivity and viscosity models and their extension using the dynamic procedure based on the Germano identity are briefly discussed.

2.3. Eddy viscosity and diffusivity models

The eddy viscosity model (EVM) is often used to model the deviatoric part of the SGS stress tensor. It is expressed as

\[ \tau_{ij} - \frac{\tau_{kk}}{3} \delta_{ij} = -2\nu_{\text{SGS}} \tilde{S}_{ij}, \quad \nu_{\text{SGS}} = (C_s \tilde{\Delta})^2 |\tilde{S}|, \]  (2.8)

where \( \tilde{S}_{ij} \) and \( |\tilde{S}| \) are the resolved strain-rate tensor and its magnitude (e.g. the square root of its second invariant), \( \nu_{\text{SGS}} \) is the SGS eddy viscosity, \( \tilde{\Delta} \) is the grid scale and \( C_s \) is the model coefficient. The EVM is an adaptation of the corresponding RANS model and originates from the relation between the stress and shear in laminar flows. It is clearly insufficient for the description of the SGS stress tensor, the reasons for which were already given in chapter [1].

Similar to \( \nu_{\text{SGS}} \) an SGS eddy diffusivity, \( D_{\text{SGS}} \), is defined for the scalar field

\[ D_{\text{SGS}} = \frac{\nu_{\text{SGS}}}{\text{Pr}_{\text{SGS}}}, \]  (2.9)

where \( \text{Pr}_{\text{SGS}} \) is the SGS Prandtl number. The SGS scalar flux, \( q_i \), according to the eddy diffusivity model (EDM) reads

\[ q_i = -D_{\text{SGS}} \frac{\partial \tilde{\theta}}{\partial x_i}. \]  (2.10)

The SGS Prandtl number appears as an adjustable parameter in the EDM. Different values for \( \text{Pr}_{\text{SGS}} \) can be found in the literature ranging from 0.1 to 1.0 with the commonly used value \( \text{Pr}_{\text{SGS}} = 0.6 \) (Sagaut 2010). There are a number of deficiencies related to the EDM as discussed in chapter [1].

The EDM and EVM are both isotropic models in the sense that \( \nu_{\text{SGS}} \) and \( D_{\text{SGS}} \) are constants rather than dependent on the direction. The EDM and
EVM can be further improved using the Germano identity for computing $Pr_{\text{SGS}}$ and $C_s$, see the next section.

### 2.4. Germano identity and the dynamic procedure

Germano et al. (1991) proposed a procedure, based on the scale invariance assumption that uses the resolved scales to dynamically compute the model coefficient in the EVM during the simulation, rather than prescribing it \textit{a priori}. The Germano identity is expressed as

\[
\mathcal{L}_{ij} = T_{ij} - \hat{\tau}_{ij},
\]

where $\hat{\cdot}$ denotes filtering at a larger scale than the grid filter, usually called the test filter, $T_{ij}$ are the SGS stresses at the test filter level and $\mathcal{L}_{ij} = \hat{u}_i \hat{u}_j - \hat{\bar{u}}_i \hat{\bar{u}}_j$.

The commonly used value for the test filter size is $\hat{\Delta} = 2 \hat{\bar{\Delta}}$. $\hat{\bar{\Delta}}$ can be defined in several ways but usually defined as $\hat{\bar{\Delta}} = \sqrt[3]{\Omega}$, where $\Omega$ is the volume of a computational cell. For the EVM $\tau_{ij}$ and $T_{ij}$ are deduced from (1) and one obtains

\[
\mathcal{L}_{ij} = \frac{1}{3} \mathcal{L}_{kk} \delta_{ij} = -2C_s M_{ij},
\]

where $M_{ij}$ is

\[
M_{ij} = \hat{\Delta}^2 |\hat{S}|\hat{\bar{S}}_{ij} - \hat{\bar{\Delta}}^2 |\hat{S}|\hat{S}_{ij}.
\]

The value of $C_s$ cannot be determined from (2.12) since the system of equations is over-determined. Germano et al. (1991) contracted (2.12) with $\hat{S}_{ij}$ and obtained

\[
C_s = \frac{1}{2} \frac{\langle \mathcal{L}_{ij} \hat{S}_{ij} \rangle}{\langle \hat{S}_{ij} M_{ij} \rangle},
\]

where $\langle \cdot \rangle$ denotes a spatial averaging to smooth out the variations of $C_s$. Lilly (1992) has proposed a least-square method to find $C_s$ from equations (2.12), to improve the predictions. The dynamic procedure significantly improves the performance of the EVM. Also, the correct asymptotic near-wall behaviour of $\nu_{\text{SGS}}$ is also obtained.

The Germano identity has also been used for the dynamic computation of $Pr_{\text{SGS}}$ in the EDM (2.10) (Moin et al. 1991). This leads to

\[
\mathcal{L}_{i\theta} = Q_i - \hat{q}_i,
\]

and the SGS Prandtl number is found as

\[
Pr_{\text{SGS}} = -\frac{\langle M_{i\theta} M_{i\theta} \rangle}{\langle M_{i\theta} L_{i\theta} \rangle},
\]

where

\[
M_{i\theta} = \nu_{\text{SGS}}(\hat{\Delta}) \frac{\partial \hat{\theta}}{\partial x_i} - \nu_{\text{SGS}}(\hat{\bar{\Delta}}) \frac{\partial \bar{\theta}}{\partial \bar{x}_i}.
\]
2.5. SGS DISSIPATION AND ASSESSMENT OF ACCURACY LIMITATIONS

Application of the Germano identity is not limited to the SGS fluxes. It has, for instance, been used in many different fields including modelling of the reaction rate in premixed turbulent combustion and many other cases (Meneveau 2012). In this thesis the Germano identity is used for derivation of the model coefficients for the explicit algebraic SGS models as well as computation of the SGS kinetic energy.

2.5. Subgrid-scale dissipation and assessment of accuracy limitations in LES

The most important statistical feature of \( \tau_{ij} \) and \( q_i \) is their effect on the resolved kinetic energy \( K = \tilde{u}_i \tilde{u}_i / 2 \) and scalar intensity \( K_\theta = \tilde{\theta} \tilde{\theta} / 2 \) (Meneveau 1993; Meneveau & Katz 2000). This is best illustrated by the governing equations of \( K \) (Sagaut 2010) and \( K_\theta \) (Jiménez et al. 2001)

\[
\begin{align*}
\frac{\partial K}{\partial t} + \frac{\partial}{\partial x_j} (\tilde{u}_j K) &= \left[ \nu \frac{\partial \tilde{u}_i}{\partial x_j} \right]_{\text{viscous dissipation}} - \nu \frac{\partial K}{\partial x_i} - \tilde{u}_i \tau_{ij} + \tau_{ij} \tilde{S}_{ij} \quad (2.17) \\
\frac{\partial K_\theta}{\partial t} + \frac{\partial}{\partial x_j} (\tilde{u}_j K_\theta) &= \left[ \nu \frac{Pr \tilde{\theta}}{\partial x_j} \right]_{\text{molecular dissipation}} - \nu \frac{\partial^2 K_\theta}{\partial x_j} - \frac{\partial}{\partial x_i} (\tilde{\theta} q_j) + q_j \frac{\tilde{\theta}}{\partial x_j} \quad (2.18)
\end{align*}
\]

The advection, viscous and molecular dissipation and diffusion terms are denoted in the equations. The viscous and molecular dissipation terms are often negligible in the simulations since the grid scale is much larger than the Kolmogorov one. The diffusion terms transfer energy in space but do not dissipate energy in a volume-averaged sense. The last terms on the right-hand sides represent the transfer of kinetic energy and scalar intensity from the resolved scales to SGS and are called SGS dissipation

\[
\begin{align*}
\Pi &= -\tau_{ij} \tilde{S}_{ij}, & \chi &= -q_j \frac{\tilde{\theta}}{\partial x_j} \quad (2.19)
\end{align*}
\]

The mean SGS dissipation terms are sink terms and dissipate energy. They act as source terms in the corresponding equations of the SGS kinetic energy and scalar intensity. The instantaneous SGS dissipation can attain both positive (forward scatter) and negative (backscatter) values meaning a transfer of energy to or from the subgrid-scales. The SGS dissipation is further discussed in chapter 5.

Characterisation of the various error sources in LES has been the subject of many investigations, see e.g. Chow & Moin (2003), Ghosal (1996) and Kravchenko & Moin (1997). Geurts & Fröhlich (2002) introduced the SGS activity parameter \( s \) defined as

\[
s = \frac{\langle \varepsilon^{\text{SGS}} \rangle}{\langle \varepsilon^{\text{GS}} \rangle + \langle \varepsilon^{\mu} \rangle},
\]
to assess the SGS stress parameterisation errors. Here, $\varepsilon^\mu = 2\nu \tilde{S}_{ij} \tilde{S}_{ij}$ is the viscous dissipation and $\varepsilon^{\text{SGS}} = -\tilde{\tau}_{ij} \tilde{S}_{ij}$ is the SGS dissipation. With increasing resolution, the SGS dissipation becomes smaller and at the same time viscous dissipation becomes larger, hence $s$ tends to smaller values. Theoretically, the maximum value of $s = 1$ occurs at high Reynolds number LES when the cutoff frequency is well in the inertial subrange and the viscous dissipation is negligible. When coarse resolutions are used at moderate Reynolds numbers, simulation results show that $s$ tends to increase as the resolution becomes coarser. In order to analyze the accuracy of LES using this SGS activity parameter, Geurts & Fröhlich (2002) defined an error norm as

$$\delta_E = \left| \frac{E_{\text{LES}} - \tilde{E}_{\text{DNS}}}{\tilde{E}_{\text{DNS}}} \right|, \quad (2.21)$$

where $E_{\text{LES}}$ is the mean resolved kinetic energy in LES integrated over the flow domain and $\tilde{E}_{\text{DNS}}$ is the corresponding value obtained from the DNS field after filtering it to the LES resolution. Here, LES data of turbulent channel flow with the explicit algebraic SGS stress model (EASSM) (Marstorp et al. 2009) at $Re_\tau = 934$ for six different resolutions (Rasam 2011) are used to demonstrate the method. The results, see figure 11(a), show that the relative error $\delta_E$ drops almost exponentially with decreasing $s$ (increasing resolution) which shows that the EASSM reasonably well predicts the SGS dissipation in this range of resolution. Thus, parameterisation errors do not spoil the predictions at coarse resolutions and the errors become small at fine resolutions. This method has been used in paper I as a diagnostic tool for the comparison of various SGS models.
In (Rasam et al. 2013), we introduced a similar SGS activity parameter for the scalar field $s_\theta$, see paper IV. Figure 11(b) shows the behaviour of the error norm with $s_\theta$ for four different resolutions in LES of channel flow with the explicit algebraic SGS scalar flux model (EASSFM) (Rasam et al. 2013) at $Re_\tau = 590$. A similar behaviour of $\delta_E$ for scalar and velocity fields in LES with the EASSM and EASSFM is observed with changing $s_\theta$, see figure 11(b).
CHAPTER 3

Nonlinear subgrid-scale stress models

As pointed out in chapter 1, a priori analysis of the filtered DNS data shows that the SGS stress tensor is not aligned with the resolved strain-rate tensor (see e.g. Borue & Orszag 1998; Tao et al. 2002; Horiuti 2003). This implies that the isotropic eddy viscosity model (EVM), equation (1), cannot correctly predict the individual SGS stresses since the correlation between the EVM prediction and true SGS stress is poor. It is therefore only possible to get an overall mean drain of energy from the resolved scales by the EVM, which is sufficient for a reasonable prediction of some of the resolved statistics if the grid is fine enough to resolve the SGS anisotropy. At coarse resolutions, by virtue of its isotropic formulation and the appreciable anisotropy of the SGS, the model gives poor predictions (see e.g. Rasam 2011; Rasam et al. 2014).

There have been many efforts to develop SGS models that provide for a better prediction of SGS anisotropy, see the summary given in chapter 1. Nonlinear SGS models, a sub-category of the structural models, are examples of such models and are of particular interest in this thesis, since the explicit algebraic SGS stress model belongs to that category. In the following, we introduce the concept of constituent relations, as described by Lund & Novikov (1992), for development of some of the nonlinear models.

3.1. Tensorial polynomial representation of the SGS stress tensor

The tensorial expansion of the SGS stress tensor in terms of the strain- and rotation-rate tensors is based on the idea developed for the closure of the Reynolds stress equations in RANS (Pope 1975). Following this approach, Lund & Novikov (1992) expressed the deviatoric part of the SGS stress tensor \( \tau^d_{ij} \) as a general tensorial function of the filtered strain-rate \( \tilde{S}_{ij} \) and rotation-rate \( \tilde{\Omega}_{ij} \) tensors, the unit tensor \( \delta_{ij} \) and the filter size \( \tilde{\Delta} \) as

\[
\tau^d_{ij} = \tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = f(\tilde{S}_{ij}, \tilde{\Omega}_{ij}, \delta_{ij}, \tilde{\Delta}),
\]

where

\[
\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right), \quad \tilde{\Omega}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right).
\]
The most general form of (3.1) consists of a tensor polynomial with ten elements of different powers of \( \tilde{S}_{ij} \) and \( \tilde{\Omega}_{ij} \) and their combination, with coefficients that are functions of the invariants of \( \tilde{S}_{ij} \) and \( \tilde{\Omega}_{ij} \) or both, obtained using the Cayley-Hamilton theorem, as proposed by Pope (1975) to describe the Reynolds stresses in RANS

\[
\tau^d = \sum_{k=1}^{10} \beta_k T^{(k)},
\]

where \( \beta_k \) are scalar coefficients, functions of the five irreducible tensorial invariants given by

\[
\begin{align*}
\text{II}_S &= \text{tr}(\tilde{S}^2), & \text{II}_\Omega &= \text{tr}(\tilde{\Omega}^2), \\
\text{III}_S &= \text{tr}(\tilde{S}^3), & IV &= \text{tr}(\tilde{S}\tilde{\Omega}^2), \\
V &= \text{tr}(\tilde{\Omega}^2),
\end{align*}
\]

where \( \text{tr}() \) is trace of a matrix. In the rest of this chapter the nonlinear models by Lund & Novikov (1992), Wong (1992), Kosovic (1997) and Wang & Bergstrom (2005) are discussed. Then the explicit algebraic SGS stress model (Marstorp et al. 2009) is introduced and its application to various flows is briefly discussed.

### 3.2. Nonlinear model of Lund and Novikov

Following the tensorial polynomial expansion of the SGS stress tensor, equation (3.3), Lund & Novikov (1992) proposed a set of five symmetric tensorial elements using additional simplifications and expressed the deviatoric part of the SGS stress tensor as

\[
\tau^d = C_1 \tilde{\Delta}^2 |S| S + C_2 \tilde{\Delta}^2 (\tilde{S}^2 - \frac{1}{3} |S| I) + C_3 \tilde{\Delta}^2 (\tilde{\Omega}^2 - \frac{1}{3} I_S I) + C_4 \tilde{\Delta}^2 (\tilde{S}\tilde{\Omega} - \tilde{\Omega} S) + C_5 \tilde{\Delta}^2 S, \quad (3.4)
\]

where \( |S| = \sqrt{2|S|} \). The model coefficients \( C_{1-5} \) were evaluated in a priori analysis of filtered DNS data of isotropic turbulence. The coefficients were computed by a least-square method to minimise the error in the model predictions and then variability and dependence on the tensor invariants were studied (see also Meneveau et al. 1992). It was found that the model coefficients have a weak dependence on the invariants. The correlation coefficient between the
modelled and exact SGS stresses were also examined using different combinations of the terms in (2). It was found that if only two terms in (2) are used, the highest correlation coefficient ($\approx 0.7$) is obtained by considering the first and fourth terms on the right-hand side of (2) and if three terms are to be used the first, fourth and the fifth terms give the highest correlation coefficient ($\approx 0.8$). If constant coefficients obtained through a least-square global optimisation of errors are used, the correlation coefficient drops to 0.28.

### 3.3. Dynamic nonlinear model of Wong

The dynamic nonlinear model of Wong (1992) is expressed as

$$
\tau_{ij} = \frac{2}{3} K_{SGS} \delta_{ij} - 2 C_1 \bar{\Delta} \sqrt{K_{SGS}} S_{ij} - C_2 \bar{N}_{ij},
$$

(3.5)

where $C_1$ and $C_2$ are model coefficients, $K_{SGS} = \tau_{kk}/2$ is the SGS kinetic energy and

$$
\bar{N}_{ij} = \bar{S}_{ik} \bar{S}_{kj} - \frac{1}{3} \bar{S}_{ij} \bar{S}_{kl} \delta_{ij} - \frac{1}{3} \bar{S}_{mn} \bar{S}_{mn} \delta_{ij},
$$

(3.6)

where $\bar{S}_{ij}$ is the Oldroyd derivative of $\bar{S}_{ij}$

$$
\bar{S}_{ij} = \frac{D \bar{S}_{mn}}{Dt} - \frac{\partial \bar{u}_i}{\partial x_k} \bar{S}_{kj} - \frac{\partial \bar{u}_j}{\partial x_k} \bar{S}_{ki},
$$

(3.7)

and $D/Dt = \partial / \partial t + \bar{u}_k \partial / \partial x_k$ is the material derivative based on the resolved velocity field. The model parameters $C_1$ and $C_2$ are found by a dynamic procedure using the Germano identity. This model needs the SGS kinetic energy and the sub-test filter kinetic energy to be computed using either two transport equations for each or a model based on the resolved velocity gradient and the filter size.

### 3.4. The simplified nonlinear SGS model of Kosovic

Kosovic (1997) proposed the following simplified version of (2) by neglecting higher-order terms based on an analysis of their order of magnitude

$$
\tau_{ij}^d = -(C_s \bar{\Delta})^2 \left[ 2 \sqrt{\bar{S}_{ij}} + C_1 \left( \bar{S}_{ik} \bar{S}_{kj} - \frac{1}{3} \bar{S}_{ij} \delta_{ij} \right) + C_2 (\bar{S}_{ik} \bar{\Omega}_{kj} - \bar{\Omega}_{ik} \bar{S}_{kj}) \right],
$$

(3.8)

where $C_s$ is the Smagorinsky constant. An additional partial differential equation for $K_{SGS}$ was solved and the velocity scale in the eddy viscosity part of the model was computed using the $K_{SGS}$ to improve the model prediction near the walls (Lilly 1967). The $C_1$ coefficient was found from the balance between the viscous dissipation $\varepsilon$ and production of $K_{SGS}$

$$
\langle \varepsilon \rangle = - \langle \tau_{ij} \bar{S}_{ij} \rangle = (C_s \bar{\Delta})^2 \left[ 2 \left( \bar{S}_{ij} \right)^2 + C_1 \bar{S}_{ij} \right].
$$

(3.9)

Based on the theory of isotropic turbulence with an infinite inertial range and assuming a sharp spectral filter expressions for $\langle \bar{S}_{ij} \rangle$ in terms of the resolved quantities are proposed and the model coefficient $C_1$ is determined,
3.6. EXPLICIT ALGEBRAIC SUBGRID-SCALE STRESS MODEL

see Kosovic (1997) for details. The other parameter $C_2$ cannot be determined in this way and is assumed to be equal to $C_1$. The model can also account for backscatter, which is adjusted by a parameter. Kosovic (1997) used his model for LES of a shear-driven atmospheric boundary layer and found improvements compared to the eddy viscosity model.

3.5. Dynamic nonlinear SGS model of Wang and Bergstrom

The dynamic nonlinear model (DNM) of Wang & Bergstrom (2005) is expressed as

$$
\tau_{ij}^d = -2C_S \Delta^2 |\tilde{S}| \tilde{S}_{ij} - 4C_W \Delta^2 (\tilde{S}_{ik} \tilde{\Omega}_{kj} - \tilde{\Omega}_{ik} \tilde{S}_{kj}) - 4C_N \Delta^2 (\tilde{S}_{ik} \tilde{S}_{kj} - \frac{1}{3} \langle I_S \delta_{ij} \rangle),
$$

(3.10)

where $C_S$, $C_W$ and $C_N$ are model coefficients which are determined dynamically using the Germano identity and the least-square method of Lilly (1992). The DNM is validated in the case of plane Couette flow. Simulation results show that the model coefficients without any smoothing or local averaging do not become singular. Their model also gives backscatter, which has been shown to be of the order of 10 percent of the forward scatter. The alignment of the predicted SGS stress is also improved in comparison to the EVM.

3.6. Explicit algebraic subgrid-scale stress model

In the previous sections nonlinear SGS stress models were presented which are based on the expansion (3.3). The explicit algebraic SGS stress model (EASSM) (Marstorp et al. 2009) is also a nonlinear model. Similar to the differential SGS stress models (see e.g. Sagaut 2010), the EASSM is derived from the modelled transport equations of the SGS stress anisotropy following the approach that led to the RANS model of Wallin & Johansson (2000). The equilibrium between the SGS kinetic energy production and dissipation in combination with the weak equilibrium assumption (Rod 1972) is used to obtain the following algebraic formulation

$$
c_1 a_{ij} = -\frac{11}{15} \tilde{S}_{ij}^* + \frac{4}{9} (a_{ik} \tilde{\Omega}_{kj}^* - \tilde{\Omega}_{ik}^* a_{kj}),
$$

(3.11)

where $c_1$ is a model coefficient, $a_{ij} = \tau_{ij}^d / K_{SGS}$ is the SGS stress anisotropy and $\tilde{S}_{ij}^*$ and $\tilde{\Omega}_{ij}^*$ are the resolved strain- and rotation-rate tensors, respectively, normalised by the SGS time scale $\tau^*$. For statistically two-dimensional flows, $T^1$, $T^2$ and $T^4$ form an integrity basis and there are two independent invariants $I_S$ and $I_\Omega$ (Gatski & Speziale 1993). Therefore, the tensorial expansion (3.3) can be written for $a_{ij}$ in terms of $\tilde{S}_{ij}^*$ and $\tilde{\Omega}_{ij}^*$ as

$$
a_{ij} = \beta_1 \tilde{S}_{ij}^* + \beta_4 \left( \tilde{S}_{ik} \tilde{\Omega}_{kj}^* - \tilde{\Omega}_{ik}^* \tilde{S}_{kj}^* \right),
$$

(3.12)

It is worth mentioning that the combination of the terms used above was found by Lund & Novikov (1992) to give the highest correlation between the real
and modelled SGS stresses among the two component tensorial expansions, see section 3.2. The EASSM is expressed for the SGS stress tensor as

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

(3.13)

The second term on the right-hand side is an eddy-viscosity term which controls the SGS dissipation, while the third term provides for anisotropy of the SGS stresses and is responsible for the non-alignment of the SGS stress and resolved strain-rate tensors (Horiuti 2003). The EASSM uses Yoshizawa’s model (Yoshizawa 1986) for modelling $K_{SGS}$ using a dynamic procedure as

$$
K_{SGS} = c \tilde{s}_2 \tilde{\Omega}^*,
$$

(3.14)

where the model coefficient $c$ is dynamically determined using the Germano identity

$$
c = \frac{1}{2} \tilde{u}_k \tilde{u}_k - \tilde{\Omega}^* \tilde{\Omega}^* \tilde{s}_2 |\tilde{\Omega}^*|^2.
$$

One of the differences between the EASSM and other nonlinear models is that the expansion coefficients $\beta_1$ and $\beta_4$ are obtained by substituting (3.12) in the modelled transport equations (7) of $a_{ij}$ and are given as

$$
\beta_1 = \frac{9}{4} c_1, \quad \beta_4 = -\frac{33}{20} \frac{1}{\left(9 c_1/4\right)^2 + |\tilde{\Omega}^*|^2},
$$

(3.15)

where $|\tilde{\Omega}^*| = \sqrt{2 \tilde{\Omega}_{ij}^* \tilde{\Omega}_{ij}^*}$. The model parameter $c_1$ is determined from the dynamic coefficient $c$ and the SGS time scale, $\tau^*$, is modelled as

$$
c_1 = c'_1 \sqrt{c'_3} \left(2 C_\kappa\right)^{2.5}, \quad \tau^* = C_\kappa \frac{1.5 C_\kappa^{1.5}}{2 C_s} |\tilde{S}|^{-1},
$$

(3.16)

where $c'_1 = 3.12$, $c'_3 = 0.91$, $C_\kappa = 1.5$ is the Kolmogorov constant and $C_s = 0.1$. For details of the model derivation and the model coefficients $\beta_1$ and $\beta_4$ see Marstorp et al. (2009) and Rasam et al. (2014a).

In the following a summary of the simulation results obtained with the EASSM in the framework of this thesis are given. These include channel flow simulations at $Re_\tau = 934$ and 2003, channel flow with system rotation and channel flow with streamwise periodic hill-shaped constrictions.

### 3.6.1. Turbulent channel flow at $Re_\tau = 934$ and 2003

LES results of turbulent plane channel flow with two bulk Reynolds numbers corresponding to the DNSs of Hoyas & Jiménez (2008) with $Re_\tau = 2003$, based on friction velocity and channel half-width, and del Alamo & Jiménez (2003) with $Re_\tau = 934$ are presented. The LES results at $Re_\tau = 934$ are taken from paper I (Rasam 2011). LESs are performed at four different resolutions using the EASSM and DEVM with a constant mass flux constraint. The effect of resolving the SGS anisotropy by the EASSM on the mean velocity and Reynolds stress predictions is demonstrated by comparing with the LES results using
3.6. EXPLICIT ALGEBRAIC SUBGRID-SCALE STRESS MODEL

Figure 3.1. Resolution diagram displaying the grid resolution in streamwise and spanwise directions in wall units, i.e. \( \Delta_x^+ \) and \( \Delta_z^+ \), for the four different grids; • : \( Re_\tau = 934 \); Figures also show percentage of the error in LES predictions of \( Re_\tau \), i.e. \( \% E_{Re_\tau} = (Re_{\tau}^{LES} - Re_{\tau}^{DNS}) / Re_{\tau}^{DNS} \) vs the streamwise grid resolution \( \Delta_x^+ \) for the EASSM (a) and DEVM (b); • : \% \( E_{Re_\tau} \) at \( Re_\tau = 2003 \); • : \% \( E_{Re_\tau} \) at \( Re_\tau = 934 \);

The mean velocity profiles in wall units are shown in figure 3.2(a). The EASSM predictions are close to the DNS profile and are similar at all resolutions. In contrast, the DEVM strongly over-predicts the mean velocity profile at coarser resolutions and is only close to the DNS at the finest resolution. Reynolds stresses are shown in figures 3.2(b)–(d). Due to the presence of the wall, the turbulence is highly anisotropic. The \( \langle v'v' \rangle \) and \( \langle w'w' \rangle \) stresses are suppressed by the wall and both are much smaller than \( \langle u'u' \rangle \). The turbulent energy in the streamwise direction is transferred to the other components by the action of the pressure and velocity gradients. At coarser resolutions the SGS is more anisotropic and is more affected by the anisotropic dynamics of

the isotropic DEVM. The streamwise and spanwise resolutions of each grid are shown in the resolution diagrams in figures 3.1(a) and (b). The error in \( Re_\tau \) predictions relative to the DNS results at various resolutions is also displayed in these figures. The DEVM gives larger errors, especially at coarse resolutions, than the EASSM. The error in the EASSM predictions is small at all resolutions.
the resolved flow field and this needs to be properly modelled. Due to the misprediction of the SGS anisotropy by the DEVM at coarser resolutions, the peak of \( \langle u'u' \rangle \) is largely over-predicted, see [3.2] (b). This is also observed in other studies (see e.g. [Kravchenko et al. 1996; Rasam et al. 2011]). The over-prediction decreases with increasing resolution since the subgrid-scales become more isotropic. It has to be pointed out that the Reynolds stresses in figure [3.2] only contain the resolved part for the DEVM, hence the over-prediction of the \( \langle u'u' \rangle \) peak value should be actually higher. The EASSM computes the total Reynolds stress and the comparison between DNS and LES is complete [Winckelmans & Jeanmart 2002]. The \( \langle v'v' \rangle \) and \( \langle w'w' \rangle \) are under-predicted by the DEVM due to the reasons discussed before. The DEVM predictions at the coarsest resolution differ significantly from those at the finest resolution.
3.6. EXPLICIT ALGEBRAIC SUBGRID-SCALE STRESS MODEL

whereas the EASSM predictions are always reasonably close to the DNS results and are less resolution dependent. This better performance of the EASSM can be attributed to the proper modelling of the anisotropy of the subgrid-scales.

**Figure 3.3.** Horizontal snapshots (x-z) of (a-b): streamwise velocity fluctuations $u^+$; (c-d): spanwise velocity fluctuations $w^+$; (e-f): scalar fluctuations $\theta^+$ in wall units at $y^+ \approx 15$. Upper row: DNS of channel flow without system rotation (Rasam et al. 2013). Lower row: DNS of channel flow with system rotation in the wall-normal direction with $Ro_\tau = 0.054$ (Rasam et al. 2013).

A considerable reduction in the required computational resources can thus be achieved by using a coarse mesh with the EASSM and yet obtain comparable predictions to LES with the DEVM. In channel flow predictions given in this section, the EASSM predictions of the mean velocity and Reynolds stresses for the coarsest mesh are roughly comparable with those of the DEVM for the finest mesh. The number of grid points used for the EASSM is approximately 1/11 of the number of grid points used for the DEVM. The EASSM thus reduces the computational costs by approximately one order of magnitude and perhaps even more since the coarser mesh allows for a larger time step.
3. NONLINEAR SUBGRID-SCALE STRESS MODELS

Figure 3.4. (a): Mean streamwise (left half) and spanwise (right half) velocity profiles normalized with the friction velocity. (b): Angle of the mean velocity vector relative to the streamwise direction, $\alpha$, as a function of the distance from the wall for $Ro_{\tau} = 0.018$ (left figure) and $Ro_{\tau} = 0.054$ (right figure). Arrows point in the direction of increasing rotation rate. DNS, solid line; EASSM, dashed line; DEV, dotted line.

3.6.2. Turbulent channel flow with system rotation

Turbulence subject to rotation has many complex features, (see e.g. Cambon et al. 1997; Brethouwer 2005; Grundestam et al. 2008; Mehdizadeh & Oberlack 2010) and can be substantially different from non-rotating flows. Figure 3.3 (a-f) shows snapshots of the instantaneous fluctuations of streamwise and spanwise velocity and temperature, in the buffer layer of turbulent channel flow with and without system rotation around the wall-normal direction in DNS of Rasam et al. (2013). One can immediately observe the differences in the near-wall turbulent structures in the two cases. The streaks are more elongated in the rotating flow and are aligned with the mean flow direction, which is tilted towards the spanwise direction.

One of the most important implications of rotation for the SGS dynamics is the increase in the SGS anisotropy. Isotropic SGS models such as the DEV can give a reasonable prediction of turbulent flows with system rotation as long as the grid is fine enough and the resolved scales capture most of the effects of rotation (Tafti & Vanka 1991; Pallares & Davidson 2000; Cui & Street 2001). SGS models that are specifically designed to handle rotation are scarce. Rotational effects are accounted for, to some extent, in the formulation of the EASSM. But the weak equilibrium assumption used in the derivation of the model is not strictly valid for the subgrid-scales and in particular for rotating flows. Nevertheless, the EASSM has been shown to give good predictions in these flows as well (Marstorp et al. 2009; Rasam et al. 2013).
3.6. EXPLICIT ALGEBRAIC SUBGRID-SCALE STRESS MODEL

3.6.1. Turbulent channel flow with streamwise periodic constrictions

LES of turbulent channel flow with streamwise periodic hill-shaped constrictions with spanwise homogeneity (periodic hill flow) is studied using the EASSM and DEVM for three coarse grids. The geometry of the flow is shown in figure 3.6 where snapshots of the instantaneous velocity are presented. The computational domain sizes in the streamwise, spanwise and cross-stream directions are $L_x = 9h$, $L_z = 4.5h$ and $L_y = 3.035h$ where $h$ is the hill height. The dimension of the hills in the streamwise direction is $L_h = 3.86h$ and the distance between two successive hills is $5.14h$. The bulk Reynolds number of the flow, based on the hill height and the bulk velocity $u_b$ on top of the hill, is $Re_b = u_b h/\nu = 10595$.

The periodic hill flow features separation from a curved surface, subsequent reattachment, a strong shear layer and rapid acceleration and deceleration of...
3. NONLINEAR SUBGRID-SCALE STRESS MODELS

Figure 3.6. Streamlines of the mean flow at three resolutions with contour plot of the mean resolved shear stress in outer units \( \langle u'v' \rangle / \langle u_b \rangle^2 \), for the finest grid; EASSM (a) and DEVM (b). Different resolutions are separated by a shift in the plot. Arrows point in the direction of decreasing resolution.

The flow. The separation point has a high spatial variation in time. These characteristics of this flow make it a challenging test case for LES. It has been studied in several papers using DNS, LES and experiments at various resolutions and Reynolds numbers (Almeida et al. 1993; Temmerman et al. 2003; Fröhlich et al. 2005; Breuer et al. 2009; Manhart et al. 2011).

Code Saturne (Archambeau et al. 2004), an unstructured collocated finite volume solver for incompressible flows, has been used in the present study. It uses a second-order central difference scheme for spatial discretisation. The inherent numerical dissipation of this low-order code has a significant effect on the LESs, as shown in LES of channel flow (Rasan et al. 2014). LES results with the EASSM are assessed against LES with the DEVM and reference LES data of Breuer et al. (2009).

The effects of the SGS stresses and dissipation on the development of the separated shear layer in such a complex flow are obvious and LES results are
found to be very sensitive to the performance of the SGS model at these coarse resolutions, e.g. an over-dissipative SGS model gives a too short separation bubble. Streamlines of the mean flow for three resolutions give an overview of the influence of the models, see figure 4(a) and (b) (see paper III for the details of the grid resolutions). Both the shape and size of the separation bubble are different in the LES with the EASSM and DEVM. The EASSM gives a reasonable prediction of the streamlines at all resolutions, while the DEVM predicts a very small separation bubble at the coarsest resolution.

Besides the shape and size of the separation bubble, the location of the separation and reattachment points are also very sensitive to the SGS model, see figure 5. The EASSM predictions are much closer to the reference LES data than the DEVM predictions.

The good performance of the EASSM in LES of the periodic hill flow at various resolutions makes it a good candidate for LES of flows in complex geometries with low-order numerical methods.
Tensor eddy diffusivity subgrid-scale models

The scalar eddy diffusivity model (EDM) assumes an alignment between the scalar flux and scalar gradient. Hence, it cannot correctly predict all the individual components of the mean scalar flux vector, for example, in shear flows when the scalar flux is not aligned with the mean scalar gradient, see also the discussion in chapter 1. Figure 4.1 shows the SGS scalar fluxes computed from DNS data of channel flow with heat transfer between the two walls at constant different temperatures at $Re_\tau = 590$, see Rasam et al. (2013) for details of the DNS. Although the mean temperature gradient is in the wall-normal direction, the mean SGS scalar flux in the streamwise direction is large while the EDM does not predict any streamwise SGS flux. The angle of the mean SGS scalar flux vector, relative to the streamwise direction, also shows large variations across the channel, see figure 4.1(c).

The deficiency of the EDM extends to its predictions of the anisotropy in the SGS dissipation of the resolved scalar intensity (see e.g. Kang & Meneveau 2001). It should also be noted that unlike velocity, local isotropy does not completely hold for passive scalars neither in the inertial range nor in the dissipation range in the presence of a mean gradient, see e.g. Warhaft 2000. A proper modelling of the SGS anisotropy is thus even more important for the scalar field than the velocity field.

Improvements in the EDM predictions can be obtained by replacing the scalar eddy diffusivity formulation with a tensor one, as first devised by Batchelor (1949). In the RANS community, a number of tensor eddy diffusivity models have been developed, two examples are the models by Daly & Harlow (1971) and Wikström et al. (2000). The tensor eddy diffusivity in the former is related linearly to the Reynolds stress tensor and in the latter it is a nonlinear function of strain- and rotation-rate tensors and the Reynolds stress tensor.

In LES, a number of tensor EDMs have been proposed, see Rasam et al. (2013) for a summary, to improve the geometrical and physical representation of the SGS scalar fluxes and to properly resolve the SGS anisotropy. In this chapter we introduce the three dynamic tensor EDMs of Wang et al. (2008) and the explicit algebraic SGS scalar flux model of Rasam et al. (2013). The performance of the latter in LES of turbulent channel flow with system rotation is briefly discussed and compared to the results with the dynamic EDM of Moin et al. (1991).
4.1. Dynamic tensor eddy diffusivity models of Wang et al.

Wang et al. (2008) proposed a set of SGS scalar flux models based on extensions of the generalised gradient hypothesis of Daly & Harlow (1970). The first proposed model is a simple adaptation of this model and expresses the SGS scalar flux $q_i$ as

$$q_i = -C_{\theta iG} \tau_{\theta \delta} \partial_{x_j} \tilde{\theta},$$  \hspace{1cm} (4.1)

where $\tau_{\theta \delta}$ is a characteristic SGS time scale expressed as $\tau_{\theta} = 1/|\tilde{S}|$, and $|\tilde{S}| = \sqrt{2\tilde{S}_{ij} \tilde{S}_{ij}}$. The model coefficient $C_{\theta iG}$ is computed by a dynamic procedure with least-squares minimisation of errors. The corresponding tensor eddy diffusivity of this model is

$$D_{ij} = C_{\theta iG} \tau_{\theta \delta} \tau_{ij}^d.$$

The second model proposed by Wang et al. (2008) is obtained by changing the tensor diffusivity from a homogeneous linear tensor function to an inhomogeneous linear one as

$$D_{ij} = C_{\theta P} \tau_{\theta |\tilde{S}|} \delta_{ij} + C_{\theta iG} \tau_{\theta \delta} \tau_{ij}^d.$$
where \(|\tau| = \sqrt{\sum i j \tau d i j \tau d i j}\). The following model for \(q_t\) is then obtained

\[ q_t = -C_{\theta P} \tau |\tilde{\theta}| \frac{\partial \tilde{\theta}}{\partial x_i} - C_{\theta G} \tau d i j \frac{\partial \tilde{\theta}}{\partial x_j}. \]  (4.2)

The model coefficients \(C_{\theta P}\) and \(C_{\theta G}\) are again computed by a dynamic procedure.

The third proposed model is obtained using the theory of tensor invariants and functions by expressing \(q_t\) in terms of the resolved scalar gradient vector and the SGS stress tensor based on Noll’s formula (Zheng 1994) as

\[ q_t = -C_{\theta P} \tau |\tilde{\theta}| \frac{\partial \tilde{\theta}}{\partial x_i} - C_{\theta G} \tau d i j \frac{\partial \tilde{\theta}}{\partial x_j} - C_{\theta Q} \tau d i k j \frac{\partial \tilde{\theta}}{\partial x_j}, \]  (4.3)

where the model coefficients \(C_{\theta P}\), \(C_{\theta G}\) and \(C_{\theta Q}\) are obtained by a dynamic procedure. This model has a quadratic nonlinear tensor eddy diffusivity given by

\[ D_{ij} = C_{\theta P} \tau |\tilde{\theta}| \delta_{ij} + C_{\theta G} \tau d i j \frac{\partial \tilde{\theta}}{\partial x_j}. \] 

### 4.2. Explicit algebraic subgrid-scale scalar flux model

The explicit algebraic SGS scalar flux model (EASSFM) of Rasam et al. (2013) is derived from the modelled transport equations of the SGS scalar flux. A weak equilibrium assumption for the normalised SGS scalar flux is assumed. This is an extension of the weak equilibrium assumption for the SGS stress anisotropy (Marstorp et al. 2009) shown to be reasonably valid, in a mean sense, away from the solid walls. It states that the advection and diffusion of the normalised SGS scalar flux is negligible. A local equilibrium assumption between the production and dissipation of the SGS scalar intensity as well as the SGS kinetic energy are also assumed to further simplify the equations in a manner similar to Wikström et al. (2000). The final simplified system of equations gives an implicit relation for \(q_t\), see Rasam et al. (2013) for details, as

\[ A_{ij} q_j = -(1 - c_{4\theta}) \tau^{*} \tau_{ij} \frac{\partial \tilde{\theta}}{\partial x_j}, \]  (4.4)

where \(\tau^{*}\) is the SGS time scale, \(c_{4\theta}\) is a model coefficient to be determined and the matrix \(A_{ij}\) is given as

\[ A_{ij} = c_{1\theta} \delta_{ij} + c_S \tilde{S}_{ij}^* + c_D \tilde{\Omega}_{ij}^*, \]  (4.5)

where \(c_S = 0.2\), \(c_D = 0.5\) and \(c_{1\theta}\) is given as

\[ c_{1\theta} = c_{1\theta}' \left( \frac{\tau^{*} K^{\text{SGS}}}{(0.1 \Delta |\tilde{S}_{ij}^*|)^2} \right)^{0.7}, \quad c_{1\theta}' = 0.2, \]  (4.6)
4.2. EXPLICIT ALGEBRAIC SUBGRID-SCALE SCALAR FLUX MODEL

The EASSFM is obtained by inverting $A_{ij}$ and reads

$$q_i = -(1 - c_{4\theta}) \tau^* A^{-1}_{ij} \tau_{jk} \frac{\partial \tilde{\theta}}{\partial x_k},$$  

(4.7)

The inverse of tensor $A_{ij}$ is obtained using the Cayley–Hamilton theorem

$$A^{-1} = \frac{(c_{1\theta}^2 - \frac{1}{2} Q_1) I - c_{1\theta}(c_S \tilde{S}^* + c_\Omega \tilde{\Omega}^*) + (c_S \tilde{S}^* + c_\Omega \tilde{\Omega}^*)^2}{c_{1\theta}(c_{1\theta}^2 - \frac{1}{2} Q_1) + \frac{1}{2} Q_2},$$  

(4.8)

where boldface denotes tensor notation and

$$Q_1 = c_S^2 tr(\tilde{S}^*^2) + c_\Omega^2 tr(\tilde{\Omega}^*^2), \quad Q_2 = \frac{2}{3} c_S^2 tr(\tilde{S}^*^3) + 2 c_S c_\Omega tr(\tilde{S}^* \tilde{\Omega}^*^2),$$  

(4.9)

and $tr(\cdot)$ denotes the trace of a tensor. The tensor diffusivity of the EASSFM can also be written as

$$D_{ij} = (1 - c_{4\theta}) \tau^* A^{-1}_{ik} \tau_{kj}.$$  

The model coefficient $c_{4\theta}$ is obtained by a dynamic procedure and the SGS time scale is computed from equation (10). The EASSFM is best used in...
Figure 4.3. Mean streamwise (a), wall-normal (b) and spanwise (c) resolved plus modeled scalar fluxes in wall units, \( \langle u' \theta' \rangle^+, \langle v' \theta' \rangle^+ \) and \( \langle w' \theta' \rangle^+ \) respectively. Statistics are taken from Rasam et al. (2013).

4.2.1. Turbulent channel flow with system rotation

In this section, some LES results of scalar transport in turbulent channel flow with system rotation around the wall-normal direction using the combination of EASSM and EASSFM (EA–EA) are presented. The results are compared to the DNS and LES results using the EASSM combined with the dynamic EDM (EA–ED), see paper IV (Rasam et al. 2013) for details. Two rotation rates are considered, i.e. \( Ro_r = 2 \Omega y u_r / \delta = 0.018 \) and 0.054, and the Prandtl number is \( Pr = 0.71 \).

Rotation induces anisotropy and affects the subgrid-scales. This needs to be properly modelled, hence this flow is a suitable test case for anisotropy resolving SGS models. The EASSM predictions of the mean velocity profiles in LES of this flow was already discussed in chapter 3. Rotation also creates a mass flux and heat in the spanwise direction. Therefore, the mean scalar flux is three-dimensional and cannot be correctly predicted by the EDM.
Figure 4.2(a-c) shows the SGS scalar fluxes predicted in the two cases EA–EA and EA–ED. It shows that in case EA–ED, $q_1$ and $q_3$ are identically zero due to the incorrect formulation of the EDM, discussed earlier, while case EA–EA gives reasonable predictions at both rotation rates. Figure 4.3(a-c) shows the resolved plus modelled scalar fluxes. It shows that the streamwise and spanwise scalar fluxes are better predicted in case EA–EA than EA–ED.
CHAPTER 5

Stochastic extensions of subgrid-scale models

5.1. Motivation

Contrary to the deterministic formulation of most SGS models, the subgrid-scales contain an appreciable amount of stochastic noise (Destefano et al. 2005). The deterministic nature of the modelled SGS stresses and scalar fluxes leads to longer correlations of the resolved statistics both in time and space in LES (Rasam 2011). The energy transfer between the resolved and unresolved scales in LES is also widely known to be very intermittent featuring both a forward and a backward flow of energy across the cutoff (see e.g. Piomelli et al. 1991; HärTEL et al. 1994; Domardzaki et al. 1994). However, most SGS models assume an equilibrium between production and dissipation of SGS kinetic energy, and hence are not able to model the reverse energy cascade (backscatter of energy). This backscatter of energy is of physical importance to the dynamics of the wall-bounded flows (Leslie & Quarini 1979; Piomelli et al. 1991; HärTEL et al. 1994; Domardzaki et al. 1993, 1994; Dunn & Morrison 2003; Cimarelli & De Angelis 2012). One way to incorporate backscatter in the explicit algebraic SGS models will be briefly outlined in this chapter. An important implication of stochastic extensions of SGS models concerns the modelling of the SGS dissipation of the scalar variance which plays a central role in the prediction of the small-scale mixing in LES of reactive flows (Pouransari et al. 2013; Pitsch 2006; Pitsch & Fedotov 2006). The small scale dynamics in particle dispersion and multiphase flows also involves stochastic processes that could be incorporated through a stochastic extension of the SGS force which could lead to improvements in the LES predictions (Bianco et al. 2012; Jones et al. 2010; Geurts & Kuerten 2012; Shotorban & Mashayek 2006).

5.2. Langevin stochastic diffusion process

Stochastic processes are of various kinds. A particular process of interest is the diffusion process, which is a continuous-time Markov process. These diffusion processes are not differentiable. Therefore ordinary differential calculus tools are not suitable and itô calculus is used instead. The diffusion processes are described by stochastic differential equations (SDE) of the form

\[ d\mathcal{X}(t) = \mu(t)dt + \sigma(t)dW(t), \]

where \( \mathcal{X} \) is the stochastic process, \( W \) is a Wiener process and \( \mu \) and \( \sigma \) are called drift and diffusion coefficients, respectively. The Wiener process is the
most fundamental diffusion process with drift and diffusion coefficients of zero and one, respectively. Using the solution of the Fokker-Planck equation with $\sigma = 1$ and $\mu = 0$, one can show that the increment of the Wiener process, $dW$, with the time increment $\Delta t$ has a normal distribution with a zero mean and $\Delta t$ variance, i.e. $\mathcal{N}(0, \Delta t)$. The diffusion process of equation (5.1) is described by its drift and diffusion coefficients and can be interpreted as an extension of the Wiener process.

The Langevin stochastic process is also a diffusion process. As described in paper V, its SDE is expressed as

$$dX(x, t) = -X(x, t)\frac{dt}{\tau_X} + b\sqrt{2\tau_X}dW(x, t),$$

(5.2)

or in the following discretised form

$$X(x, t + \Delta t) = \left(1 - \Delta t\right)X(x, t) + b\sqrt{2\Delta t/\tau_X}dW(x, t),$$

(5.3)

where $dW(x, t)$ is a random number with $\mathcal{N}(0, 1)$ and $\Delta t$ is the time step of the numerical simulation. $\tau_X$ is modelled using dimensional analysis, as

$$\tau_X = C_X \frac{\Delta}{\sqrt{K_{SGS}}}$$

(5.4)

where $C_X = 0.05$ is a model constant obtained from a posteriori analysis of LES of channel flows.

### 5.2.1. Statistical moments of the stochastic process

In order to find the first and second moments of $X$, i.e. mean and variance, the solution to equation (5.2) is expressed as

$$X = e^{-at}X_0 + \sigma \int_0^t e^{-a(t-s)}dW,$$

(5.5)

where $\sigma = b\sqrt{2/\tau_X}$, $a = \frac{dt}{\tau_X}$ and $X_0$ is the initial condition of the stochastic process. Now we take the mean of (5.5)

$$\langle X \rangle = e^{-at} \langle X_0 \rangle.$$  

(5.6)

Therefore, as $t \to \infty$ the mean of the stochastic process will tend to zero, $\langle X \rangle = 0$. The mean square of $X$ is

$$\langle X^2 \rangle = \left\langle e^{-2at}X_0^2 + 2\sigma e^{-at}X_0 \int_0^t e^{-a(t-s)}dW + \sigma^2 \left(\int_0^t e^{-a(t-s)}dW\right)^2\right\rangle =$$

$$e^{-2at} \langle X_0^2 \rangle + 2\sigma e^{-at} (\langle X_0 \rangle) \left\langle \int_0^t e^{-a(t-s)}dW\right\rangle + \sigma^2 \int_0^t e^{-2a(t-s)}ds =$$

$$e^{-2at} \langle X_0^2 \rangle + \frac{\sigma^2}{2a} \left(1 - e^{-2at}\right).$$

(5.7)
Figure 5.1. Length scale of the SGS kinetic energy (a) and scalar variance dissipation (b) normalized with the grid-scale
\( \Delta = \sqrt[3]{\Delta x (\Delta y) \Delta z} \). 
- : DNS, - - : stochastic EASSM and EASSFM; - - - : EASSM and EASSFM; + - : stochastic EASSM and stochastic EASSFM.

The variance of \( \mathcal{X} \) is computed from equations (5.7) and (5.6) as
\[
\text{var}[\mathcal{X}] = \langle \mathcal{X}^2 \rangle - \langle \mathcal{X} \rangle^2 = \frac{\sigma^2}{2a} (1 - e^{-2at}),
\]
which will be \( \sigma^2/2a = b^2 \) as \( t \to \infty \).

### 5.3. Stochastic explicit algebraic subgrid-scale models

In paper V (Rasam et al. 2014a), we extend the eddy viscosity part of the explicit algebraic SGS stress model (EASSM), equation (5.11), with the stochastic process \( \mathcal{X}_1 \) as
\[
\tau_{ij} = \frac{2}{3} K_{\text{SGS}} \delta_{ij} + (1 + \mathcal{X}_1(x,t)) \beta_1 K_{\text{SGS}} \bar{S}_{ij}^* + \beta_4 K_{\text{SGS}} (\bar{S}_{ik}^* \bar{\Omega}_{kj}^* - \bar{\Omega}_{ik}^* \bar{S}_{kj}^*), \quad (5.8)
\]
and in the same way, the explicit algebraic SGS scalar flux model (EASSFM), equation (4.7), is extended with the stochastic process \( \mathcal{X}_2 \) as
\[
q_i = -(1 - c_{4b}) r^* A_{ij}^{-1} \tau_{jk} \frac{\partial \theta}{\partial x_k} (1 + \mathcal{X}_2(x,t)). \quad (5.9)
\]

LES of channel flow with a passive scalar at \( Re_\tau = 590 \) and \( Pr = 0.71 \) using the stochastic extensions of the EASSM and EASSFM shows that the models provide for reasonable amounts of backscatter of energy both for the velocity and scalar, while the original models do not provide for backscatter. Other statistics of the SGS energy dissipation such as variance and length scales were also improved. The latter is shown in figure (7a) and (b). The length scale are reduced by the introduction of the stochastic term, giving a better agreement with filtered DNS data, both for the velocity and scalar quantities. Some of the
resolved statistics were also improved, although the predictions of the original models already were in very good agreement with the DNS data.
CHAPTER 6

Summary of the papers

Paper 1

*Effects of modelling, resolution and anisotropy of subgrid-scales on large eddy simulations of channel flow*

The performance of the anisotropy resolving explicit algebraic subgrid-scale (SGS) stress model (EASSM), the isotropic dynamic eddy viscosity model (DEVM) and the high-pass filtered DEVM (HPF) are studied in large eddy simulations (LESs) of turbulent channel flow at $Re_{\tau} = 934$, at moderate to very coarse resolutions. LESs without a SGS model (NM) are also carried out for comparison.

The convergence of the wall friction with increasing resolution towards the DNS value was non-monotonic in the LES using the EASSM, HPF and HPF, while it was monotonic for the DEVM. LES results at the coarser resolutions show that the isotropic DEVM, HPF and NM strongly over-predict the streamwise Reynolds stress, while the EASSM predictions are reasonably close to the DNS. The isotropic model predictions varied considerably with resolution, while the anisotropy resolving EASSM had the least sensitivity to the resolution among the three SGS models, owing to its ability to predict the anisotropy of the SGSs.

The LES results reasonably captured the large energy containing scales, although the near wall structures were not correctly represented due to the coarse resolutions. Spatial two-point correlations revealed that the significant SGS dissipation of the DEVM and EASSM results in longer correlation lengths in the near-wall region, while for the HPF and NM, that provide very little and no SGS dissipation, the length scales were in better agreement with the DNS.

Paper 2

*Large eddy simulation of channel flow with and without periodic constrictions using the explicit algebraic subgrid-scale model*

LESs of separated flow in a channel with periodic hill-shaped constrictions and spanwise homogeneity (periodic hill flow) are carried out with the EASSM,
DEVM and no SGS model (NM) at a moderate resolution. CodeSaturne (CS), an unstructured collocated second-order finite volume solver for incompressible flows is used in the simulations. It has inherent numerical dissipation due to the Rhie-Chow interpolation used to avoid odd-even oscillations. Channel flow simulations at \( Re_\tau = 590 \) are also carried out to quantify the effect of numerical errors in the LES with the EASSM and DEVM using CS and compare with similar LESs using a pseudo-spectral method (PSM).

In LES of channel flow at different resolutions, it was found that the EA-SSM predictions were less accurate with the CS than with the PSM. The inherent numerical dissipation was found to be sufficient for a proper description of the mean velocity profiles but not the Reynolds stresses. The computed SGS dissipation by the EASSM was substantially lower in simulations with CS than in the simulations with the PSM, but its performance was generally better than the DEVM.

In LES of separated flow in the periodic hill case, the anisotropy resolving EASSM predicted the separation and reattachment points more accurately than the isotropic DEVM and NM. The mean velocity profiles, the streamlines of the mean flow and Reynolds stresses were other quantities that were in better agreement with the reference data with the EASSM. The paper demonstrates the advantages of using an anisotropy-resolving SGS model also in complex flows computed with low-order scheme codes. This has significant implications for practical CFD applications.

**Paper 3**

*An comparison between isotropic and anisotropy-resolving closures in large eddy simulation of separated flow*

A comparative study of the anisotropy resolving EASSM and the isotropic DEVM in LES predictions of highly anisotropic, separated flow in a channel with periodic constrictions and spanwise homogeneity (periodic hill flow) in the limit of coarse resolutions is performed. CodeSaturne (CS), an unstructured collocated second-order finite volume solver for incompressible flows with inherent numerical dissipation is used in the simulations. LES results are compared to those of a well-resolved LES and no SGS model (NM) simulations with the CS.

The EASSM predictions of the mean location of the separation and reattachment points, the shape of the separation bubble and the mean velocity profiles were found to be much more accurate than the DEVM and NM prediction and in better agreement with the reference LES data at all resolutions studied. An interesting observation was that at the coarsest resolution the NM did not predict flow separation, the DEVM predicted a very small separation bubble, while the EASSM prediction was reasonable.
Paper 4

An explicit algebraic model for the subgrid-scale passive scalar flux

A new SGS passive scalar flux model, based on the explicit algebraic solution of the modelled transport equations for the SGS scalar fluxes, is proposed (EASSFM). The new EASSFM has a nonlinear tensor eddy diffusivity formulation with a natural incorporation of the SGS stress tensor. It resolves the SGS anisotropy and is able to predict mean shear effects on SGS scalar fluxes.

LESs of heat transfer in turbulent channel flows with system rotation around the wall normal direction and without system rotation at different resolutions were carried out using the EASSM for the SGS stresses and EASSFM (EA–EA) and the dynamic eddy diffusivity model (DEDM) (EA–ED) for the SGS scalar fluxes. Moreover, LESs using the DEVM for the SGS stresses and the DEDM for the SGS scalar fluxes (EV–ED) were performed. The LESs were at different Reynolds numbers and were also studied by DNS in this paper.

The EA–EA results of the resolved statistics were in good agreement with the DNS data in both test cases. The resolved scalar fluxes showed appreciable improvements in channel flow simulations with system rotation, compared to the EV–ED and EA–ED. The EA–EA predictions of the Nusselt number were also more accurate and less resolution dependent, a characteristic attributed to the anisotropy resolving feature of the explicit algebraic SGS models. The EASSFM was able to predict the shear-induced streamwise SGS scalar flux in channel flow simulations with and without system rotation, and the rotation-induced spanwise SGS scalar flux in channel flow simulations with system rotation. The DEDM predicted these SGS scalar fluxes to be zero due to its formulation.

Paper 5

Stochastic explicit algebraic subgrid-scale stress and scalar flux models

The EASSM and EASSFM were extended with stochastic terms based on the Langevin equation formalism for the subgrid-scales. The extended models were tested in LES of passive scalar transport in channel flow at $Re_T = 590$ and the results were compared to those of the standard EASSM and EASSFM and DNS data.

Although the EASSM predictions of the resolved quantities were in excellent agreement with the DNS data, the stochastic extension led to better predictions of the streamwise Reynolds stress by reducing the wall-distance of its peak. The improvements in the predicted resolved velocity statistics by the stochastic extension, although limited, led to appreciable improvements of the resolved scalar statistics of the EASSFM, i.e. the mean and root-mean-square of the scalar fluctuations and the streamwise scalar flux.
The streamwise two-point correlations of velocity showed reasonable improvements due to the stochastic extension for the EASSM, but the corresponding correlation for the scalar did not show any improvements.

The SGS dissipation characteristics were substantially improved through the stochastic extension for both EASSM and EASSFM. The extended models were able to predict some backscatter, while the original models did not. Moreover, the length scale and variance of the SGS dissipation were in better agreement with DNS. The probability density functions of the SGS dissipation showed a better statistical description of the SGS dissipation in comparison with the original models.
CHAPTER 7

Conclusions and outlook

This study was focused on the further development and validation of the explicit algebraic subgrid-scale (SGS) models for the SGS stresses (EASSM) and passive scalar fluxes (EASSFM). These SGS models resolve the SGS anisotropy and improve the prediction of the individual SGS stresses and scalar fluxes at a very wide range of resolutions. Owing to this fact, large eddy simulation (LES) with the explicit algebraic models can have a comparable accuracy to LES with isotropic SGS models, like the conventional dynamic eddy viscosity model, at a much coarser resolution. Hence, the computational cost of LES with the explicit algebraic SGS models can be much lower. Yet the computational over-head of these models is relatively low.

The EASSM was extensively tested in channel flows with and without system rotation and in LES of separated flows at a wide range of resolutions. A further step in this direction would be to explore the possibility of hybrid modelling using the EASSM and its RANS counterpart, which shares many of its favourable characteristics.

The EASSFM was developed and successfully tested in channel flows with and without system rotation with different Prandtl numbers. The EASSFM is suitable for LES of passive scalar transport in complex geometries. Therefore, the next step is to apply it to LES of flows in complex geometries, and to extend it to the situation with active scalar (as in density-stratified flows).

A stochastic extension of the EASSM and EASSFM was proposed which improved the prediction of the SGS dissipation further and even improved the predictions of the resolved quantities and allowed for backscatter of energy. There are several possibilities for application of stochastic models in simulations of turbulent flows such as resolving the interface problem in hybrid LES–RANS simulations, improving LES predictions in multiphase flows and combustion where small-scale turbulence plays an important role.
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