DEVELOPMENT OF A NEAR-WALL DOMAIN DECOMPOSITION METHOD FOR TURBULENT FLOWS

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Development of a near-wall domain decomposition method for turbulent flows
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In computational fluid dynamics (CFD), there are two widely-used methods for computing the near-wall regions of turbulent flows: high Reynolds number (HRN) models and low Reynolds number (LRN) models. HRN models do not resolve the near-wall region, but instead use wall functions to compute the required parameters over the near-wall region. In contrast, LRN models resolve the flow right down to the wall. Simulations with HRN models can take an order of magnitude less time than with LRN models, however the accuracy of the solution is reduced and certain requirements on the mesh must be met if the wall function is to be valid. It is often difficult or impossible to satisfy these requirements in industrial computations.

In this thesis the near-wall domain decomposition (NDD) method of Utyuzhnikov (2006) is developed and implemented into the industrial code, Code_Saturne, for the first time. With the NDD approach, the near-wall regions of a fluid flow are removed from the main computational mesh. Instead, the mesh extends down to an interface boundary, which is located a short distance from the wall, denoted \( y^* \). A simplified boundary layer equation is used to calculate boundary conditions at the interface. When implemented with a turbulence model which can resolve down to the wall, there is no lower limit on the value of \( y^* \). There is a Reynolds number-dependent upper limit on \( y^* \), as there is with HRN models. Thus for large \( y^* \), the model functions as a HRN model and as \( y^* \to 0 \) the LRN solution is recovered.

NDD is implemented for the \( k - \varepsilon \) and Spalart-Allmaras turbulence models and is tested on five test cases: a channel flow at two different Reynolds numbers, an annular flow, an impinging jet flow and the flow in an asymmetric diffuser. The method is tested as a HRN and LRN model and it is found that the method behaves competitively with the scalable wall function (SWF) on simpler flows, and performs better on the asymmetric diffuser flow, where the NDD solution correctly captures the recirculation region whereas the SWF does not.

The method is then tested on a ribbed channel flow. Particular focus is given to investigating how much of the rib can be excluded from the main computational mesh. It is found that it is possible to remove 90% of the rib from the mesh with less than 2% error in the friction factor compared to the LRN solution.

The thesis then focuses on the industrial case of the flow in an annulus where the inner wall, referred to as the pin, has a rib on its surface that protrudes into the annulus. Comparison is made between CFD calculations, experimental data and empirical correlations. It is found that the experimental friction factors are significantly larger than those found with CFD, and that the trend in the friction factor with Reynolds number found in the experiments is different. Simulations are performed to quantify the effect that a non-smooth surface finish on the pin and rib surface has on the flow. This models the situation that occurs in an advanced gas-cooled nuclear reactor, when a carbon deposit forms on the fuel pins. The relationship between the friction factor and surface finish is plotted. It is demonstrated that surface roughness left over by the manufacturing process in the experiments is not the source of the discrepancy between the experimental and CFD results.
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Chapter 1

Introduction

1.1 Commercial motivation for project

At the time of writing, EDF Energy Generation currently operates 15 nuclear reactors in the UK, shared over 8 sites. One of these reactors is a pressurised water reactor and the remaining 14 are advanced gas-cooled reactors (AGRs). Nuclear power comprises around three quarters of EDF Energy’s total electricity generation, and around one sixth of the total electricity generation in the UK.

AGRs were developed in the UK in the 1960s and commercial power stations became operational in the 1970s and 1980s. The fuel is enriched uranium in the form of pellets, which are stacked in stainless steel pins that are held in a fuel assembly. Carbon dioxide flows up the fuel assembly and acts as the coolant, taking heat away from the fuel pins to the reactor boiler. The stainless steel pins have helical ribs on their surfaces which enhance the heat transfer between the pin and coolant. The geometry of a fuel pin, the rib on the fuel pin, and the organisation of fuel pins in a fuel assembly is shown in Figure 1.1. Each fuel assembly comprises 36 fuel pins arranged in three rings with the rib helices arranged to enhance mixing of the coolant, a central guide tube and an outer graphite sleeve.

Under normal operating circumstances, radiation within the AGR core would ionise the carbon dioxide coolant. To prevent this, small amounts of carbon monoxide and methane are added to the coolant. However this has the effect of causing a solid carbon deposit to form over time on the fuel pin (Sykes et al., 1993; Gras and Stanley, 2008).

The power output of the reactor per fuel assembly is related to the rate of enthalpy change of the coolant flowing through a fuel assembly, $\dot{q}$, which can be computed in terms of the mass...
1.1. Commercial motivation for project

(a) Fuel pins
(b) Rib profile
(c) End-on view of a fuel assembly

Figure 1.1: The geometry of an AGR fuel assembly.

flow rate of the coolant through the assembly, $\dot{m}$, as

$$\dot{q} = \dot{m}c_p\Delta T_b,$$

(1.1)

where $c_p$ is the specific heat capacity of the coolant and $\Delta T$ is the bulk temperature change of the coolant between the inlet and outlet of the assembly.

The power output of the reactor can also be measured by measuring the neutron flux outside the reactor core. It has been found recently that the values of $\dot{q}$ calculated by these two methods do not match to within their expected uncertainties. Hence there is uncertainty in the operating power of the reactor. This degrades the confidence in both methods and all other uses that depend on the two methods. For safety reasons, the larger value of $\dot{q}$ is assumed to be the correct value, since this is more conservative. This imposes a limit on the power of each channel in the core that may be lower than the true limit. In normal operation this is not restrictive, since the reactor is not usually operated near to the channel power limit. However, decay heats for discharged fuel are calculated using the channel power limit. Assuming a larger channel power increases the time taken for the decay heat to fall below acceptable limits, which extends the time required for performing irradiated fuel handling tasks. This additional, and possibly unnecessary, delay makes refuelling take longer, which reduces the time the reactor is operating. This leads to increased costs. Part of the commercial motivation for this EngD project is to investigate the source of this discrepancy in the predicted values of $\dot{q}$.

The effect of the carbon deposit on the heat transfer properties of the fuel assembly is not well understood. However $\Delta T_b$ in Equation (1.1) can be measured using thermocouples in
the reactor and is therefore known. Thus $\dot{m}$ is the only parameter in Equation (1.1) whose value might be uncertain. This would be the case if the carbon deposit on the fuel pins affects the pressure drop in the reactor core. There is very little experimental data on the effects of carbon deposition on the pressure drop. Physical experiments are impossible due to the high levels of radiation in the core. Hence computational modelling is the only means by which the effects of carbon deposition can be studied.

This thesis addresses two industrial aims:

1. To compare computed predictions of the pressure drop of flow over a fuel pin to existing experimental data. This is achieved by reproducing the experiments of two reports produced in the 1970s using computational fluid dynamics (CFD).

2. To quantify the effect of carbon deposition on this pressure drop. This is achieved using a rough wall function to model the roughness on the fuel pin wall caused by the carbon deposit.

1.2 Academic motivation for project

The flows in AGR fuel assemblies have very large Reynolds numbers. Hence the flow field, which is a solution of the Navier-Stokes equations, contains motions on a vast range of scales. Computing this solution by direct solution of the Navier-Stokes equations is unfeasible. Therefore it is necessary to make a trade-off, and reduce the accuracy of the solution for a decrease in the computational requirements. Methods of making this trade-off are a significant topic of research in CFD. With a class of models known as Reynolds-averaged Navier-Stokes (RANS) methods, only the average flow field is computed; all turbulent motions are modelled with a turbulence model. This greatly reduces the computational requirements of the simulation and allows a solution to be obtained in a relatively short space of time.

However even with the speed advantages of RANS methods, the computation power required to solve flows at high Reynolds numbers can still be prohibitively large. The motion in the near-wall region of fluid flows can be responsible for as much as 90\% (Utyuzhnikov, 2012) of the computation time. Numerous models of the near-wall behaviour of fluid flows have been developed to try to reduce the computational cost. These are often semi-empirical functions based on experimental data for statistically one-dimensional flows. Recently, however, some more advanced models have been developed.

In this thesis, the near-wall domain decomposition (NDD) method of Utyuzhnikov (2006) is developed. With the NDD method, the near-wall region of a fluid flow is excluded from the main computational mesh and is treated separately. The main computational mesh
1.2. Academic motivation for project

stops a surface within the flow a short distance from the wall, called an interface boundary. Special boundary conditions, called interface boundary conditions (IBCs) are imposed on this interface boundary. The IBCs model the response of the main flow to the near-wall region, without explicitly calculating the solution in the near-wall region.

In this thesis, the NDD method of Utyuzhnikov (2006) is developed and applied for the first time in an industrial code. The method is applied to four different turbulence models and used to study a greater range of flows than has been studied with NDD before. An example is given of how NDD can be used for efficient design optimisation studies, without requiring a new mesh when the geometry changes.

CFD results are often not thought of as reliable enough for use in industry. Therefore it is important to perform verification and validation tests of any new methods and to compare CFD results, particularly with NDD, against experimental data for similar flows. Hence in this thesis, a number of academic test cases are performed with the NDD method to assess the accuracy of the method.

In a project sponsored by British Energy, Keshmiri (2011) studied the flow in a simplified fuel element, in which the ribs form continuous rings rather than helices. This reduced the portion of the fuel element that had to be meshed from a $120^\circ$ sector to a $30^\circ$ sector. In this thesis, two-dimensional flows over a single pin are studied, instead of the full three-dimensional geometry of Figure 1.1. This not only reduces the computation time but also allows comparisons to be made between CFD and experimental results. Thus, the accuracy of the CFD results can be assessed. Although Keshmiri (2010) argued that a three-dimensional study of a fuel assembly is required if the results are to be accurate, EDF Energy Generation have transformation methods that can transform two-dimensional results into their three-dimensional equivalents. Therefore the two-dimensional simulations performed as part of this project are commercially useful. There are also correlations that have been developed to allow a friction factor for the flow over a single pin to be computed given just a pin geometry and a Reynolds number. The correlations of Maubach (1972) and Dalle Donne and Meyer (1977) are discussed and used in Chapter 8 to assess the accuracy of experimental and CFD results on studies of a single fuel pin.

The major academic aims of this project are:

1. To implement the NDD method of Utyuzhnikov (2006) in an industrial code and assess its accuracy on a range of test cases.

2. To assess the accuracy of CFD models in application to flows over the types of pins found in AGRs.
3. To investigate the extent to which NDD can be used to simplify these flows.

4. To demonstrate the use of NDD in efficient design optimisation studies.

5. To study flows over ribbed pins similar to those found in an AGR fuel assembly and to assess how much of a rib can be excluded from the main computational mesh.

1.3 The engineering doctorate (EngD)

The engineering doctorate (EngD) is a four year postgraduate research degree funded by the EPSRC and a sponsoring company, which for this project is EDF Energy R&D UK Centre Limited. Of the four years, approximately six months is devoted to taught technical courses and another six months is devoted to a postgraduate diploma in enterprise management and professional development courses. The remaining three years are devoted to a PhD level research project.

As an industrial doctorate there are both academic and commercial objectives for this thesis. The research topic addressed by this thesis was suggested by EDF Energy Generation. In addition, Code_Saturne, a computational code developed and maintained by EDF R&D, has been used.

1.4 Structure of this thesis

The thesis begins with an overview of computational fluid dynamics in Chapter 2, which focusses on the modelling techniques used in this thesis. Chapter 3 contains a description of the structure of a turbulent boundary layer and a detailed review of the different techniques used to model the near-wall regions of fluid flows, which is a topic of particular importance in this thesis. A detailed overview of Code_Saturne, which is the computational code used in this work, is provided in Chapter 4. Particular attention is given to the implementation of boundary conditions in Code_Saturne.

The NDD method of Utyuzhnikov (2006), which is further developed in this thesis, is introduced in Chapter 5. The treatment of the velocity and pressure, and the implementation of the method for two turbulence models, are described. The NDD method is compared to conventional wall functions and some notes on numerical implementation of the method are given.

Chapter 6 contains the results of five distinct test cases of the NDD method. The test cases are two channel flows at different Reynolds numbers, an annular flow, an impinging jet flow
and the flow in an asymmetric diffuser. A comparison of the computation time with NDD against conventional models is also given.

The application of the NDD method to a heated ribbed channel flow is the focus of Chapter 7. This case is used as a testing ground for the industrial flows studied in this thesis and ends with an example of how NDD can be used for efficient design optimisation studies.

Chapter 8 contains a detailed study of flows over ribbed fuel pins in annular passages. These flows are of particular importance to EDF Energy Generation as the results can be directly related to the performance of an AGR fuel assembly. The flow is studied with a number of CFD models as well as correlations from academic literature.

Conclusions are given after each results chapter. Further conclusions and possible future research topics that could build on the work in this thesis are given in Chapter 9.
Chapter 2

Computational fluid dynamics

The velocity of a fluid, \( \mathbf{U} = (U, V, W)^T \), with molecular viscosity \( \mu \) and density \( \rho \) is governed by the Navier-Stokes equations

\[
\rho \frac{\partial \mathbf{U}}{\partial t} + \rho \mathbf{U} \cdot \nabla \mathbf{U} = -\nabla P + \nabla \cdot (\mu \nabla \mathbf{U}) + \mathbf{F},
\]

(2.1)

and the continuity equation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0.
\]

(2.2)

The vector \( \mathbf{F} \) represents any external forces and \( \nabla P \) is the pressure gradient. Equation (2.1) may be thought of as conservation of momentum through a form of Newton’s second law. The right hand side represents the forces per unit volume and the left hand side is mass per unit volume multiplied by the acceleration of the fluid. The left hand side contains the total derivative

\[
\rho \frac{\partial \mathbf{U}}{\partial t} + \rho \mathbf{U} \cdot \nabla \mathbf{U} \equiv \frac{\rho \mathbf{U}}{D^t},
\]

(2.3)

which describes the rate of change of a function transported by the fluid\(^1\).

In an incompressible flow where the density is constant, the continuity equation simplifies to

\[
\nabla \cdot \mathbf{U} = 0.
\]

(2.4)

Hence in an incompressible flow, the velocity is divergence-free.

Using the continuity equation, the total derivative can be re-written in conservative form as

\[
\rho \frac{D\mathbf{U}}{Dt} = \frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} \equiv \frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}),
\]

(2.5)

where \( \mathbf{U} \mathbf{U} \) is a dyadic tensor.

\(^1\)The total derivative is sometimes written as \( \frac{d\mathbf{U}}{dt} \) instead of \( \frac{\partial \mathbf{U}}{\partial t} \). It is also sometimes called the material derivative.
2.1 Poisson equation for the pressure

Other quantities, such as the enthalpy of the fluid or the concentration of a dye, are transported by the motion of the fluid. These quantities obey their own transport equations, which are of a similar form to Equation (2.1). The archetypal transport equation for a function \( \Phi \) is

\[
\rho \frac{D \Phi}{Dt} = \nabla \cdot (\rho \gamma \nabla \Phi) + S_\Phi,
\]

where \( \gamma \) is the diffusivity and \( S_\Phi \) contains any source terms. The Navier-Stokes equations are reached by setting \( \Phi = U \), \( S_U = -\nabla P \) and \( \gamma = \nu \equiv \mu/\rho \), where \( \nu \) is called the kinematic viscosity.

2.1 Poisson equation for the pressure

An equation for the pressure can be found by taking the divergence of the Navier-Stokes equations. With no external forces, this yields

\[
\nabla \cdot (\nabla P) = \nabla^2 P = -\nabla \cdot \left( \frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U U) - \nabla \cdot (\mu \nabla U) \right),
\]

which can be written for each Cartesian component as

\[
\partial_i \partial_i P = -\partial_i \partial_i (\rho U_i) - \partial_i \partial_j (\rho U_i U_j) + \partial_i \partial_j (\mu \partial_j U_i),
\]

where the Einstein summation convention has been used to imply summation over repeated indices. This convention will be used throughout this thesis, except where it is explicitly stated otherwise.

For incompressible flow the result simplifies further to

\[
\nabla^2 P = -\rho \nabla \cdot (U \cdot \nabla U).
\]

If the pressure satisfies this Poisson equation then the continuity equation is also satisfied. For incompressible flows there is no relation between the pressure and other fluid variables such as density or temperature. Therefore in such flows the pressure can be regarded as a function which acts in order to ensure that the continuity equation is obeyed.

2.2 Boundary conditions

At a wall with unit normal \( \mathbf{n} \), moving with velocity \( \mathbf{V}_w \), the fluid velocity must obey

\[
\mathbf{U} \cdot \mathbf{n} = \mathbf{V}_w \cdot \mathbf{n},
\]

where \( \mathbf{U} \) is the fluid velocity.
Chapter 2. Computational fluid dynamics

otherwise fluid would penetrate the wall. Furthermore it is observed experimentally that the tangential velocity also vanishes at the wall. This condition is called the “no slip condition” and means that at the wall the fluid velocity obeys

\[ \mathbf{U} \times \mathbf{n} = \mathbf{V}_w \times \mathbf{n}. \] (2.11)

The two conditions can be combined so that the boundary condition on the fluid velocity is

\[ \mathbf{U} = \mathbf{V}_w. \] (2.12)

For a stationary wall, this becomes \( \mathbf{U} = 0 \).

Physically, the no slip condition is a statement that the fluid interacts with solid walls in the same way that it interacts with the fluid itself. Therefore any viscous stresses \( \mu \nabla \mathbf{U} \) must be finite. Hence the velocity must be continuous at the wall.

For incompressible flows, another boundary condition for \( \mathbf{U} \) can be obtained on smooth manifolds. For a flow past a wall in the \((x, z)\) plane with \( \mathbf{U} = (U, V, W)^T \), the no slip condition ensures not only that \( \mathbf{U}_w = 0 \) but also that

\[ \frac{\partial U}{\partial x} \bigg|_w = \frac{\partial W}{\partial z} \bigg|_w = 0, \] (2.13)

where the subscript \( w \) means a quantity is evaluated at the wall. The continuity equation requires that \( \nabla \cdot \mathbf{U} = 0 \), therefore

\[ \frac{\partial V}{\partial y} \bigg|_w = 0. \] (2.14)

This can be written more generally as

\[ \frac{\partial (\mathbf{U} \cdot \mathbf{n})}{\partial n} \bigg|_w = 0. \] (2.15)

At the wall, Equations (2.12) and (2.15) mean that the Navier-Stokes equations become

\[ \frac{\partial P}{\partial n} = \mu \frac{\partial^2 (\mathbf{U} \cdot \mathbf{n})}{\partial n^2}, \] (2.16)

which is the boundary condition for the pressure at the wall.

2.3 The Reynolds number

The non-dimensional parameter

\[ Re = \frac{UL}{\nu}, \] (2.17)

is called the Reynolds number and is used to classify solutions to the Navier-Stokes equations. Typically \( L \) is computed from the geometry and \( U \) is an average speed across the flow domain.
Solutions to the Navier-Stokes equations exist for all Reynolds numbers. However, it is observed that steady flow only exists for flows below certain Reynolds numbers. When the Reynolds number is small, flows are laminar and are characterised by a smooth, ordered velocity field with smooth streamlines. As the Reynolds number increases, flows eventually become turbulent and are characterised by unsteady coherent structures with a wide range of velocity scales. The range of length and time scales in turbulent flows is what makes them so challenging to compute.

### 2.4 Boundary layers

As the Reynolds number increases, viscous effects become negligible. However, near to a wall, the viscosity is responsible for the no-slip condition and the velocity at a stationary wall is always zero. This leads to the development of boundary layers near to walls, which are thin regions characterised by large velocity gradients.

Boundary layers can be laminar, turbulent or contain regions of both flow regimes. Immediately adjacent to a wall lies a viscous sub layer, where the viscosity is dominant. In this region the average wall-parallel component of the fluid velocity varies linearly with distance from the wall and the fluid appears to move in layers in the plane of the wall. The turbulent part of a boundary layer is further from the wall. In this region the flow no longer appears to move in layers. Mathematical analysis of boundary layers shows that the thickness of the boundary layer scales as $\delta \sim L/\sqrt{Re}$, which means that the boundary layer becomes thinner as $Re$ increases. This creates further computational challenges, as fine meshes are needed near to walls in order to resolve the high gradients that occur there. Meshes must become finer as the Reynolds number increases.

Additionally it can be shown that as $Re \to \infty$, the boundary condition on the pressure at the wall tends to

$$\frac{\partial P}{\partial n} = 0. \tag{2.18}$$

Since engineering flows often have large Reynolds numbers, this is a widely-used result.

### 2.5 Structure of turbulence

In turbulent flows the velocity at each point varies about some mean value. The mean varies smoothly throughout the domain, whereas the deviations from the mean vary on smaller length and time scales. The deviation can be thought of as being caused by a combination of eddies of different sizes. There is no strict definition of what constitutes an eddy but they
are characterised by a velocity scale $u$ and a length scale $L$, which is related to the region over which the velocity fluctuation occurs.

Each eddy has a Reynolds number associated with it, $Re_{\text{eddy}} = uL/\nu$. The size of the largest eddies in a flow is determined by the geometry. The velocity associated with these eddies is of the order of magnitude of the size of the change in mean velocity over the flow domain, $\Delta u$. Since $\Delta u$ increases with the Reynolds number, $Re_{\text{eddy}}$ also increases with the Reynolds number.

The viscosity is responsible for dissipation of kinetic energy by diffusion. However in the largest eddies, convection dominates over diffusion. Therefore in large eddies the viscosity has a negligible effect and little energy is dissipated. In contrast, viscous effects dominate in the smallest eddies. Thus, energy dissipation occurs on the smallest scales.

Richardson (1922) proposed the concept of an energy cascade, whereby the energy carried by the largest eddies is gradually transferred to smaller eddies until it reaches the smallest eddies in the flow, whereupon it is dissipated as heat. Kolmogorov (1941) introduced three hypotheses which allow the size of the smallest eddies, and the energy contained within them, to be estimated. They are based on dimensional analysis and observed experimental behaviour. The hypotheses are applicable to flows at high Reynolds numbers.

1. The first hypothesis is that turbulence is isotropic at the smallest scales.

2. The second is that the behaviour of the smallest eddies is determined entirely by the kinematic viscosity, $\nu$, and the rate of energy dissipation, $\varepsilon$. 

3. The third hypothesis is that at intermediate length scales the behaviour of the eddies does not depend on $\nu$ but depends only on the rate at which they receive energy, $\varepsilon$.

The rate of energy dissipation is the same as the rate at which the largest eddies lose energy. Therefore $\varepsilon$ also determines the size of the largest eddies, $L_t$. The Kolmogorov hypotheses and dimensional analysis can be used to determine that

$$L_t \sim \frac{\Delta u^3}{\varepsilon},$$

and that the length scale of the smallest eddies, $\eta$ scales as

$$\eta \sim \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}.$$ 

Eddies of size $L \sim L_t$ are in the “energy range”. These eddies contain the bulk of the kinetic energy of the turbulence. Eddies of size $L \sim \eta$ are in the “dissipation range” and are responsible for dissipating the turbulent kinetic energy. Length scales between $\eta$ and $L_t$ are in the “inertial sub-range”.

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The energy contained within all eddies, $k$, can be expressed as an integral over a spectral energy density, which depends on the wavenumber of the eddies, $\kappa = 2\pi/L$, as

$$k = \int E(\kappa) \, d\kappa.$$ (2.21)

Eddies in the inertial sub-range are characterised by $\kappa$ and $\varepsilon$. Therefore, by dimensional analysis, the form of $E(\kappa)$ in the inertial sub-range is

$$E(\kappa) = C \kappa^{2/3} \kappa^{-5/3}.$$ (2.22)

This form of the spectral energy density is called the Kolmogorov $-5/3$ spectrum and is observed experimentally. The typical form of the total energy spectrum in a turbulent flow is shown in Figure 2.1.

![Figure 2.1: The spectral energy density of eddies in a turbulent flow, showing the Kolmogorov $-5/3$ spectrum.](image)

Analytical solutions to the Navier-Stokes equations for all but the simplest cases of laminar flow are either intractable or do not exist. For this reason, a wealth of computational methods for solving the Navier-Stokes and continuity equations have been developed. These are outlined in the remainder of this chapter.

### 2.6 Direct numerical simulation

Direct numerical simulation (DNS) involves solving the Navier-Stokes equations directly by discretising them on a computational domain. All time and length scales of the flow are resolved, including the smallest Kolmogorov scale, $\eta$. 

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In order to achieve such detail, very fine computational grids are required. To resolve a Kolmogorov length $\eta$ over a length $L$, the number of cells required can be shown to scale as $L/\eta = Re^{3/4}$, where $Re = UL/\nu$ is the Reynolds number based on the largest structures in the geometry. Thus, in three dimensions the number of cells requires scales as $Re^{9/4}$.

The number of time steps can be found by requiring a total simulation time of at least the turbulence time scale $\tau = \Delta u^2 / \varepsilon$, computed with a time step $\Delta t$ that limits the motion of a fluid element to the less than the length a single cell. This means that

$$\frac{\tau}{\Delta t} \sim \Delta u^3 / (\varepsilon \Delta x) \sim L/\Delta x \sim L/\eta \sim Re^{3/4}. \quad (2.23)$$

Considering both spatial and temporal resolution requirements, the total number of computations required to perform a DNS scales as

$$N \sim Re^3. \quad (2.24)$$

At the present time the computational power required is insurmountably high for industrial engineering applications, which have Reynolds numbers $Re \gtrsim 10^7$.

A DNS solution provides an exact solution for one realisation of a flow. However solutions to the Navier-Stokes equations are sensitive to the initial conditions, especially on the smallest scales. Therefore, for engineering purposes, knowing the solution on the smallest scales is unnecessary. For many practical purposes it is sufficient to know only the average velocity and pressure in the domain. Therefore more-efficient computational methods exist, which discard the finest details of the flow and seek to resolve only the motion on the largest scales.

### 2.7 Large eddy simulation

Kolmogorov’s first hypothesis states that turbulence is isotropic on the smallest scales. This means that the smallest scales should be simpler to model than the largest scales. In the technique called large eddy simulation (LES), the large scale motions are solved with a differential equation, while the smallest scales are modelled with algebraic equations. The large scale velocity, $\tilde{U}$, is obtained by passing the instantaneous velocity through a low pass filter $G(r, x)$ (Leonard, 1974),

$$\tilde{U}(x, t) = \int G(r, x) U(x - r, t) \, d^3r. \quad (2.25)$$

The instantaneous and filtered velocities define the sub-grid scale (SGS) motions, $u'(x, t)$, as

$$u'(x, t) = U(x, t) - \tilde{U}(x, t). \quad (2.26)$$
For constant density and viscosity the filtered Navier-Stokes and continuity equations are

\[
\frac{\partial \tilde{U}}{\partial t} + \nabla \cdot \left( \tilde{U} \tilde{U} \right) = -\frac{1}{\rho} \nabla \tilde{P} + \nu \nabla^2 \tilde{U} - \nabla \cdot \tau_{SGS}, \tag{2.27}
\]

\[
\nabla \cdot \tilde{U} = 0. \tag{2.28}
\]

The second order tensor \( \tau_{SGS} \) contains the sub-grid scale stresses, which are decomposed in Cartesian coordinates as

\[
\tau_{ij}^{SGS} = L_{ij} + C_{ij} + R_{ij}. \tag{2.29}
\]

The three components are the Leonard stress, \( L_{ij} = \tilde{U}_i \tilde{U}_j - \tilde{U}_i \tilde{U}_j \), the cross stress, \( C_{ij} = \tilde{U}_i u'_j + \tilde{U}_j u'_i \), and the Reynolds stress, \( R_{ij} = u'_i u'_j \). The Leonard stress involves products of the filtered velocity, the cross stress involves products of the filtered velocity and the unresolved velocity, and the Reynolds stress involves products of the unresolved velocity.

With a Reynolds averaging methodology, the Leonard and cross stresses would be identically zero. Typically the dominant stress is the Reynolds stress (Pletcher et al., 2012, p. 282). To proceed, it is necessary to model \( \tau_{ij}^{SGS} \). Many methods exist, including the widely-used Smagorinsky model (Smagorinsky, 1963), in which the deviatoric part of \( \tau_{ij}^{SGS} \) is related to the gradient of the filtered velocity.

LES is less computationally expensive than DNS because of the modelled SGS motion. A coarser grid and larger time step can be used since motions on scales smaller than the filter size are not fully resolved. Hence LES calculations run more quickly than DNS calculations. However the number of computations required for LES scales with \( Re^a \) with \( 3/2 < a < 2 \). This makes LES uneconomical for flows in large geometries at high Reynolds numbers.

LES and DNS results are used in this work, but no simulations are performed. They are presented here for reference. This work uses a third method of simulation, known as Reynolds-averaged Navier Stokes (RANS) methods. RANS simulations are even faster than LES simulations.

## 2.8 Reynolds-averaged Navier-Stokes methods

Reynolds-averaged Navier-Stokes (RANS) methods use a Reynolds decomposition (Reynolds, 1895) to split the instantaneous velocity, from this point on referred to as \( \tilde{U} \), into its mean part, \( U \), and fluctuating part, \( u \), as

\[
\tilde{U} = U + u. \tag{2.30}
\]
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The pressure is also decomposed the same way as \( \tilde{P} = P + p \). All instantaneous quantities are denoted with a tilde, mean quantities are denoted with upper case letters and fluctuating quantities are denoted with lower case letters. In general, the fluctuating quantities cannot be considered small compared to their mean counterparts. The averaging process is not important. It could be an ensemble average or a time average over a particular time interval. The averaging process means that the average of a fluctuating quantity is always zero.

Substituting Equation (2.30) into the Navier-Stokes and continuity equations yields the RANS momentum and continuity equations, which are respectively

\[
\rho \frac{D\mathbf{U}}{Dt} = \frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} U) = \nabla \cdot (\mu \nabla \mathbf{U} - \rho \mathbf{uu}) - \nabla P, \tag{2.31}
\]

and

\[
\nabla \cdot \mathbf{U} = \nabla \cdot \mathbf{u} = 0, \tag{2.32}
\]

where the total derivative is now written in terms of the mean velocity instead of the instantaneous velocity. Note that the time derivative is included in Equation (2.31). If the RANS averaging procedure is defined as an infinite time average then the solution must be steady. However if the solution is unsteady then the averaging process can be understood as an ensemble or period average. Unsteady solutions to Equation (2.31) are known as unsteady RANS (URANS) solutions.

The dyad \( \mathbf{uu} \) is the Reynolds stress tensor. This tensor obeys its own transport equation, which can be written in Cartesian coordinates as

\[
\frac{D(u_i u_j)}{Dt} = P_{ij} - \varepsilon_{ij} + \phi_{ij} + d_{ij}, \tag{2.33}
\]

where \( P_{ij} \) is the production tensor, \( \varepsilon_{ij} \) is the dissipation tensor, \( d_{ij} \) is the diffusion tensor, and \( \phi_{ij} \) is the pressure-strain tensor. The forms of these tensors are

\[
P_{ij} = - \left( \frac{u_i u_k}{u_j u_k} \frac{\partial U_j}{\partial x_k} + \frac{u_j u_k}{u_i u_k} \frac{\partial U_i}{\partial x_k} \right), \tag{2.34}
\]

\[
\varepsilon_{ij} = 2\nu \frac{\partial u_i}{\partial u_j} - \frac{\partial u_j}{\partial u_i}, \tag{2.35}
\]

\[
\phi_{ij} = \frac{p}{\rho} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \tag{2.36}
\]

and

\[
d_{ij} = - \frac{\partial}{\partial x_k} \left( u_i u_j u_k + \frac{p u_j}{\rho} \delta_{ik} + \frac{p u_i}{\rho} \delta_{jk} \right) - \nu \frac{\partial^2 u_i}{\partial x_k}, \tag{2.37}
\]
2.8.1 Near-wall behaviour of the Reynolds stresses

The no-slip wall boundary condition is unaffected by the Reynolds decomposition. Therefore, Equations (2.12) and (2.15) remain valid. In this section the wall is treated as stationary so that \( \nu_w = 0 \), the wall-normal velocity is \( V \) and the wall-normal points in the \( y \) direction. Therefore Equations (2.12) and (2.15) become respectively

\[
U = V = W = 0, \tag{2.38}
\]

and

\[
\frac{\partial V}{\partial y} = 0. \tag{2.39}
\]

In general the wall-parallel gradients \( \partial_y U \) and \( \partial_y W \) are non-zero and give rise to a wall shear stress, \( \tau_w \).

The fluctuating velocity components \( u, v \) and \( w \) can be expanded about the wall to reveal their \( y \) dependence. For a small distance from the wall, \( \delta y \),

\[
\begin{align*}
    u(\delta y) &= a_1 + b_1 \delta y + c_1 \delta y^2, \\
v(\delta y) &= a_2 + b_2 \delta y + c_2 \delta y^2, \\
w(\delta y) &= a_3 + b_3 \delta y + c_3 \delta y^2. \tag{2.40}
\end{align*}
\]

Equation (2.12) means that \( a_1 = a_2 = a_3 = 0 \) and Equation (2.15) means that \( b_2 = 0 \). Therefore as \( y \to 0 \),

\[
\begin{align*}
    \bar{u}^2 &= \mathcal{O}(y^2), \quad \bar{v}^2 = \mathcal{O}(y^4), \quad \bar{w}^2 = \mathcal{O}(y^2), \\
    \bar{uv} &= \mathcal{O}(y^3), \quad \bar{uw} = \mathcal{O}(y^2), \quad \bar{vw} = \mathcal{O}(y^3). \tag{2.41}
\end{align*}
\]

This shows that \( \bar{v}^2 \) tends to zero at the wall more quickly than \( \bar{u}^2 \) or \( \bar{w}^2 \). Hence the tensor \( \bar{u}_i u_j \) is anisotropic near to the wall.

2.8.2 The \( k \) equation

A widely-used quantity in turbulence modelling is the turbulent kinetic energy, \( k \). It can be found by contracting the Reynolds stress tensor

\[
k = \frac{1}{2} u_i u_i = \frac{1}{2} (\bar{u}^2 + \bar{v}^2 + \bar{w}^2). \tag{2.42}
\]

Equation (2.41) shows that \( k = \mathcal{O}(y^2) \) at the wall and therefore \( \partial_y k = 0 \). The transport equation for \( k \) can be found by contracting Equation (2.33), which yields

\[
\frac{Dk}{Dt} = -\bar{u}_i \bar{w}_j \frac{\partial U_j}{\partial x_i} - \nu \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \frac{1}{2} \bar{u}_j \bar{u}_j u_i + \frac{\bar{w}_i \rho}{\rho} - \nu \frac{\partial k}{\partial x_i} \right) \tag{2.43}
\]
Each term on the right hand side of Equation (2.43) has a name. These names are standard in the literature and will be used throughout the rest of this thesis. The first term is known as the production term:

\[ P = -u_i u_j \frac{\partial U_i}{\partial x_j}. \]  

(2.44)

It is so-called because the same term appears in the transport equation for the mean kinetic energy with the opposite sign. It is understood to represent the transfer of energy from the mean part of the flow to the turbulent part of the flow. The second term on the right hand side of Equation (2.43) is called the dissipation:

\[ \varepsilon = \nu \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}. \]  

(2.45)

The final three terms in Equation (2.43) are grouped into the “diffusion term”, which comprises molecular diffusion of \( k \),

\[ D_k^\nu = \frac{\partial}{\partial x_j} \left( \nu \frac{\partial k}{\partial x_j} \right), \]  

(2.46)

which needs no modelling, pressure diffusion of \( k \),

\[ \Pi_k = -\frac{\partial}{\partial x_j} \left( \frac{u_j p}{\rho} \right); \]  

(2.47)

and turbulent diffusion of \( k \)

\[ T_k = -\frac{\partial}{\partial x_j} \left( \frac{1}{2} u_i u_j u_i u_j \right). \]  

(2.48)

The production, dissipation and diffusion tensors in Equation (2.33) have scalar counterparts in the \( k \) equation. However the pressure-strain tensor has no counterpart because it is traceless.

The five terms on the right-hand side of Equation (2.43) are shown in Figure 2.2 for a one-dimensional channel flow at \( Re = 13750 \) computed by Moser et al. (1999). The wall is located at \( y = 0 \) and the half-height of the channel is \( h \). The flow is steady with no mean convection, which means that the total derivative of \( k \) is zero. Therefore the sum of the five source terms in Equation (2.43) is zero. Far from the wall in Figure 2.2 the production approximately balances the dissipation. Near to the wall however molecular diffusion and dissipation are \( O(1) \) and the other terms tend to zero. Pressure diffusion is not dominant anywhere in the channel.

RANS models are classified by how they model the Reynolds stresses. The remainder of this chapter is devoted to a discussion of some of the different methods that exist.
2.8. Reynolds-averaged Navier-Stokes methods

2.8.3 Reynolds stress models

Reynolds stress models (RSMs) solve a different equation for each independent Reynolds stress. The starting point for the derivation is Equation (2.33). Since $P_{ij}$ contains only Reynolds stresses and mean velocity gradients, it requires no modelling. However the dissipation, diffusion and pressure-strain tensors all require modelling in order to solve the equation.

Because the first hypothesis of Kolmogorov states that turbulence is isotropic on the smallest scales, $\varepsilon_{ij}$ is often modelled as (Rotta, 1951)

$$\varepsilon_{ij} = \frac{2}{3} \varepsilon.$$  \hspace{1cm} (2.49)

Although an exact form of the $\varepsilon$ transport equation can be derived (Hanjalić and Launder, 1972), most of the terms in it would need to be modelled. Therefore the $\varepsilon$ equation is often defined empirically. For example, Hanjalić and Launder (1972) used

$$\frac{D\varepsilon}{Dt} = c_{\varepsilon 1} \frac{P_{\varepsilon}}{k} - c_{\varepsilon 2} \frac{\varepsilon^2}{k} + c_{\varepsilon 3} \frac{\partial}{\partial x_k} \left( \frac{k}{\varepsilon} \frac{\partial u_i}{\partial x_l} \frac{\partial \varepsilon}{\partial x_l} \right),$$  \hspace{1cm} (2.50)

where the constants $c_{\varepsilon 1}$, $c_{\varepsilon 2}$ and $c_{\varepsilon 3}$ are tuned to experimental data.

The diffusion term in Equation (2.37) comprises three terms: a triple velocity fluctuation,
pressure-diffusion and viscous diffusion. Molecular diffusion can be included in its exact form, however it is generally small except for in near-wall regions. Pressure diffusion is typically neglected because it is generally small, except for in near-wall regions (Pope, 2000, p. 430). The remainder of the diffusion term is often modelled using the generalised gradient diffusion hypothesis (GGDH) (Daly and Harlow, 1970), whereby the turbulent fluctuations of a quantity $\phi$ are modelled as

$$\overline{u_i \phi} = -c \varepsilon \overline{u_i u_j} \frac{\partial \phi}{\partial x_j},$$

(2.51)

for some constant $c$.

The pressure-strain redistributes energy between the Reynolds stresses. It does not affect the turbulent kinetic energy because it is traceless. It can be shown that the fluctuating pressure obeys a Poisson equation, which can be solved with a Green’s function (Chou, 1945). The solution is conventionally split into three parts; the rapid pressure, which depends on mean velocity gradients; the slow pressure, which depends on gradients of the Reynolds stresses; and the pressure reflection term. The pressure reflection term is active near to wall boundaries and is required in order to impose a homogeneous Neumann boundary condition on the fluctuating pressure. Consequently, the pressure strain is often modelled as three terms,

$$\phi_{ij} = \phi_{ij,1} + \phi_{ij,2} + \phi_{ij,w},$$

(2.52)

where $\phi_{ij,1}$ is the slow part, $\phi_{ij,2}$ is the rapid part $\phi_{ij,w}$ is the pressure reflection term.

The slow part of the pressure strain is responsible for the return to isotropy of the turbulence (Rotta, 1951; Speziale et al., 1991). The rapid term is often modelled with a term that is active when the production tensor is anisotropic. This model is given the name “isotropisation of production” (Naot et al., 1970). The pressure reflection term is often split into its rapid and slow parts (Shir, 1973; Gibson and Launder, 1978). It is used to make the model predict $\overline{v^2} < \overline{w^2} < \overline{u^2}$ in the near wall region, in order to be consistent with Equations (2.41) and experimental observations.

RSMs are theoretically the most accurate of the existing RANS models. They are the most computationally expensive RANS models but are still cheaper than LES or DNS.

The EBRSM model of Manceau and Hanjalić (2002) is used in a small part of this work. The model solves for the six independent Reynolds stresses, the dissipation and an elliptic blending parameter, $\alpha$. The elliptic blending parameter obeys an elliptic equation that reproduces the blocking effect of the wall. Hence $\alpha$ appears in the model for the pressure-strain tensor. The method is tuned to reproduce the correct limiting behaviour of $\phi_{ij} - \varepsilon_{ij}$ at the wall. Hence $\alpha$ also appears in the definition of the dissipation tensor. The full equations for the EBRSM model can be found in Manceau and Hanjalić (2002).
2.8. Reynolds-averaged Navier-Stokes methods

2.8.4 Eddy viscosity models

Eddy viscosity models (EVMs) use algebraic expressions to calculate the Reynolds stresses. This is computationally cheaper than solving a differential equation. Typically the Reynolds stresses are computed in terms of some mean flow parameters and a turbulent viscosity, $\mu_t$.

Two commonly-used parameters are the mean strain tensor

$$S_{ij} \equiv \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right), \quad (2.53)$$

and the mean vorticity tensor

$$\Omega_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right). \quad (2.54)$$

These are used to define the mean strain invariant, $S = \sqrt{2S_{ij}S_{ij}}$ and the mean vorticity invariant, $\Omega = \sqrt{2\Omega_{ij}\Omega_{ij}}$.

Eddy viscosity models are often classified by the relationship between the Reynolds stresses and $S$ or $\Omega$. Relationships that are linear in $S_{ij}$ and $\Omega_{ij}$ are called linear eddy viscosity models (LEVMs), non-linear relationships are called non-linear eddy viscosity models (NLEVMs).

Linear eddy viscosity models

The most commonly used eddy viscosity model is the Boussinesq hypothesis, which links the Reynolds stresses to the mean strain,

$$\rho \bar{u}_i \bar{u}_j = \frac{2}{3} \rho k \delta_{ij} - 2 \mu_t S_{ij}, \quad (2.55)$$

where $\mu_t$ must be computed somehow.

Substituting Equation (2.55) into Equation (2.31) yields

$$\rho \frac{D\mathbf{U}}{Dt} = \nabla \cdot ((\mu + \mu_t) \nabla \mathbf{U}) - (\nabla \mathbf{U})^T \cdot \nabla \mu_t - \nabla P, \quad (2.56)$$

where the pressure on the right hand side has been redefined as

$$P \rightarrow P + \frac{2}{3} \rho k. \quad (2.57)$$

Thus, when the Boussinesq hypothesis is used, the turbulent fluctuations are modelled by a turbulent viscosity that can be added to the dynamic viscosity of the fluid.

Equation (2.55) works well in many flows. However it has well known weaknesses.

1. With Equation (2.55), the normal Reynolds stresses, $\bar{u}^2$, $\bar{v}^2$ and $\bar{w}^2$, are always isotropic.
2. Near to curved boundaries, the wall-limiting behaviour of the off-normal Reynolds stresses (shown in Equation (2.41)) has a significant effect on the production tensor. This effect is lost when Equation (2.55) is used.

3. Rotating homogeneous shear flows are seen experimentally to exhibit increasing asymmetry in the velocity profile as the rotation rate increases. However in a rotating frame, Equation (2.55) is completely insensitive to the rotation rate and always produces the same results (Gatski and Speziale, 1993).

More complex expressions can be used for the Reynolds stresses that help to ameliorate some of these issues.

Non-linear eddy-viscosity models

Equation (2.55) only uses the mean strain tensor. However, any combination of $S_{ij}$, $\Omega_{ij}$ and $\delta_{ij}$ could be used with an expression of the form

$$u_i u_j = \frac{2}{3} k \delta_{ij} - \nu_t S_{ij} + F(S_{ij}, \Omega_{ij}),$$

(2.58)

provided that the general function $F$ satisfies the necessary transformation and contraction properties. NLEVMs contain more model constants and can be tuned to fit a wider range of flow phenomena than LEVMs. The additional computational cost of a simulation with a NLEVM compared to a LEVM is small compared to the difference between RANS and LES or DNS (Craft et al., 1996).

2.8.5 Computing the turbulent viscosity

The final parameter that is required is the turbulent viscosity, $\mu_t$. There are many ways of calculating it, some of which are now discussed.

2.8.6 Algebraic models

Algebraic models use an algebraic equation to link $\mu_t$ to mean flow properties. The earliest method is that of Prandtl (1925), who proposed a mixing length hypothesis to model wall-bounded shear flows. For a mixing length, $l_m$, and a characteristic velocity, $v_m$, the turbulent viscosity is $\mu_t = \rho l_m v_m$. The characteristic velocity is related to the mean shear as

$$v_m = l_m \left| \frac{\partial U}{\partial y} \right|,$$

(2.59)
where $U$ is the wall-parallel velocity and $y$ is the wall-normal direction, so that the turbulent viscosity is

$$
\nu_t = \rho l^2 \frac{\partial U}{\partial y}.
$$

(2.60)

The mixing length is flow-dependent and varies with position. The turbulent viscosity must vanish at the wall in order to create a viscous region in the boundary layer. Near-wall damping terms, which reduce $l_m$ near to the wall, are often used to achieve this. A widely used example is the van Driest (1956) damping function.

Despite their simplicity, algebraic models have been finely tuned to certain types of flow and are often used today in specific industries (Absi, 2009). They are typically used in flows where boundary layers remain attached. This is because they are incapable of accounting for non-local effects, which are important near separation points (Bredberg, 2001). They are also useful for obtaining approximations to solutions of the Navier-Stokes equations, which may be used to initialise more detailed calculations.

### 2.8.7 One equation models

The mixing length hypothesis predicts that turbulence will vanish whenever the mean strain is zero, which is not observed experimentally. Kolmogorov (1942) and Prandtl (1945) proposed taking the velocity scale from turbulent kinetic energy as

$$
v_m = c \sqrt{k},
$$

(2.61)

where the constant $c$ must be determined. These models are called one-equation models because a transport equation must be solved to find $k$.

**The Spalart-Allmaras model**

A more advanced one equation model is the Spalart-Allmaras model (Spalart and Allmaras, 1994; Spalart, 2000). The model is known to perform well in wall-bounded aerospace applications with either attached or separated boundary layers (Wilcox, 2006). This model solves an ad hoc transport equation for a function $\tilde{\nu}$, which is used to calculate $\nu_t$ as

$$
\nu_t = \rho \tilde{\nu} f_{\nu_1},
$$

(2.62)

with

$$
f_{\nu_1} = \frac{\chi^3}{\chi^3 + c_{\nu_1}^3},
$$

(2.63)
and $\chi = \rho \tilde{v} / \mu$. This model is widely used in this work. The full equations are given in Appendix A.5.

### 2.8.8 Two equation models

Two equation turbulence models are widely used in CFD and solve two differential equations in order to compute the turbulent viscosity. It is common for one of the two functions to be the turbulent kinetic energy, which provides a velocity scale. The other function provides the length scale needed to specify the turbulent viscosity, $\mu_t = \rho v_m l_m$.

The turbulent kinetic energy is governed by Equation (2.43). Some of the terms in Equation (2.43) must be modelled in order to close the set of equations. The terms $\Pi_k$ and $T_k$ are often modelled as

$$ T_k + \Pi_k = \nabla \cdot \left( \frac{\mu_t}{\rho \sigma_k} \nabla k \right), \quad (2.64) $$

so that the $k$ equation becomes

$$ \rho \frac{Dk}{Dt} = \rho P - \rho \varepsilon + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right). \quad (2.65) $$

The boundary conditions on $k$ at the wall are $k = 0$ and $\partial n k = 0$ where $n$ is the wall normal. In $k - \varepsilon$ models, $\varepsilon$ obeys its own transport equation.

### $k - \varepsilon$ models

$k - \varepsilon$ models solve for $k$ and $\varepsilon$. The earliest model was developed by Jones and Launder (1972), and computes the turbulent viscosity as

$$ \mu_t = c_\mu \frac{k^2}{\varepsilon}, \quad (2.66) $$

with $c_\mu = 0.09$. The $\varepsilon$ equation is empirical in nature and is written

$$ \rho \frac{D\varepsilon}{Dt} = c_{\varepsilon 1} \frac{\rho P \varepsilon}{k} - c_{\varepsilon 2} \frac{\rho \varepsilon^2}{k} + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right), \quad (2.67) $$

where the constants $c_{\varepsilon 1}, c_{\varepsilon 2}$ and $\sigma_\varepsilon$ are tuned to experimental data. The asymptotic behaviour of $\varepsilon$ at the wall is

$$ \varepsilon_w = \nu \frac{\partial^2 k}{\partial y^2} = 2\nu \left( \frac{\partial \sqrt{k}}{\partial y} \right)^2. \quad (2.68) $$

This wall boundary condition is computationally awkward. Jones and Launder (1972) introduced a transport equation for $\tilde{\varepsilon} = \varepsilon - \varepsilon_w$, so that the boundary condition becomes $\tilde{\varepsilon}_w = 0$. In this work, the standard $k - \varepsilon$ model of Launder and Spalding (1974), and the LRN model of Chien (1982) are used. The full equations are given in Appendices A.2 and A.3, respectively.
Other two equation models

The second equation does not have to be for $\varepsilon$. For example, $k - \omega$ models (Wilcox, 2006) solve for $\omega \equiv \varepsilon/k$ and the turbulent viscosity is computed as

$$\mu_t = \frac{k}{\omega}. \quad (2.69)$$

A brief overview of the $k - \omega$ model and the full equations for the related $k - \omega$ SST model (Menter, 1994; Menter et al., 2003) are given in Appendix A.4.

2.8.9 Four equation (elliptic relaxation) models

The correct near-wall behaviour of the Reynolds stresses, expressed in Equation (2.41), can rarely be achieved by two equation EVMs. Durbin (1991) introduced a four equation model, known as the $v^2 - f$ model, which solves for $k$, $\varepsilon$, $v^2$ and an elliptic relaxation function, $f$. The model uses $v^2$ to calculate the turbulent viscosity as $\mu_t = c_\mu \rho v^2 T$, where $T$ is the turbulent time scale, which is computed as

$$T = \max \left( \frac{k}{\varepsilon}, c_T \left( \frac{\mu}{\rho \varepsilon} \right)^{1/2} \right), \quad (2.70)$$

where $c_T$ is a constant. The equation for $v^2$ has the form

$$\rho \frac{Dv^2}{Dt} = \rho k f - \rho \varepsilon \frac{v^2}{k} + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_{v^2}} \right) \nabla v^2 \right). \quad (2.71)$$

The term $\rho k f$ can be thought of as modelling the pressure-strain, pressure diffusion and the dissipation tensors (Billard, 2011). The elliptic relaxation function obeys an equation of the form

$$L_D^2 \nabla^2 f - f = \frac{1}{T} (c_1 - 1) \left( \frac{v^2}{k} - \frac{2}{3} \right) - c_2 \frac{P}{k}, \quad (2.72)$$

for constants $c_1$ and $c_2$. The turbulent length scale, $L_D$ is computed as

$$L_D = c_L^2 \left( \frac{k^{3/2}}{\varepsilon} + c_\eta \frac{\mu^{3/4}}{\rho^{3/4} \varepsilon^{1/4}} \right). \quad (2.73)$$

The function $f$ contains a measure of the non-local effects on $v^2$ within a sphere of radius $L_D$. The effect of $f$ is to impose the correct near-wall behaviour on $v^2$, which, according to Equation (2.41), is $v^2 = O(y^4)$. The boundary condition is $v^2 = 0$ and the boundary condition on $f$ is

$$f \to \left( \frac{-20 \mu^2 v^2}{\rho^2 \varepsilon y^4} \right) \text{ as } y \to 0, \quad (2.74)$$
which is numerically stiff due to the explicit ratio of functions of order $y^4$ at the wall (Billard, 2011). Consequently, a small time-step must be used to achieve convergence.

Modern $\vec{v}^2 - f$ models solve an equation for the ratio $\varphi = \vec{v}^2 / k$ instead of $\vec{v}^2$ (Laurence et al., 2004; Hanjalić et al., 2004; Billard and Laurence, 2012). At the wall, $\varphi = O(y^2)$ with the boundary condition $\varphi = 0$. A change of variables is also made to $f$ to transform the boundary condition into something less numerically stiff. For example, the $\varphi - f$ model (Laurence et al., 2004) solves for a variable $\overline{f}$, where

$$\overline{f} = f + \frac{2\mu \nabla \varphi \cdot \nabla k}{\rho k} + \frac{\mu}{\rho} \nabla^2 \varphi$$

Equation (2.75)

The boundary condition on $\overline{f}$ at the wall is $\overline{f} = 0$, which is less numerically stiff than Equation (2.74).

Two $\vec{v}^2 - f$ models are used in this work, the $\varphi - f$ model (Laurence et al., 2004) and the BL-$\vec{v}^2 / k$ model (Billard, 2011). The full equations for these models can be found in Appendices A.6 and A.7, respectively.

### 2.8.10 Curvature and rotation and corrections for LEVMs

The effects of rotation and streamline curvature can be included explicitly in RSMs. For example, in a rotating frame with rotation vector $\Omega'_k$ there is an additional turbulence generation rate (Piquet, 1999, p. 569)

$$G_{ij} = -2\Omega'_k \left( \overline{u_j u_n} \varepsilon_{ikn} + \overline{u_i u_n} \varepsilon_{jkn} \right).$$

Equation (2.76)

However in many EVMs the effects are not captured adequately.

The effects of frame rotation and streamline curvature are similar. The turbulent shear stresses are observed to be significantly affected even by only weak streamline curvature (Spalart and Shur, 1997). Curvature can be both global and local; global curvature is caused by the geometry of the flow domain and local curvature is caused by the flow behaviour. For example, local curvature manifests as streamline curvature in a recirculation region or in a vortex. Therefore, although all calculations in this thesis are performed in a static frame, some simulations are performed with a rotation correction algorithm in order to assess the effects of streamline curvature.

Bradshaw (1969) identified a similarity between stratified flows and flows with streamline curvature. An important parameter in stratified flows is the flux Richardson number, which is the ratio of turbulence production due to buoyancy forces to turbulence production due to shear forces. For flux Richardson numbers less than zero the flow is unstable, whereas for flux
Richardson numbers greater than zero, the buoyancy enhances the stability of the flow. By analogy to this, a curvature Richardson number, $Ri_c$, can be computed for flows with streamline curvature. Conceptually, the curvature Richardson number is the ratio of turbulence production due to curvature to turbulence production due to shear stresses (Piquet, 1999, p. 570). Many different definitions of $Ri_c$ exist, a selection of which can be found in Hellsten (1998) and Cazalbou et al. (2005). It usually depends on the mean vorticity and mean strain rate. The most important feature is that for $Ri_c < 0$, streamline curvature reduces the stability of the flow. This occurs in flows with concave curvature. For positive $Ri_c$, streamline curvature enhances stability of the flow. This occurs in flows with convex curvature. The curvature Richardson number can be used to define a further parameter called the Bradshaw Richardson number, (Piquet, 1999, p. 571)

$$B_R = Ri_c(1 + Ri_c).$$

Another parameter, which is useful in rotating frames is the Rossby number, $Ro$, which is the ratio of the magnitude of the inertial forces to the Coriolis force.

Many methods exist to sensitise turbulence models to streamline curvature and rotating frames. Two different methods are used in this thesis. The first type of curvature correction is that of Cazalbou et al. (2005). The constant $c_{ε^2}$ in the $ε$ equation is no longer treated as a constant. Instead it is sensitised to the Rossby number and the Bradshaw-Richardson number. The effect of the correction is to increase $c_{ε^2}$ in regions of rotation or convex curvature, which reduces the dissipation. In turn this increases the turbulent viscosity which stabilises the flow. This approach is used with the $k−ε$, BL-$\overline{v^2}/k$ and $ϕ−f$ models, which solve for $ε$. The Spalart-Allmaras model does not solve for the dissipation and so the method of Cazalbou et al. (2005) cannot be used.

The second type of correction is that of Shur et al. (2000), which modifies the production to account for the Bradshaw Richardson number. The effect of the correction is to reduce the production in regions of the flow where the mean vorticity is larger than the mean strain. In turn, the correction reduces the turbulent viscosity and therefore damps the vortices less, making the flow less stable. This type of correction can be used for every turbulence model used in this thesis. In this work it is used with the BL-$\overline{v^2}/k$, $ϕ−f$ and Spalart-Allmaras models.

A comparison of the two rotation correction methods can be found in (Dufour et al., 2008), who tested both methods on the flow in a centrifugal compressor. They report that both approaches reproduce the desired physical effects and produce results in agreement with experimental data.

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Only the correction methods of Cazalbou et al. (2005) and Shur et al. (2000) are used in this thesis, because they are already implemented in Code_Saturne. The full equations of the two correction methods are given in Appendix A.9. Other correction methods exist, such as the correction of Pettersson Reif et al. (1999), who made \( c_\mu \), and hence \( \mu_t \), directly dependent on the rotation rate.

### 2.8.11 Scalar transport equations

Scalars such as temperatures or concentrations can also be decomposed using a Reynolds decomposition and obey analogous equations to Equation (2.31). After the usual Reynolds decomposition of a scalar \( \tilde{\Phi} \) into its mean and fluctuating parts, \( \tilde{\Phi} = \Phi + \phi \), the transport equation obeyed by the mean, \( \Phi \), is found to be

\[
\rho \frac{D\Phi}{Dt} = \nabla \cdot \left( \Gamma_\Phi \nabla \Phi - \rho \bar{u} \phi \right) + \overline{S_\Phi},
\]  

(2.78)

where \( \overline{S_\Phi} \) represents any source terms. The coefficient \( \Gamma_\Phi \) is often related to the viscosity with a Prandtl number, \( \sigma_\Phi \), as

\[
\Gamma_\Phi = \frac{\mu}{\sigma_\Phi}.
\]  

(2.79)

The turbulent heat fluxes, \( \bar{u} \phi \), must be modelled. They are often modelled using a gradient diffusion hypothesis, which relates \( \bar{u} \phi \) to the gradients of \( \Phi \). The simple gradient diffusion hypothesis (SGDH) is used in this work. Under this approach the turbulent fluxes are calculated as

\[
\bar{u} \phi = - \frac{\mu_t}{\sigma_t,\Phi} \sigma_\Phi \rho \nabla \Phi,
\]  

(2.80)

where \( \sigma_t,\Phi \approx 1 \) is the turbulent Prandtl number. With the SGDH, Equation (2.78) becomes

\[
\rho \frac{D\Phi}{Dt} = \nabla \cdot \left( \left( \frac{\mu}{\sigma_\Phi} + \frac{\mu_t}{\sigma_t,\Phi} \right) \nabla \Phi \right) + \overline{S_\Phi}.
\]  

(2.81)

It is experimentally observed that the SGDH is incorrect. For example, in a flat plate boundary layer with its wall in the \((x,z)\) plane, the turbulent flux \( |\bar{u} \phi| \) is seen in experiments to be greater than \( |\overline{v \phi}| \) even though \( |\partial_y \Phi| > |\partial_x \Phi| \). The GGDH in Equation (2.51) can be used to improve the model for the heat fluxes. However it has not been used in this work for two reasons:

1. The predictions of scalars with the SGDH on the test cases in Chapter 6 in this thesis with are sufficiently accurate and therefore the GGDH is not needed.

2. On the more complex flows in Chapters 7 and 8, the solution of the momentum equations (expressed through the friction factor) is often so inaccurate that the priority is to
improve it before focusing on passive scalars. If the flow field is not accurately predicted then predictions of transported scalars contain errors. Thus, if the GGDH were used in Chapters 7 and 8 and the heat transfer results were accurate, they could not be treated with confidence since the flow field is so poorly predicted. Hence the immediate priority is to improve the flow field predictions. In addition, in Chapter 8, when an RSM is used, the friction factor does not change significantly compared to its value with eddy-viscosity models, which indicates that the difference in capability of the GGDH and SGDH on the flows in Chapter 8 is small.
Chapter 3

Near-wall models

As mentioned in Section 2.4, the no slip boundary condition at the wall leads to the development of boundary layers. In these thin regions near to the wall, the velocity gradient normal to the wall is typically large compared to the velocity gradients elsewhere in the flow. Therefore in order to resolve the flow in these regions, a fine mesh is required. This greatly increases the computational expense of performing a simulation. For example, resolution of the boundary layer can be responsible for over 90% of the total computation time in two-dimensional flows, and even an even larger fraction in three-dimensional flows (Craft et al., 2006).

Flows in engineering typically have high Reynolds numbers. Therefore there will usually be a turbulent boundary layer next to any walls. Boundary layers have a common structure that can be discussed in terms of the distance from the wall. In this chapter, the wall will be assumed to be stationary and span the \((x, z)\) plane. The wall-normal coordinate is denoted \(y\), the wall-normal velocity component is \(V\) and the local wall-parallel velocity is denoted \(U\).

The chapter begins with a description of the structure of an attached, one-dimensional boundary layer. Turbulence models are classified by the approach used to simulate the boundary layer.

- Low Reynolds number (LRN) turbulence models compute the flow in the boundary layer. The turbulence model equations are valid down to the wall. The name comes from the low turbulent Reynolds number near the wall. When a LRN turbulence model is used, the computational mesh often contains prism layers near to the wall, in order to increase the mesh resolution there.

- High Reynolds number (HRN) turbulence models use empirical models called wall functions to model the boundary layer. The turbulence model equations are not valid near to the wall. Typically the mesh for a HRN model contains large cells near to the wall.
This means that while HRN calculations run faster than LRN calculations, the accuracy of the solution is often, though not always, reduced.

The chapter ends with a discussion of boundary layers next to rough walls.

3.1 Notation

Before starting, it is useful to introduce the velocity and length scales that appear throughout the rest of this thesis.

- An important velocity scale is the friction velocity, \( u_\tau = \sqrt{\tau_w/\rho} \), where \( \tau_w \) is the wall shear stress, which, in the local coordinate system, is \( \mu \partial_y U \). This is used to define the non-dimensional velocity scale \( U^+ = U/u_\tau \).

- Another velocity scale is the turbulence velocity \( u_k = c_1^{1/4} k^{1/2} \), which is sometimes used in place of \( u_\tau \). This velocity scale is useful in regions where \( \tau_w = 0 \), and hence \( u_\tau = 0 \).

- The dimensionless distances that are widely used are distinguished by subscripts, which indicate which velocity scale is used to compute them:
  \[
  y_+^\tau = \frac{y u_\tau}{\nu}, \quad \text{(3.1)}
  \]
  \[
  y_+^k = \frac{y u_k}{\nu}. \quad \text{(3.2)}
  \]

3.2 Turbulent boundary layers

In statistically steady flow the RANS equations can be simplified. Variations in \( z \) are ignored, as are the \( x \) derivatives of all quantities apart from the pressure. The pressure gradient is retained because it drives the flow. Since the flow is statistically one-dimensional and steady, the total derivative of all functions is zero. Therefore, the \( U \) and \( V \) RANS momentum equations become

\[
0 = -\frac{\partial P}{\partial x} + \mu \frac{\partial^2 U}{\partial y^2} - \frac{\partial (\rho \overline{uv})}{\partial y}, \quad \text{(3.3)}
\]
\[
0 = -\frac{\partial P}{\partial y} - \frac{\partial (\rho \overline{v^2})}{\partial y}. \quad \text{(3.4)}
\]

Since \( \overline{v^2} = \mathcal{O}(y^2) \) as \( y \to 0 \) it follows that \( \partial_y P = 0 \) near to the wall.

With a LEVM the Reynolds stress \( \overline{uv} \) is

\[
\rho \overline{uv} = -\mu_i \frac{\partial U}{\partial y}, \quad \text{(3.5)}
\]
which turns Equation (3.3) into
\[ \frac{\partial}{\partial y} \left( (\mu + \mu_t) \frac{\partial U}{\partial y} \right) = \frac{\partial P}{\partial x}. \] (3.6)

The earliest wall models ignored the pressure gradient. With this approach, the \( U \) boundary layer equation is written as
\[ \frac{\partial}{\partial y} \left( (\mu + \mu_t) \frac{\partial U}{\partial y} \right) = 0. \] (3.7)

### 3.2.1 The viscous sublayer

In the viscous region of the boundary layer (see Section 2.4), viscous effects dominate and therefore \( \nu T \) (or equivalently \( \mu_t \)) can be neglected. Under these conditions, Equation (3.7) becomes
\[ \frac{\partial^2 U}{\mu \partial y^2} = 0, \] (3.8)
which can be solved to give
\[ U = \frac{y \tau_w}{\mu}, \] (3.9)
or
\[ U^+ = y_r^+. \] (3.10)

This equation is valid only in the viscous sublayer, which is thin and typically exists for \( y_r^+ \lesssim 5 \).

### 3.2.2 The logarithmic layer

Further out from the wall, the Reynolds stresses become more important until eventually they dominate over the viscous stresses. At this wall distance, the molecular viscosity can be ignored. Therefore Equation (3.7) becomes
\[ \frac{\partial}{\partial y} \left( \mu_t \frac{\partial U}{\partial y} \right) = 0. \] (3.11)

Integration gives
\[ \mu_t \frac{\partial U}{\partial y} = \tau_w. \] (3.12)

A mixing length model can be used to calculate the turbulent viscosity. The size of the turbulent eddies is proportional to the distance to the wall so that the mixing length (see Section 2.8.6) is
\[ l_m = \kappa y, \] (3.13)
where $\kappa = 0.42$ is the von Kármán constant. According to Equation (2.60) the turbulent viscosity is

$$\mu_t = \rho \kappa^2 y^2 \left| \frac{\partial U}{\partial y} \right|. \tag{3.14}$$

so that Equation (3.12) becomes

$$\kappa^2 y^2 \left( \frac{\partial U}{\partial y} \right)^2 = \frac{\tau_w}{\rho}. \tag{3.15}$$

Integration of Equation (3.15) yields

$$U = \sqrt{\frac{\tau_w}{\rho \kappa}} \log(y) + A, \tag{3.16}$$

which can be re-written as the so-called log law

$$U^+ = \frac{1}{\kappa} \log(y^+_r) + C. \tag{3.17}$$

The constant $C$ must be tuned to experimental data. A common value is $C = 5.2$. Sometimes Equation (3.17) is written as

$$U^+ = \frac{1}{\kappa} \log(E y^+_r), \tag{3.18}$$

with $E \approx 9$.

The logarithmic layer begins around $y^+_r = 30$ but at large enough wall distances, most flows eventually deviate from it. For a channel flow with half-height $h$, deviation from Equation (3.17) occurs around $y/h \approx 0.3$ (Pope, 2000, p. 276), which can correspond to a relatively small value of $y^+_r$. In all flows, the upper limit on the validity of the log law is Reynolds number-dependent. Equation (3.10), the log law and the DNS results of Moser et al. (1999) for a channel flow with half-height $h$ at $Re_r = u_r \tau / \nu = 590$ are plotted in Figure 3.1. The log law matches the DNS for $30 \lesssim y^+_r \lesssim 100$ (that is, up to $y/h \approx 0.2$) and Equation (3.10) is accurate for $y^+_r < 5$. Figure 3.1 demonstrates that Equation (3.17) is inaccurate at the wall.

### 3.2.3 The buffer layer

For $5 \lesssim y^+_r \lesssim 30$ there is another layer where neither the viscosity nor the Reynolds stresses dominate. This region is visible in Figure 3.1 and is called the buffer layer. No simple analytical expression exists to determine the velocity in this layer. However, with a mixing length hypothesis, Equation (3.7) can be written in non-dimensional form as

$$\frac{\tau}{\tau_w} = \left( \frac{\partial U^+}{\partial y^+_r} \right)^2 + \left( l^+ \frac{\partial U^+}{\partial y^+_r} \right)^2, \tag{3.19}$$
where $\tau = \tau(y)$. Assuming that $\tau/\tau_w = 1$ (which is true only for small $y$), this equation can be solved to give (van Driest, 1956)

$$U^+ = \int_0^{y^+} \frac{2d\xi}{1 + \sqrt{1 + 4l_m^+(\xi)^2}}. \quad (3.20)$$

Equation (3.10) is found by setting $l_m^+ = 0$. Equation (3.17) can be obtained by setting $l_m^+ = \kappa y^+$ and restricting the limits of integration to the turbulent region of the boundary layer. However if a van Driest (1956) damping function is used to compute the mixing length

$$l_m = \kappa y \left(1 - \exp\left(-y^+ / A^+\right)\right), \quad (3.21)$$

where $A^+ \approx 26$, then a formal solution to Equation (3.7) is obtained.

The damping function is not always accurate. For example, with the Boussinesq approximation in Equation (2.55), Equation (3.21) produces $\overline{uu} = \mathcal{O}(y^4)$ when at the wall, according to Equation (2.41), $\overline{uu}$ should be $\mathcal{O}(y^2)$. 

Figure 3.1: The analytical solution for the velocity in the logarithmic and viscous layers and the DNS solution for a channel flow of Moser et al. (1999).
3.2.4 The velocity defect layer

For large enough $y^+$, the log law becomes inaccurate. This can be seen in Figure 3.1 around $y^+ \approx 100$. At larger $y^+$, the flow is said to be in the velocity defect layer until eventually the boundary layer ceases to exist at all. In general, the $y^+$ at which the velocity defect layer begins increases as the Reynolds number increases. However the limit is not well-defined and cannot be computed a priori.

Coles (1956) demonstrated that the flow in the defect layer can be adequately approximated as the sum of the “law of the wall” and the “law of the wake” as

$$U^+ = f(y^+) + \frac{\Pi}{\kappa} w(y/L),$$

where $L$ is a characteristic lengthscale of the mean velocity, $\Pi$ is a constant that depends on the type of flow and $w$ is the “wake function”, which is a tabulated function that contains the effects of momentum loss to the bulk flow. The wake function is zero at the wall, and increases non-linearly as $y/L$ increases (Coles, 1956).

On a practical level, the velocity defect layer is the region nearest to the wall where the boundary layer equations (Equations 3.3 and 3.4) cannot be accurately used. Therefore models based on the boundary layer equations, such as wall functions or the near-wall domain decomposition method developed in this thesis, cease to be accurate in the velocity defect layer. This places a Reynolds number-dependent upper limit on the near-wall cell size that can be used with near-wall models.

However for computations, the velocity defect layer does not cause many issues because the full HRN or LRN RANS equations can be used in this region.

3.3 Low Reynolds number models

The governing equations of LRN turbulence models remain valid to the wall. Hence the equations must be capable of producing the structure of a boundary layer. LRN models often introduce additional functions to produce the correct near-wall behaviour. The procedure followed depends on the turbulence model.
3.3.1 Two equation models

LRN $k-\varepsilon$ models modify the computation of the turbulent viscosity by introducing a damping function $f_\mu$:

$$\mu_t = f_\mu c_\mu \rho \frac{k^2}{\varepsilon}. \quad (3.23)$$

In a shear layer, $\overline{uv}$ is calculated as

$$\overline{uv} = -\frac{\mu_t}{\rho} \frac{\partial U}{\partial y} = -f_\mu c_\mu \frac{k^2}{\varepsilon} \frac{\partial U}{\partial y}. \quad (3.24)$$

Therefore it follows that

$$f_\mu c_\mu = -\frac{\overline{uv} \varepsilon}{k^2} \frac{\partial U}{\partial y}. \quad (3.25)$$

This is plotted in Figure 3.2 for a channel flow with half-height $h$ at $Re_\tau = h u_\tau / \nu = 590$ using the DNS data of Moser et al. (1999). Although $f_\mu c_\mu$ is approximately constant for $y_+^\tau \gtrsim 100$, the need for a damping function at small $y_+^\tau$ is clear.

![Figure 3.2: $f_\mu c_\mu$ across a channel flow at $Re_\tau = 590$, computed from the DNS data of Moser et al. (1999).](image)

Often the $\varepsilon$ equation is modified in the near-wall region. This is reasonable because the $\varepsilon$ equation is only empirical in nature. As discussed in Section 2.8.8, a change of variables is often made to a variable that obeys more convenient boundary conditions at the wall, $\tilde{\varepsilon}$. The $\tilde{\varepsilon}$ equation often has the form

$$\rho D \tilde{\varepsilon} \frac{D}{Dt} = f_1 c_{21} \rho P \frac{\tilde{\varepsilon}^2}{k} - f_2 c_{22} \rho \frac{\tilde{\varepsilon}^2}{k} + \rho E + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_{\tilde{\varepsilon}}} \right) \nabla \tilde{\varepsilon} \right), \quad (3.26)$$
3.3. Low Reynolds number models

where $f_1$, $f_2$ are damping functions chosen to ensure that the model recreates observed experimental behaviour in certain flows. For example, Hanjalić and Launder (1976) chose the form of $f_2$ to reproduce the behaviour of decaying grid turbulence. The extra function $E$ is introduced to capture the peak in turbulent kinetic energy in the buffer layer more accurately (Jones and Launder, 1972).

A full review of LRN $k - \varepsilon$ models can be found in Rodi and Mansour (1993). Two of the most commonly used LRN $k - \varepsilon$ models are those of Launder and Sharma (1974) (LS) and Chien (1982) (CH). They are summarised in Table 3.1, where $y$ is the wall-normal direction and $Re_t = \nu k^2/\varepsilon$. The full equations of the Chien (1982) turbulence model can be found in Appendix A.3. Many other LRN $k - \varepsilon$ models exist such as those of Nagano and Tagawa (1990) or Yang and Shih (1993).

<table>
<thead>
<tr>
<th>$c_{\varepsilon 1}$</th>
<th>$c_{\varepsilon 2}$</th>
<th>$f_1$</th>
<th>$f_2$</th>
<th>$E$</th>
<th>$\sigma_\varepsilon$</th>
<th>$f_\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LS</td>
<td>1.44</td>
<td>1.92</td>
<td>1</td>
<td>$1 - 0.3e^{-Re_t^2}$</td>
<td>$2\nu \nu_t (\partial^2 U/\partial y^2)^2$</td>
<td>1.3</td>
</tr>
<tr>
<td>CH</td>
<td>1.35</td>
<td>1.8</td>
<td>1</td>
<td>$1 - 2\nu \nu_t^2/36$</td>
<td>$2\nu \nu_t^2 e^{-y/w^+}$</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Table 3.1: Constants and damping functions for the LRN $k - \varepsilon$ models of Launder and Sharma (1974) and Chien (1982).

Other correction terms exist which can be introduced into LRN $k - \varepsilon$ models. For example Yap (1987) introduced the so-called “Yap term” into the $\varepsilon$ equation to prevent the turbulent length scale from growing too large in near-wall regions. The number of additional terms can result in the model equations becoming long and laborious to deal with.

Damping functions are also introduced into the $k - \omega$ (Wilcox, 2006) and $k - \omega$ SST (Menter et al., 2003) to account for the damping effect of walls.

A drawback of creating LRN turbulence models with damping functions is that they may not apply in certain flow regions and can be numerically inconvenient. For example, the $E$ term in the LS $k - \varepsilon$ model contains the second derivative of the velocity, which is not straightforward to calculate in unstructured codes, and the use of $y^+_w$ in the CH model can cause problems at separation points where $\tau_w = 0$.

3.3.2 Four equation (elliptic relaxation) models

Elliptic relaxation models do not use damping functions. Instead, a separate equation is solved for $\overline{v^2}$, which imposes the behaviour $\overline{v^2} = \mathcal{O}(y^4)$ at the wall. The elliptic variable, which obeys its own transport equation, models the blocking effect of the wall (Durbin, 1991). The operator $\nabla^2 - 1/L^2$, which is similar to the operator that appears in the equation
Chapter 3. Near-wall models

for the elliptic variable, has the Green’s function

\[ G(\mathbf{x}, \mathbf{x}') = e^{-|\mathbf{x} - \mathbf{x}'|/L}. \]  

(3.27)

Thus, as mentioned in Section 2.8.9, the elliptic variable can be loosely thought of as including non-local effects within a sphere of radius \( L \).

There are also limiters placed on the turbulent time and length scales to prevent them becoming smaller than the Kolmogorov scales near to the wall (Durbin, 1991).

3.4 High Reynolds number models

A fine mesh is required in the viscous and buffer layers in order to capture the velocity gradients there. This increases the number of cells in a simulation dramatically and increases the time it takes to compute the solution. It can take many hundreds of times the amount of time to resolve the viscous sublayer of a flow than it does to resolve the outer region, especially in three-dimensional flows (Craft et al., 2006). However, as seen in Equation (3.10), the viscous sublayer is relatively straightforward to model. Therefore many methods that avoid the need for such fine grids near the walls have been developed.

These methods are often called “wall functions”. Wall functions typically use analytical or empirical correlations to link the properties of a flow at a point near to the wall with the properties at the wall. This means that the near-wall cell can be large, and therefore results can be obtained more quickly. However the accuracy of the solution now depends on both the turbulence model and the wall function. Turbulence models that use wall functions are called high-Reynolds number models because the turbulent Reynolds number in the first near-wall cell is large.

The wall function provides boundary conditions for the velocity, any scalars and all turbulence model functions. The details of the implementation depend on the numerical solver type. That means that the implementation of a wall function differs in finite difference, volume or element solvers, and in structured or unstructured codes. In this section, wall function implementations in finite volume codes for the velocity, passive scalars and turbulence model functions are discussed.

3.4.1 Velocity boundary conditions

There are two regions of the boundary layer in which the velocity boundary conditions are straightforward to calculate.
3.4. High Reynolds number models

The logarithmic region

In the logarithmic region of the boundary layer, the log law can be used to compute the velocity boundary conditions. To use this, the first near-wall cell centre must be at \( y^+ \gtrsim 30 \). The velocity itself is not imposed, nor is the no slip condition. Rather, Equation (3.17) is used to compute the wall shear stress and velocity gradient the cell centre, \( I' \). The wall shear stress can be computed iteratively using the definitions of \( U^+ \) and \( y^+ \). The velocity gradient at \( I' \) can be computed from differentiation of Equation (3.17). With this approach, the buffer layer and viscous sub layers do not need to be resolved.

A weakness of Equation (3.17) is its dependence on the wall shear stress, which means that the wall function fails if \( \tau_w = 0 \) because the logarithm is undefined. This issue is often addressed by using the velocity scale, \( u_k = c_1^{1/4} k^{1/2} \) (Launder and Spalding, 1974). This is justified by the experimental observation that \( k \) is roughly constant over the range \( 20 \lesssim y^+ \lesssim 60 \) and approximately equal to \( c_1^{1/2} k \approx \tau_w/ \rho \) (Ciofalo and Collins, 1989), such that in this range of \( y^+ \), \( u_r = u_k \). Hence in this region, \( k \) can be used to define \( y^+_k \), as in Equation (3.2). In this notation, the log law is written

\[
U^+ = \frac{1}{\kappa} \log(y^+_k) + C, \tag{3.28}
\]

or

\[
U^+ = \frac{1}{\kappa} \log(Ey^+_k), \tag{3.29}
\]

for the same constants \( C \) and \( E \) as in Equations (3.17) and (3.18).

Wall functions can use both \( u_r \) and \( u_k \). These are categorised as “two velocity scale wall functions”. With two velocity scale wall functions, the wall shear stress is calculated from (Launder and Spalding, 1974; Chieng and Launder, 1980; Johnson and Launder, 1982)

\[
\frac{u_k}{u_r}U^+ = \frac{1}{\kappa} \log \left( Ey^+_k \right). \tag{3.30}
\]

If quantities evaluated at the first near-wall node are denoted with a subscript \( I' \) then the wall shear stress is

\[
\tau_w = \frac{\kappa c_{1}\mu_{r}^{1/4}}{\log \left( E c_{1}^{1/4} k^{1/2} y_{I'}/\nu \right) } . \tag{3.31}
\]

The viscous sub layer

When the cell centre lies in the viscous sub layer, which is often taken as \( y^+_r < 11.6 \) (Gant, 2002), then the wall shear stress can be calculated using Equation (3.10),

\[
\tau_w = \mu \frac{U_{I'}}{y_{I'}} . \tag{3.32}
\]
Chapter 3. Near-wall models

This is a first-order approximation of the derivative of $U$ at the wall. If the near-wall cell centre lies in the viscous sub layer then the turbulence model should include damping functions or another mechanism to account for the buffer layer. Therefore it is usually advised that the near-wall cell centres lie in the logarithmic region when using HRN turbulence models. On the other hand, LRN models can use Equation (3.32) if $y_+^+$ is small enough.

The wall-normal velocity

The wall-normal velocity is specified with the impermeability condition at the wall, $V = 0$, as well as the condition from the continuity equation, $\partial_y V = 0$. This means that while $U$ can be calculated accurately with a wall function approach, $V$ can not. However this approach is accurate enough because in the boundary layer $V$ is small compared to $U$.

3.4.2 Scalar boundary conditions

The transport equation for a scalar (Equation (2.78)) has exactly the same form as the transport equation for the mean velocity (Equation (2.31)). Therefore, as with the velocity, if there are no source terms, and convection and stream-wise diffusion are ignored in the near-wall boundary layer, the transport equation reduces to

$$\frac{\partial}{\partial y} \left( \mu \frac{\partial \Phi}{\partial y} - \rho v \Phi \right) = 0. \quad (3.33)$$

This can be integrated and, if $\Phi$ is the enthalpy, the wall heat flux $q''_w$ can be used as a boundary condition to find

$$\frac{\mu}{\sigma_\Phi} \frac{\partial \Phi}{\partial y} - \rho v \Phi = q''_w. \quad (3.34)$$

The SGDH (Equation (2.80)) can be used to model the turbulent flux

$$\rho v \Phi = -\frac{\mu_t}{\sigma_{t, \Phi}} \frac{\partial \Phi}{\partial y}. \quad (3.35)$$

so that Equation (3.34) now becomes

$$\left( \frac{\mu}{\sigma_\Phi} + \frac{\mu_t}{\sigma_{t, \Phi}} \right) \frac{\partial \Phi}{\partial y} = q''_w. \quad (3.36)$$

Note that under the assumptions that led to Equation (3.34), the GGDH would give the same result as the SGDH. In the logarithmic region, a mixing length is used to compute the turbulent viscosity as

$$\mu_t = \rho \kappa^2 y^2 \left| \frac{\partial U}{\partial y} \right|, \quad (3.37)$$
where the velocity gradient is computed using the log law so that

\[ \mu_t = \rho \kappa^2 y^2 \frac{u''}{\tau} = \rho \kappa y u', \] (3.38)

In the logarithmic region of the boundary layer, molecular diffusion can be ignored. Therefore Equation (3.36) becomes

\[ \frac{\rho \kappa y u'}{\sigma_{t, \Phi}} \frac{\partial \Phi}{\partial y} = \dot{q}_w, \] (3.39)

which has the solution

\[ \Phi(y) = \Phi_w + \frac{\dot{q}_w}{\rho u_r} \frac{\sigma_{t, \Phi}}{\kappa} \log(y), \] (3.40)

where \( \Phi_w \) is the value of the scalar at the wall. By introducing

\[ \Phi^+ = \frac{\rho u_r (\Phi - \Phi_w)}{\dot{q}_w}, \] (3.41)

the scalar log law is obtained

\[ \Phi^+ = \frac{\sigma_{t, \Phi}}{\kappa} \log \left( \frac{y^+}{\tau} \right) + C_\Phi, \] (3.42)

where \( C_\Phi \) is a constant that depends on the Prandtl number and must be tuned to experimental data. Many such tunings exist. The most well-known and widely used is that of Jayatilleke (1969), who developed the so-called “P-function” which states that

\[ C_\Phi = C + P \left( \frac{\sigma_\Phi}{\sigma_{t, \Phi}} \right), \] (3.43)

where \( C \) is the constant from the velocity log law in Equation (3.17), and

\[ P \left( \frac{\sigma_\Phi}{\sigma_{t, \Phi}} \right) = 9.24 \left( \left( \frac{\sigma_\Phi}{\sigma_{t, \Phi}} \right)^{3/4} - 1 \right) \left( 1 + 0.28 \exp \left( -0.007 \frac{\sigma_\Phi}{\sigma_{t, \Phi}} \right) \right). \] (3.44)

This allows Equation (3.42) to be written as

\[ \Phi^+ = \sigma_t \left( U^+ + P \left( \frac{\sigma_\Phi}{\sigma_{t, \Phi}} \right) \right). \] (3.45)

As with the velocity wall function, \( y_k^+ \) is sometimes used instead of \( y_\tau^+ \).

Equation (3.42) is used to compute boundary conditions for \( \Phi \) in the same way that Equation (3.17) is used to compute boundary conditions for \( U \). These boundary conditions are only accurate in the logarithmic region of the boundary layer.

### 3.4.3 Boundary conditions for turbulence model functions

Wall functions must also produce boundary conditions for any turbulence model functions. A brief outline of some methods that are used to do this in \( k - \varepsilon \) models is now given.
Treatments for more advanced turbulence models are given in Section 3.5.

The earliest wall functions used the log law to compute cell-average values of $P$ and $\varepsilon$ (written $\overline{P}$ and $\overline{\varepsilon}$), which are fed directly into the numerical solver such that the near-wall cell centre value is calculated analytically. Implementations differ in how they calculate these values. It is usual to assume that the dominant Reynolds stress is $\overline{uv}$ and to ignore all other Reynolds stresses.

Many implementations assume that there is an equilibrium layer in the logarithmic region where $P = \varepsilon$ and $k$ is constant. This allows a useful result to be obtained:

$$
\varepsilon = P = \frac{\mu_t}{\rho} \left( \frac{\partial U}{\partial y} \right)^2 = c_p \frac{\kappa^2}{\varepsilon} \frac{u_k^2}{\kappa^2 y^2}
$$

where Equation (3.28) has been used to evaluate the velocity derivative. This gives

$$
\varepsilon = \frac{c_l^{3/4} k^{3/2}}{\kappa y} = \frac{k^{3/2}}{c_l y},
$$

where $c_l = \kappa c_p^{-3/4} = 2.55$. This expression, or variants using the same derivation, are often used in wall function implementations. Some widely-used implementations are summarised below for codes that use structured, hexahedral solvers. The subscript $I'$ denotes quantities evaluated at the near-wall cell centre and the subscript $N$ refers to quantities evaluated at the hexahedral face farthest from the wall, as shown in Figure 3.3.

![Diagram](image)

Figure 3.3: The notation used to describe the implementation of many wall functions.
3.4. High Reynolds number models

Launer and Spalding (1974) calculated $\bar{P}$ as

$$\bar{P} = -\frac{1}{y_N} \int_0^{y_N} \rho \frac{\partial U}{\partial y} dy = \tau_w \frac{U_I^'}{y_I^'},$$  \hspace{1cm} (3.48)

where the gradient has been estimated with a finite difference approximation and $\tau_w = \rho \overline{uv}$. The wall shear stress in the logarithmic layer is calculated as

$$\tau_w = \frac{\mu_t}{\rho} \frac{\partial U}{\partial y} = \frac{\rho \varepsilon k^2 U_I^'}{y_I^' \tau_w},$$  \hspace{1cm} (3.49)

which means that the cell average dissipation must be calculated as

$$\varepsilon = \frac{\rho \varepsilon k^2 U_I^'}{y_I^' \tau_w}.$$  \hspace{1cm} (3.50)

The implementation of Chieng and Launder (1980)

Chieng and Launder (1980) used a two velocity scale wall function and split the boundary layer into a viscous sublayer and a logarithmic layer. Instead of using $k$ at $I'$, the value at the edge of the viscous sublayer, $k_v$, is used. It is assumed that the viscous sublayer extends up to a distance $y_v = 20 \nu/k^{1/2}$, and $k_v$ is calculated by a linear extrapolation of $k$ from its values at the first and second nearest cells to the wall. This makes the wall-function less sensitive to the near-wall cell size. The wall shear stress is calculated with Equation (3.31) with $k_v$ instead of $k_I^'$. To calculate the production, the turbulent shear stress $\overline{uv}$ is assumed to vary linearly from $\tau_w$ at $y_v$ to $\tau_N$ at $y_N$. The velocity gradient is found by differentiating Equation (3.30). In the viscous sublayer $\overline{uv} = 0$ and so $P = 0$ there and integration is performed only over the region $[y_v, y_N]$. Hence the cell average production is

$$\bar{P} = \frac{1}{y_N} \int_{y_v}^{y_N} \frac{\tau_w \overline{uv} \partial U}{\partial y} dy,$$  \hspace{1cm} (3.51)

$$= \frac{1}{y_N} \int_{y_v}^{y_N} \left( \tau_w - \frac{\tau_N - \tau_w}{y_N} y \right) \frac{u_v^2}{\kappa u_k} dy,$$  \hspace{1cm} (3.52)

$$= \frac{1}{y_N} \left( \tau_w u_v^2 \ln \left( \frac{y_N}{y_v} \right) - \frac{\tau_N - \tau_w}{y_N} u_v^2 \left( y_N - y_v \right) \right).$$  \hspace{1cm} (3.53)

The cell average dissipation is calculated by assuming that the turbulence is in equilibrium in the interval $[y_v, y_N]$ so that equation (3.47) holds. In the viscous sublayer, $\varepsilon$ is computed as

$$\varepsilon_w = \frac{2 \nu k_v}{y_v^2}.$$  \hspace{1cm} (3.54)

This choice means that $\varepsilon$ may no longer be continuous. The linear variation of $k$ is used.
across the region \([y_v, y_N]\) and it is assumed that \(k\) varies quadratically in the interval \([0, y_v]\). This is consistent with its wall-limiting behaviour. Hence \(\varepsilon\) is obtained as

\[
\varepsilon = \frac{1}{y_N} \int_0^{y_N} \varepsilon(y) \, dy,
\]

(3.55)

\[
= \frac{1}{y_N} \left( \int_0^{y_v} \frac{2\nu k_v}{y_N^3} dy + \int_{y_v}^{y_N} \frac{1}{c_l y} \left( k_N - \frac{k_N - k_I'}{y_N - y'} (y_N - y) \right)^{3/2} dy \right). \tag{3.56}
\]

This integral must be evaluated numerically. To avoid this complexity, a simplified form is sometimes used (Gant, 2002; Ciofalo and Collins, 1989; Craft et al., 2002), where the linear variation of \(k\) and \(\bar{u}'\) across \([y_v, y_N]\) is abandoned, with the constant cell-centre value being used instead. Under these assumptions

\[
\hat{\varepsilon} = \frac{1}{y_N} \left( \frac{2\nu k_I}{y_v} + \frac{k_I'^{3/2}}{c_l} \log \left( \frac{y_N}{y_v} \right) \right), \tag{3.57}
\]

and

\[
\varepsilon = \frac{1}{y_N} \left( \frac{2\nu k_I}{y_v} + \frac{k_I'^{3/2}}{c_l} \log \left( \frac{y_N}{y_v} \right) \right). \tag{3.58}
\]

Various modifications of the implementation of Chieng and Launder (1980) were investigated by Gant (2002). These were mostly found to increase the sensitivity of the model to the near-wall cell size.

The value of \(\varepsilon_w\) was introduced to match the theoretical behaviour of \(\varepsilon\) at the wall (Jones and Launder, 1972). It also matched the experimental data available at the time these models were conceived. This data suggested that there is a peak in \(\varepsilon\) near to the wall. However, modern DNS data shows that the maximum value of \(\varepsilon\) is actually reached at the wall. Therefore, some wall functions assume that the dissipation varies as

\[
\varepsilon = \frac{k_I'^{3/2}}{c_l y_v}. \tag{3.59}
\]

across the viscous sub layer (Craft et al., 2002). This avoids the unphysical, discontinuous specification of \(\varepsilon\), however with this approach the wall-limiting behaviour of \(\varepsilon\) is incorrect. The analytical wall function (Gerasimov, 2003), described later, solves this problem by introducing a new length \(y_d\).

Johnson and Launder (1982) allowed the position of the edge of the viscous sub layer to depend on a parameter \(\lambda = (k_v - k_w)/y_v\) as

\[
y_v = \frac{20\nu}{k_v^{1/2} (1 + 3.1\lambda)} \tag{3.60}
\]

The intention was to improve the behaviour in flows where the shear stress gradient is high near to the wall. Johnson and Launder (1982) also modified the constant in the log law to
3.4. High Reynolds number models

give a continuous form of $U^+$ between the viscous sublayer and the logarithmic region.

Amano (1984) developed two new wall function methods for the $k-\varepsilon$ model: a two-layer and a three-layer model. The two layer model split the domain into a viscous sublayer ($y^+_v < 11$) and an overlap layer ($11 \leq y^+_v < 400$). The three-layer model split the domain into the viscous sublayer ($y^+_v < 5$), the buffer layer ($5 \leq y^+_v < 30$) and an overlap layer ($30 \leq y^+_v < 400$). The log law was retained for the velocity. The dissipation is calculated by considering how the terms in the $\varepsilon$ equation vary over the near-wall region. The effect was to specify piecewise continuous profiles of $k$, $\varepsilon$ and $\tau_w$ over the near-wall layer.

Ciofalo and Collins (1989) built on the work of Johnson and Launder (1982) and used experimental data to model the variation of $y_v$ with $k$. They allowed $y_v$ to depend on the turbulence intensity in the near-wall cell, $\Psi_I = k^{1/2}/U'$ and the turbulence intensity in an equilibrium boundary layer, $\Psi_E = c^{-1/2}y_{k,v}^{-1/2}$, as

$$y^+_k = y^+_{k,v0} \left( \frac{\Psi_I}{\Psi_E} \right)^{-c},$$

with $c \approx 2/3$ and where $y^+_{k,v0}$ is the value of $y^+_k$ for $\Psi_I = \Psi_E$. Their results predicted levels of heat transfer more accurately than the standard wall function, however they reported difficulties in regions upstream of reattachment points.

3.4.4 Improvements to wall functions based on the log law

Many attempts have been made to improve the predictive behaviour of wall functions based on the log law. Two major drawbacks of the log law are that it is only applicable for $y^+_r \gtrsim 30$ and that it always ignores the streamwise pressure gradient.

Spalding (1961) attempted to develop a method that would be applicable across the viscous, buffer and logarithmic layers. Solving Equation (3.7) for $y^+_r$ in terms of $U^+$ produces an expression which asymptotes to the usual log law at large values of $y^+_r$ and to Equation (3.10) at small values. The expression is

$$y^+_r = U^+ + 0.1108 \left( e^{0.4U^+} - 1 - 0.4U^+ - \frac{0.4U^{+2}}{2!} - \frac{0.4U^{+3}}{3!} - \frac{0.4U^{+4}}{4!} \right),$$

which is plotted against the DNS data of Moser et al. (1999) for a channel flow at $Re_\tau = 590$ in Figure 3.4.

Despite the appealing accuracy of this model in Figure 3.4, it never made it into widespread use. The model is still based on a local equilibrium boundary layer and ignores any source terms in the momentum equations. Numerous efforts have been made to modify the standard wall function to take non-equilibrium effects into account. For example, the effects of
pressure gradients and porous walls were considered by Spalding (1967) and Patankar and Spalding (1967). The effects of convection and diffusion of turbulence towards the wall were investigated by Wolfshtein (1969). These wall functions also failed to make it into widespread use. They were not sufficiently accurate for academic studies and often failed to improve the predictions in industrial applications compared to simpler wall functions (Craft et al., 2002).

Kim and Choudhury (1995) introduced a term to model the effects of the pressure gradient and convection terms into the log law. They approximated the sum of these two terms as

$$\frac{\partial P}{\partial x} + \rho U \cdot \nabla U \approx \frac{1}{2} \frac{\partial P}{\partial x}. \tag{3.63}$$

This is justified by consideration of numerical results from backwards-facing step and impinging jet flows (Popovac, 2006). The model was applied to recirculating flows and flows with separation and reattachment. The results were more accurate than standard wall functions, and demonstrated the benefits of including the effects of the pressure gradient.

Shih et al. (2003) introduced a velocity scale, $u_p^3 = \mu |\nabla P|/\rho^2$, which is used to define a hybrid velocity scale, $u_c = u_\tau + u_p$, which in turn is used to define a non-dimensional length $y^*_c = y u_c \rho / \mu$. The model assumes that three distinct regions exist, which are, in order of increasing wall distance, the viscous, buffer and inertial layers. Quartic curves that link the
viscous and inertial layers are used to determine the velocity in the buffer region. The result is that the velocity is related to $\tau_w$ via two functions, $\alpha_1$ and $\alpha_2$ as

$$\frac{U}{u_c} = \frac{\tau_w}{\rho u_c^2} \alpha_1 \left( y_+^+ \right) + \frac{\mu}{\rho^2} \frac{|\nabla P|}{u_c^3} \alpha_2 \left( y_+^+ \right). \quad (3.64)$$

The objective was to develop a wall function that is accurate in flows with adverse pressure gradients. The results obtained on a backwards-facing step flow were more accurate than the results with the standard wall function and competitive with a LRN model.

Despite the vast effort that has gone into improving wall functions based on the log law, most improvements have not made it into industrial use. However, one of the simplest methods is widely used. It is described in the next section.

### 3.4.5 The scalable wall function

The scalable wall function (SWF) of Grotjans and Menter (1998) was introduced in an effort to make log law-based wall functions valid at lower values of $y^+$. Methods which address this issue are sometimes called “adaptive” or “low $y^+$” wall functions. The method uses $u_k$ to calculate $y_{k,I}^+$ as

$$y_{k,I}^+ = \max \left( \frac{u_k y_{I}^+}{\nu}, y_{\text{min}}^+ \right), \quad (3.65)$$

where $y_{\text{min}}^+$ is a lower limit on the allowed value of $y_{k,I}^+$, taken as $y_{\text{min}}^+ = 11.06$. The friction velocity is calculated as

$$u_\tau = \frac{U_{I}^+}{\frac{1}{\kappa} \log(y_{k,I}^+)} + C, \quad (3.66)$$

and the wall function is implemented in the same way as the standard wall function. The SWF differs from the log law when the near-wall cell lies in the viscous sub layer. In these cases, boundary conditions are applied as if the cell were at the edge of the viscous sublayer, where the log law is used.

In cases when $k_{I}^+$ is very small, a limiter can also be placed on $u_k$ (ANSYS Inc., 2009)

$$u_k = \max \left( \frac{U_{I}^{+1/4}}{\kappa} k_{I}^{1/2}, 0.01 U_{I}^+/y_{k,I}^+ \right), \quad (3.67)$$

which prevents the shear stress, $\tau_w = \rho u_k u_\tau$, from vanishing in flows with low turbulence intensity.

The scalable wall function is a useful improvement over the log law due to its increased applicability and robustness. However it is limited by the same assumptions that went into the original formulation of the log law and does not include the effects of the pressure gradient in the boundary layer.
3.5 Wall functions without the log law

Ultimately the log law is a poor approximation in many flows because of the number of assumptions used to derive it. Most flows are not in local equilibrium and it is not always accurate enough to ignore the pressure gradient or other source terms. In many flows there simply is no logarithmic region in the boundary layer. From a practical perspective one of the biggest drawbacks of the log law is the dependence on the location of the first near-wall cell centre. When modelling complex geometries it is often challenging to generate a mesh where every near-wall cell centre has $y^+ \gtrsim 30$ without introducing distorted cells. Therefore it may be impossible to reach a mesh-independent solution. Thus in many flows, using the log law reduces the accuracy of the solution; either by invalidating the log law assumptions or distorting the mesh.

Many modern wall functions do not use the log law. In this section, a selection of such wall functions are reviewed.

3.5.1 The look-up table approach of Kalitzin et al. (2005)

Kalitzin et al. (2005) developed a robust wall function that can be applied to any RANS model. Convection, diffusion in the wall-normal direction and any source terms, including the pressure gradient, are ignored. The momentum equation is put into dimensionless form and after one integration becomes

$$
(1 + \nu^+_t) \frac{dU^+}{dy^+} = 1,
$$

where $\nu^+_t \equiv \nu_t/\nu$. The solutions to dimensionless equations of this form are assumed to be Reynolds number and flow independent, and therefore universal. Rather than attempt to integrate Equation (3.68) analytically, Kalitzin et al. (2005) solved it numerically for the flow over a flat plate with no pressure gradient. This avoids having to specify a profile of $\nu^+_t$. The result is a function, $U^+(y^+_t)$, which is assumed to be valid in any flow. The inverse of this function, $y^+_t(U^+)$, is tabulated and used to calculate the wall shear stress without an iterative process.

The approach can be followed with any turbulence model. Among others, Kalitzin et al. (2005) considered the Spalart-Allmaras, $k - \omega$ and $\overline{v^2} - f$ models. The turbulence model functions were also calculated for the flat plate flow and stored as look-up tables. These look-up tables are used to specify off-wall boundary conditions for the turbulence model functions. The near-wall cell centre value of each function is forced to be equal to its look-up table value by introducing additional source terms in the turbulence model governing
equations in the near-wall cell.

This wall function was found to be efficient and accurate. It performs well on flow over a flat plate and on flows with pressure gradient-driven separation — even though the wall function ignores the pressure gradient. The method can be extended to include transported scalars.

The method depends on the concept of “wall layer universality”, which states that the profiles of non-dimensional quantities such as $U^+$ are the same in all quasi-equilibrium boundary layers. This assumption does not hold in non-equilibrium flows. Therefore the accuracy of this method in engineering flows is difficult to ascertain.

The method has been adapted for use in the BL-$v^2/k$ model by Billard et al. (2015), where a two velocity scale model is used to improve the performance of the method in flows with heat transfer. Billard et al. (2015) also showed how the look up table can be applied over a range of cells, in order to improve the numerical performance of the wall function when there are large jumps in the size of adjacent cells in the mesh, which can occur in meshes of complex geometries.

### 3.5.2 The numerical wall function of Gant (2002)

With the numerical wall function (NWF) (Gant, 2002; Craft et al., 2004, 2001), the computational domain is split into two regions with separate, independent meshes. There is a coarse “primary mesh” in the covering the whole domain, on which the RANS equations are solved, and a fine “wall function mesh” is placed over each near-wall cell of the primary grid as shown in Figure 3.5. A parabolic, one-dimensional form of the RANS momentum equations is solved on the wall function mesh to evaluate the quantities needed in the near-wall cell of the primary mesh. These include the wall shear stress and cell-average quantities such as $P$. The two meshes are linked through their boundary conditions. For all other purposes they are treated independently. Each mesh must be considered separately when performing a mesh-independence test.

The parabolic equation solved in the wall function mesh, written for a general function $\Phi$, is

$$\rho U \cdot \nabla \Phi = \frac{\partial}{\partial y} \left( \frac{\mu}{\sigma_\Phi} + \frac{\mu_t}{\sigma_{t,\Phi}} \right) \frac{\partial \Phi}{\partial y} + S_\Phi,$$

where $S_\Phi$ represents any source terms. For example with $\Phi = U$, $S_\Phi = -\partial_x P$. In contrast to log law-based wall functions, the NWF includes the convection terms. All Reynolds stresses are included in the calculation of the production term. This is a significant improvement as many wall functions include only the contribution from $\overline{uu}$.

A LRN form of the $k - \varepsilon$ model is used in the wall function mesh in order to capture the
Chapter 3. Near-wall models

Figure 3.5: Schematic of the mesh for the numerical wall function (Gant, 2002; Craft et al., 2004, 2001).

near-wall effects. An LRN model is also used on the primary mesh to maintain consistency when the near-wall cell of the primary mesh is small. In principle, the turbulence model used in the primary mesh need not be the same as the one applied to the wall function mesh.

The wall-parallel pressure gradient is assumed to be constant over the wall function mesh, which eliminates the need for a pressure-correction algorithm on the wall function mesh. The wall-normal pressure is calculated from (Gant, 2002)

$$\frac{\partial P}{\partial y} + \frac{\partial (\rho u_j u_j)}{\partial x_j} = 0.$$  \hfill (3.70)

The wall normal velocity is found by using the continuity equation across each near-wall cell of the primary mesh and scaling the solution to ensure that the wall function and primary mesh solutions match at the face marked $N$ in Figure 3.5.

Only one iteration of a tri-diagonal matrix algorithm is performed on the wall function mesh equation for each primary mesh time step. This reduces the total computation time. The solutions on both meshes converge concurrently.

The method has been applied with a regular, Cartesian mesh to the cases of a 2-D channel flow, impinging jet, a spinning disc flow (Craft et al., 2001, 2004) and to three-dimensional body-fitted meshes (Gant, 2002). The computational times were around double the time required for a standard wall function but an order of magnitude less than the equivalent LRN simulation. The computation time required for each iteration on the primary mesh is also comparable to that of a LRN method because of the extra computations required in the wall function grid. However the total number of iterations required for convergence is smaller than it is for a LRN method. This is because the two separate matrix systems are smaller. However, the efficiency of the method in URANS calculations is unknown.
The wall function produces results that are more faithful to the LRN model than log law-based wall functions. The method is noteworthy because it is one of only a few wall functions that attempt to specify a more accurate profile of the wall-normal velocity. Many wall functions ignore $V$ on the basis that it is negligible in the viscous sublayer and small throughout the rest of the near-wall cell. Moreover its derivative at the wall is zero, so it does not contribute to the wall shear stress. However it is still important to have an accurate value of $V_I$, so that the CFD solver can calculate the correct convection terms for $U$.

Drawbacks of the method include the large storage requirements of the extra wall-function grid. Since all fluid quantities are stored in this extra grid the storage requirements are similar to those of a LRN simulation. The NWF cannot be easily modified for use on unstructured grids, which makes is unsuitable for many engineering applications. It also suffers from stability issues. Therefore the method has not been widely adopted in industry, despite the accuracy of the results obtained with it.

### 3.5.3 The analytical wall function of Gerasimov (2003)

The analytical wall function (AWF) (Gerasimov, 2003; Craft et al., 2002; Amano et al., 2014) is a wall function that can handle source terms and variable fluid properties (such as variable fluid density). The method is based on analytical integration of boundary layer equations in the near-wall cell, made possible by assumptions of the variation of fluid properties. The near-wall layer is separated into a viscous sublayer ($y \leq y_v$) and a turbulent region ($y > y_v$). Integration is then performed over these two regions.

Diffusion parallel to the wall and convection normal to the wall are ignored so that the $U$ momentum equation becomes

$$
\frac{\partial}{\partial y^*} \left( (\mu + \mu_t) \frac{\partial U}{\partial y^*} \right) = \frac{\mu_v^2}{\rho v^2 k_I'} \left( \rho U \frac{\partial U}{\partial x} + \frac{\partial P}{\partial x} \right),
$$

where $y^* \equiv \rho_v y k_{I'}^{1/2} / \mu$, $v$ marks the edge of the viscous sub layer and $I'$ is the cell centre as in Figure 3.3. Note that $y^*$ differs from $y_k^+$ by a factor of $c_{\mu}^{1/4}$. To facilitate integration, the convection terms are treated as constants across the two regions of the cell and are calculated in each region as

$$
C_i = \frac{\mu^2}{\rho v^2 k_{I'}} \left( \rho U_{I'} A_i \frac{U_E - U_W}{\Omega_i} \right),
$$

where $i = 1$ refers to the viscous sublayer and $i = 2$ refers to the turbulent region. The volume of each part of the cell is $\Omega_i$ and the cross-sectional area of the faces $E$ and $W$ (as shown in Figure 3.3) is $A_i$. The mesh is assumed to be structured and hexahedral. The
turbulent viscosity is calculated as
\[ \mu_t = \mu_v \alpha (y^* - y_v^*) = \mu_v c_{\mu} c_l (y^* - y_v^*), \] (3.73)

where \( y_v^* \) is a free parameter in the method, taken to be \( y_v^* = 10.8 \) after consideration of pipe flows (Craft et al., 2002). The value of \( y_v^* \) is approximately half that used by Chieng and Launder (1980).

With these approximations, Equation (3.71) can be integrated analytically. The result is a cumbersome expression for \( U \), which depends on the relative sizes of the viscous sublayer and the near-wall cell. The wall shear stress is given by the expression
\[ \tau_w = -\frac{\rho k^{1/2}}{\mu} A_1, \] (3.74)

where \( A_1 \) is given by a long analytical expression (Gerasimov, 2003). A scalar wall function is also derived with an analogous method.

The model was developed for a HRN \( k - \varepsilon \) model. The dissipation is computed with the analytical expression
\[ \varepsilon = \frac{k^{3/2}}{c_l \max (y, y_d)} \] (3.75)

where \( y_d = 2 \nu c_l / k^{1/2} \). Choosing \( y_d < y_v \) allows for a continuous variation of \( \varepsilon \) with the correct wall-limiting behaviour, unlike the profile of Chieng and Launder (1980). The \( \varepsilon \) equation is not solved over the near wall cell. Instead, Equation (3.75) is used to compute the cell-average value, \( \overline{\varepsilon} \). The cell-average production is calculated as
\[ \mathcal{P} = \frac{1}{y_N} \frac{\rho k^{1/2}}{\mu_v} \int_{y_v^*}^{y_N} \mu_v \alpha (y^* - y_v^*) \left( \frac{\partial U}{\partial y^*} \right)^2 dy^*, \] (3.76)

and is used along with \( \overline{\varepsilon} \) in the finite volume method in the near-wall cell.

The computation of the wall-parallel convective fluxes in the finite volume method is modified in the near wall cells. For each face with surface area \( A \), the analytical velocity profile, \( U_a \), is integrated up to the top of the face, \( y_N \), to approximate the convective flux as
\[ C = \int_{\text{face}} \rho U dA = \frac{\rho}{U} \int_{0}^{y_N} U_a^2 dy. \] (3.77)

This leads to a more accurate approximation of the convective flux than is usually the case with wall functions, which often assume the velocity to be constant across the face.

The AWF has been applied to the cases of a flow down a pipe, a mixed convection flow, and an impinging jet flow. The results show a much better agreement with LRN models than log law-based wall functions and are less sensitive to the near-wall cell size.
Although the results were encouraging, the model did not gain widespread use because it is complex to apply to unstructured meshes and can be unstable. Many of the features of the model are ad hoc, such as the treatment of the convection terms and the specification of the turbulent viscosity. The scheme must be modified for the case where all, or nearly all, of the first near-wall cell lies in the viscous sublayer (Gerasimov, 2001). In addition, the model does not generalise easily to other turbulence models, although the turbulent viscosity profile has been adopted for use in a RSM for flows over rough walls by Apsley (2007), as discussed in Section 3.6.1.

3.5.4 The generalised wall function of Popovac (2006)

Popovac (2006) and Popovac and Hanjalić (2005, 2007) applied similar approximations to those used in the AWF to develop the “generalised wall function”, which was applied to a $\overline{v^2} - f$ model. Near to the wall, the wall-normal velocity component is ignored and the wall-parallel velocity is determined using the momentum equation in the form

$$\rho \frac{\partial U}{\partial t} + \rho U \frac{\partial U}{\partial x} + \rho V \frac{\partial U}{\partial y} = \frac{\partial}{\partial y} \left( (\mu + \mu_t) \frac{\partial U}{\partial y} \right) - \frac{\partial P}{\partial x}. \tag{3.78}$$

The total derivative and pressure gradient terms are combined into a single parameter

$$C_U = \rho \frac{\partial U}{\partial t} + \rho U \frac{\partial U}{\partial x} + \rho V \frac{\partial U}{\partial y} + \frac{\partial P}{\partial x}, \tag{3.79}$$

which is assumed constant over the near-wall cell and is calculated from the solution at the previous iteration. The total viscosity over the near-wall cell is computed as

$$\mu + \mu_t = \begin{cases} \mu, & \text{if } y < y_v, \\ \rho \kappa u_\tau y, & \text{if } y \geq y_v, \end{cases} \tag{3.80}$$

where $y_v^+ = 11$. These two assumptions allow Equation (3.78) to be integrated analytically. The result is an expression for $U$ of the form

$$U^+ = \frac{1}{\kappa U} \ln \left( E y^+ \right), \tag{3.81}$$

where $E$ and $\kappa$ are the usual log law parameters. This is the same as the log law (Equation (3.17)) with an additional factor of

$$\psi_U = 1 - \frac{C_U y}{\rho \kappa u_\tau}, \tag{3.82}$$

which accounts for deviations from equilibrium.

A similar approach is followed for transported scalars, where a factor $\psi_\Phi$ is introduced so
that the scalar wall function becomes
\[ \Phi^+ = \sigma_t \left( \frac{\psi_U}{\psi} U^+ + P \left( \frac{\sigma_\Phi}{\sigma_t \Phi} \right) \right), \] (3.83)
which is analogous to Equation (3.45) with a correction factor.

An advantage of this approach is the similarity of Equation (3.81) to the log law in Equation (3.17). This makes it an appealing upgrade to the log law because it can be implemented using the same procedures. When applied to flow over a backwards-facing step, impinging jet and flat plate boundary layer, the generalised wall function produced a modest improvement over the log law-based wall function. This method is noteworthy due to its inclusion of the time derivative term, although it is only included through the ungainly \( C_U \) term, which is treated as a constant at each time step.

A drawback of this method is that the specification of \( \mu + \mu_t \) in Equation (3.80) is not continuous, which is not physically realistic. The profile was chosen to give a convenient form of the wall function. The AWF assumes a continuous viscosity profile, which leads to long expressions for \( U \) and necessitates the smaller value of \( y_v \).

### 3.5.5 The compound wall function of Popovac (2006)

The compound wall function (Popovac, 2006; Popovac and Hanjalić, 2005, 2007) was developed to be applicable over the viscous sublayer, the buffer layer and the logarithmic layer. It is an extension of the work of Kader (1981) on thermal boundary layers and was developed with a \( v^2 - f \) model, however it could be implemented for a \( k - \varepsilon \) model. Each function, \( \Phi \), is computed as a bending of a solution in the viscous sub layer, \( \Phi^\nu \), and a solution in the logarithmic layer, \( \Phi^t \). The blending function is \( \Gamma = 0.01y^+_k(1+5y^+_k) \) and \( \Phi(y) \) is determined as
\[ \Phi(y) = \Phi^\nu(y)e^{-\Gamma} + \Phi^t(y)e^{-1/\Gamma}. \] (3.84)

Expressions of this form are sought for every variable, for example, the scalar wall function is written
\[ \Phi^+ = \sigma_\Phi y_k^+ e^{-\Gamma} + \left( \frac{\sigma_\Phi}{\kappa} \ln \left( Ey_k^+ \right) + P(\sigma_\Phi) \right) e^{-1/\Gamma}, \] (3.85)
where
\[ P(\sigma) = (3.85\sigma^{1/3} - 1.3)^2 + 2.12 \log(\sigma). \] (3.86)

The wall function uses the transported variable \( \varphi = \sqrt{\nu^2}/k \) to calculate the production as
\[ P = c_\mu \varphi^2 \left( \frac{\partial U}{\partial y} \right)^2 e^{-\Gamma} + \frac{c_{3/4} \varphi^{3/2} k^{3/2}}{\psi \kappa y} e^{-1/\Gamma}, \] (3.87)
and the dissipation is calculated as

$$\varepsilon = \frac{2\mu k}{\rho y^2} e^{-\Gamma_{\varepsilon} + c_{\mu}^{3/4} k^{3/2}} \frac{e^{-1/\Gamma_{\varepsilon}}}{\kappa y}$$

with a modified blending function

$$\Gamma_{\varepsilon} = \frac{0.001 y^4_k}{1 + y_k}.$$  

(3.89)

The wall shear stress is calculated as

$$\tau_w = \mu \frac{U''}{y'} = \frac{\rho c_{\mu}^{1/4} k_{\mu}^{1/2} U' \psi_U}{y_{+}^{1/4} e^{-\Gamma} + e^{-1/\Gamma}} \ln \left( E y_{+}^{1/4} \right),$$

(3.90)

where $\psi_U$ is defined in Equation (3.82).

The compound wall function has been applied to the cases of a channel flow, a pulsating channel flow, an impinging jet flow and the flow over backwards-facing step, with accurate results in each case. It has been applied to the flow of coolant in an internal combustion engine (Tatschl et al., 2006), where it picked up many of the flow features present in experimental and LES results. It has also been applied to the flow past a car (Basara et al., 2007) and produced a reasonable approximation of the experimental data.

The compound wall function is an improvement over other wall functions because it includes non-equilibrium effects through the parameter $\psi_U$. However its development is ad hoc. Only the production term and scalars use the same blending function.

### 3.6 Wall functions for rough walls

So far this chapter has considered only flows over smooth walls. However, boundary layers are affected by surface roughness. This section contains a discussion of the effects of surface roughness on boundary layers. Only wall function treatments of roughness are considered, since these are the most widely-used methods in engineering. However there are LRN turbulence models that claim to be able to account for surface roughness by redefining the turbulent length scale and boundary conditions in terms of the roughness (Durbin et al., 2001).

On a fundamental level, surface roughness can be thought of as small, irregular protuberances on a surface. These cause additional turbulent motions near to the wall and disrupt the viscous sublayer. This leads to an increase in the wall shear stress. There is also an additional pressure force on the protuberances which further increases the pressure loss in a flow.

Roughness is often characterised with a roughness height, $R_h$, which describes how far above
Chapter 3. Near-wall models

the smooth surface the roughness elements extend. However, a number of other length scales are often used. For example, in this thesis many surfaces contain ribs whose height, $h$, can be used as a measure of the roughness. The metrics that are used to characterise rough surfaces in this work are given in Table 3.2, for reference. For a surface in the $(x, z)$ plane, the roughness average is defined with a line integral over a length, $L$ of the surface as

$$R_a = \frac{1}{L} \int_0^L |y(x) - \bar{y}| \, dx,$$  \hspace{1cm} (3.91)

where the mean height of the surface is $\bar{y}$, and $y(x)$ is the surface height at location $x$.

| $s$ | Equivalent sand grain roughness |
| $z_0$ | Roughness length |
| $R_a$ | Roughness average |
| $R_h$ | Roughness height |
| $\lambda$ | Roughness density (non-dimensional) |
| $d$ | Mean height of momentum absorption by the surface |
| $h$ | Rib height |

Table 3.2: The metrics used to describe rough surfaces.

When a wall is rough, there are new dimensionless distances in addition to those in Equations (3.1) and (3.2), which are defined as

$$y_s^+ = \frac{y}{s}, \quad y_{z_0}^+ = \frac{y}{z_0}, \quad \text{and} \quad y_h^+ = \frac{y}{h}.$$  \hspace{1cm} (3.92)

The concept of the equivalent sand grain roughness originates from the work of Nikuradse (1933), who studied turbulent flow in cylindrical pipes, the walls of which were roughened with sand grains with a well-defined mean diameter. The data of Nikuradse (1933), along with data of other authors, were compiled by Moody (1944) into the Moody chart, which links the equivalent sand grain roughness, Reynolds number and friction factor. The friction factor is defined as $f = D |\Delta P| / (2W \rho U_b^2)$, where $D$ is the pipe diameter, $\Delta P / W$ is the pressure loss per unit length of pipe, $\rho$ is the density and $U_b$ is the bulk velocity. The Moody chart is shown in Figure 3.6.

Extensive reviews of rough wall functions can be found in Raupach et al. (1991) and Jiménez (2004). Rough wall functions are built using the various correlations that exist for statistically one-dimensional shear flows. For smooth walls, the log law is used to compute the velocity in the logarithmic region of the boundary layer. When the wall is rough, there is a decrease in the velocity in the logarithmic layer, which leads to an increase in drag. This change is expressed in terms of the roughness function $\Delta U^+$, which is subtracted from the wall function:

$$U^+ = \frac{1}{K} \ln \left( y_t^+ \right) + C_{\text{smooth}} - \Delta U^+,$$  \hspace{1cm} (3.93)

where the constant $C$ in Equation (3.17) has been renamed $C_{\text{smooth}}$. There are numerous
3.6. Wall functions for rough walls

Figure 3.6: The Moody chart
functions that are used to model $\Delta U^+$ (Ligrani and Moffat, 1986). In the limit that the roughness height becomes large, the flow over the wall becomes fully rough, and the rough wall function can be written (Jiménez, 2004)

$$U^+ = \frac{1}{\kappa} \ln \left( y^+_s \right) + C_{\text{rough}}, \quad (3.94)$$

where the equivalent sand grain roughness has been used to non-dimensionalise the wall distance. If the standard log law (Equation (3.17)) is true for a fully smooth wall and Equation (3.94) is true for a fully rough wall, then there must be a transitional region in between the two, where the roughness height is insufficiently large to create a fully rough regime, but large enough for the flow not to be in the smooth regime. Flows in this regime are called transitionally rough. The motion of transitionally rough flows depends on the flow geometry, the nature of the roughness and the thickness of the boundary layer. If the boundary layer is thin, then transitionally rough flows sometimes behave like flows over a series of obstacles (Jiménez, 2004).

Different authors delimit the three flow regimes – smooth, transitionally rough and fully rough – differently. Often the limits rely on the non-dimensional roughness height $s^+_+$ or $s^+_k$. For example, Pope (2000, p. 298) delimits the transitionally rough region by $5 < s^+_+ < 70$; Jiménez (2004) uses the limits $4 < s^+_k < 80$ (Jiménez, 2004); and the documentation for the commercial CFD code FLUENT gives the limits $2.25 < s^+_k < 90$ (ANSYS Inc., 2013). The value of $s^+_+$ also has implications for the mesh; if the $y^+_+$ of the nearest cell to the wall is less than $s^+_+$ and the flow is in the smooth regime then a LRN turbulence model should be used. If the flow is fully rough and $y^+_+ < s^+_+$, then the location of the origin of the wall function becomes important. It is often taken to be the location where the mean velocity extrapolates to zero, which is beyond the wall, outside the flow domain (Durbin et al., 2001). If this is done then the rough wall function is valid right down to the wall for fully rough flows (Durbin et al., 2001).

Jiménez (2004) states that Equation (3.94) is actually the definition of $s$. There is no rule which can reliably link the equivalent sand grain roughness with more conventional roughness metrics, such as the roughness average, $R_a$. However many attempts have been made to link the two so that $s$ can be calculated a priori from experimental measurements of a surface. Adams et al. (2012) modelled computationally the process of measuring the roughness average of a surface consisting of closely-packed spheres and suggested that the equivalent sand grain roughness is related to $R_a$ as

$$s = 5.9 R_a, \quad (3.95)$$

This is a useful result and is shown in Adams et al. (2012) to always yield more accurate results than assuming that $R_a$ and $s$ are equal. However the methodology is simplistic and the accuracy of this approximation is often poor.
Another expression often used for the rough wall function in all flow regimes is (Jiménez, 2004)

\[ U^+ = \frac{1}{\kappa} \ln \left( \frac{y^+_0}{z_0} \right), \]  

(3.96)

which is based on the roughness length, \( z_0 \). The concept of the roughness length is used widely in atmospheric flows over rough surfaces. Equation (3.96) implies a shift in the origin of the coordinate \( y \) (Raupach et al., 1991). The argument of the logarithm should be \( (y - d)^+_0 \), where \( d \) is the zero-plane displacement, or the mean height of momentum absorption by the rough surface (Raupach et al., 1991). For a smooth surface, \( d = 0 \), however for rough surfaces \( d \) must be calculated and obeys the limits \( 0 < d < R_h \). This calculation is not straightforward and cannot be done a priori. The coordinate \( y \) is measured from the smooth surface upon which the rough layer is imposed. At the edge of the rough layer, \( y = R_h \). Therefore in practical applications of Equation (3.96) as a wall function, the argument \( y - d > 0 \). For large \( y^+_0 \), the effect of the zero-plane displacement is small, because the logarithm varies only slowly with its argument. When the rough wall function is used in this work, the zero-plane displacement is ignored because there is no way to calculate it reliably.

Durbin et al. (2001) used a different expression for the rough wall function,

\[ U^+ = \frac{1}{\kappa} \ln \left( \frac{y + z_0}{z_0} \right) = \frac{1}{\kappa} \ln \left( \frac{y^+_0}{1} + 1 \right), \]  

(3.97)

where the origin of \( y \) is defined to be the location where the extrapolated velocity profile is zero.

The roughness length can be related directly to the roughness function and the equivalent sand grain roughness by evaluating both Equation (3.93) and (3.96) at \( z = s \) (Durbin et al., 2001) and equating the two to find that

\[ z_0 = se^{\kappa(\Delta U^+-C_{smooth})-\log(s^+_0)}, \]  

(3.98)

which is useful though not particularly helpful since neither \( z_0 \) nor \( \Delta U^+ \) are known a priori.

In the fully rough regime, the relationship between \( z_0 \) and \( s \) is (Raupach et al., 1991)

\[ z_0 \approx s/30, \]  

(3.99)

and in the smooth regime the roughness length is (Raupach et al., 1991)

\[ z_0 = 0.14\nu/u_r, \]  

(3.100)

which is independent of \( s \).

Many attempts have been made to relate the roughness length directly to the roughness height. Such approaches do not use the concept of the equivalent sand grain roughness. In
general the relationship between \( z_0 \) and \( R_h \) depends on the geometry of the roughness, such as the aspect ratio of the roughness elements, the spacing between the elements and the roughness density, \( \lambda \), which is defined as the ratio of the frontal surface area of the roughness to the wall surface area the roughness occupies (Schlichting, 1936). The effect of \( \lambda \) on \( z_0/R_h \) has been well studied. It is generally found that as \( \lambda \) increases from zero, \( z_0/R_h \) peaks with a maximum value of around 0.1 at \( \lambda \approx 0.2 \) (Raupach et al., 1991) before decreasing as \( \lambda \) increases further. The decrease is caused by adjacent roughness elements shielding one another from the flow. This is so-called \( d \)-type roughness, in which the roughness elements are so close together that the flow cannot reattach between successive roughness elements.

As the roughness elements move apart the flow begins to penetrate into the region between adjacent roughness elements. This is called \( k \)-type roughness. The complete link between \( \lambda \) and \( z_0/R_h \) is not known, especially for larger \( \lambda \) (Jiménez, 2004), where the results depend on the experimental set-up.

When studying rough walls it is difficult to reconcile the parameter required by the wall function (\( s \) or \( z_0 \)) with the actual geometry of the roughness (\( h \), \( R_h \) or \( R_a \)). Numerous experimental studies have been performed in an attempt to determine the link between these parameters, however no universal relationship has been found. In general, the roughness length and the equivalent sand grain roughness are smaller than the roughness height (Raupach et al., 1991).

### 3.6.1 Modelling turbulence near rough walls

The motion caused by the roughness elements leads to an increase in turbulent kinetic energy near to the wall. Using a mixing length model with \( l_m = u_T/\partial y U \) and Equation (3.97) yields (Durbin et al., 2001)

\[
\mu_t = \rho u_T \kappa (y + z_0).
\]

Hence by a rough wall, turbulence can be considered to originate at \(-z_0\) (Durbin et al., 2001). Therefore, near-wall damping functions are either modified or not used in rough wall-bounded flows (Durbin et al., 2001). Wall boundary conditions for \( k \) and \( \varepsilon \) at rough walls are often different to their boundary conditions at smooth walls. It is common for \( k \) to obey a non-homogeneous boundary condition at the wall (Durbin et al., 2001).

Suga et al. (2006) modified the AWF to account for wall roughness. The parameter \( y_e \) was modified to depend on the equivalent sand grain roughness through an empirical relationship. The wall function was able to cope with this modification and produced results that were competitive with experimental data on a flow over a sand dune and a flow over a sand-roughened ramp.
Apsley (2007) used the turbulent viscosity specification of the AWF and made $y_v$ sensitive to $\Delta U^+$. The algorithm admits negative values of $y_v$, which is consistent with the suggestion that the origin of turbulence is at a negative wall distance. The wall function was able to reproduce the Moody chart with both a $k - \varepsilon$ and a Reynolds stress model and made predictions of flow over an erodible bed that compare well with experimental data.
Chapter 4

Code_Saturne

The code used in this work is Code_Saturne, which is an open-source, general purpose CFD code developed by Électricité de France Research and Development (EDF R&D). It is based on a co-located finite volume scheme for unstructured meshes. The code can compute laminar or turbulent flows using a variety of different turbulence models. It can solve scalar transport equations, which means it can be used for heat transfer studies. There are also specific modules for handling the effects of, for example, combustion or compressible flows.

The version of Code_Saturne used in this thesis is 3.0.5.

4.1 The finite volume method

The finite volume (FV) method is the method of choice for CFD. This is because conservation equations can be guaranteed to hold over the flow domain. Other methods such as finite differences or finite elements may be used for specialist applications. However ensuring that the conservation equations are satisfied with these schemes is more complicated than it is for FV schemes.

To model a particular geometry with a FV scheme, the geometry is discretised into a number of smaller control volumes, or cells, with well-defined cell centres. The number of cells is important: generally the more there are the more accurate the results will be, but the longer the computation will take. Complex engineering geometries may have of the order of $10^7$ cells, however simple geometries may have only a few tens or hundreds or cells.

In fluid dynamics, all functions apart from the pressure obey a transport equation of the form

$$\frac{\partial (\rho \Phi)}{\partial t} + \nabla \cdot (\rho U \Phi) = \nabla \cdot (\gamma \nabla \Phi) + S_\Phi,$$

(4.1)
4.1. The finite volume method

which can be integrated over a volume \( \Omega \) to become

\[
\int_{\Omega} \left( \frac{\partial (\rho \Phi)}{\partial t} + \nabla \cdot (\rho \mathbf{U} \Phi) \right) d^3x = \int_{\Omega} \nabla \cdot (\gamma \nabla \Phi) d^3x + \int_{\Omega} S_\Phi d^3x. \tag{4.2}
\]

Using the divergence theorem for a vector function \( \mathbf{F} \),

\[
\int_{\Omega} \nabla \cdot \mathbf{F} d^3x = \int_{\partial\Omega} \mathbf{F} \cdot d\mathbf{S}, \tag{4.3}
\]

where \( d\mathbf{S} = \mathbf{n} dS \) is an outwards-pointing surface element of the volume \( \Omega \), Equation (4.2) can be re-written as

\[
\int_{\Omega} \frac{\partial (\rho \Phi)}{\partial t} d^3x + \int_{\partial\Omega} \rho \mathbf{U} \Phi \cdot d\mathbf{S} = \int_{\partial\Omega} \gamma \nabla \Phi \cdot d\mathbf{S} + \int_{\Omega} S_\Phi d^3x. \tag{4.4}
\]

Discretisation of the terms in Equation (4.4) is now necessary to solve the equation. The discretisation methods used for each term are now discussed.

4.1.1 Volume integrals

The volume integrals in Equation (4.4) are often approximated as the product of the cell-average value of the integrand, multiplied by the volume of the cell, \( \Omega_I \),

\[
\int_{\Omega_I} S_\Phi d^3x \approx \overline{S_\Phi} \Omega_I. \tag{4.5}
\]

The cell-averaged value of \( S_\Phi \) is stored at the cell centre. Typically \( S_\Phi \) represents a source term in the equation. In Code_Saturne, source terms are written as

\[
S_\Phi = S'_\Phi - K \Phi, \tag{4.6}
\]

where \( K > 0 \). The source term contributions contained in \( K \) are treated implicitly in the numerical solver. This enhances the stability of the numerical method (Patankar, 1980).

4.1.2 Convection terms

The convection terms in Equation (4.4) are approximated as

\[
\int_{\partial\Omega_I} \rho \mathbf{U} \Phi \cdot d\mathbf{S} \approx \sum_{i=1}^{N_{\text{faces}}} \tilde{m}_i \Phi_i, \tag{4.7}
\]

where \( \tilde{m}_i = \rho \mathbf{U} \cdot \mathbf{S}_i \) is the mass flux through the face \( i \) with surface area vector \( \mathbf{S}_i \) and the sum is over all the faces of the control volume. Values of \( \Phi \) (and \( \rho \) for compressible flows) must be interpolated from the neighbouring cell centres, denoted \( I \) and \( J \), to the cell face, \( F \), as shown in Figure 4.1a. There are three methods that can be used to calculate \( \Phi_F \) in Code_Saturne:
Chapter 4. Code_Saturne

An upwind difference scheme, which takes

$$\Phi^{UDS}_F = \begin{cases} 
\Phi_I, & \text{if } \dot{m}_F \geq 0, \\
\Phi_J, & \text{if } \dot{m}_F < 0.
\end{cases}$$

(4.8)

This is a first order approximation. The second order error term introduces artificial diffusion into the equation. While this is not desirable, it does make the scheme stable and so the upwind difference scheme is sometimes used.

A central difference scheme, which takes

$$\Phi^{CDS}_F = \alpha \Phi_I + (1 - \alpha) \Phi_J + \frac{1}{2} (\nabla \Phi|_I + \nabla \Phi|_J) \cdot \mathbf{OF},$$

(4.9)

where $\alpha = \frac{F_J'}{F_I'}$ (see Figure 4.1a). This scheme is second order, however on coarse grids the solution may sometimes diverge or oscillate.

A second order upwind scheme, which takes

$$\Phi^{SOLU}_F = \begin{cases} 
\Phi_I + \mathbf{IF} \cdot \nabla \Phi|_I, & \text{if } \dot{m}_F \geq 0, \\
\Phi_J + \mathbf{JF} \cdot \nabla \Phi|_J, & \text{if } \dot{m}_F < 0.
\end{cases}$$

(4.10)

It is also possible to use a weighted average of the values calculated by the upwind and central difference schemes.

Slope test

There is a slope test in Code_Saturne which can automatically switch the convection scheme to an upwind scheme in regions where the gradient varies rapidly in space. This is done with
two test criteria, which estimate whether the function, $\Phi$, is monotonic between the face and the two neighbouring cell centres. The “upwind gradient” is defined at each cell centre as

$$\tilde{\nabla} \Phi |_{I} = \frac{1}{\Omega_I} \sum_{i=1}^{N_{faces}} \Phi_{U}^{i} S_{i},$$

(4.11)

then the two test criteria are computed

$$T_{F} = \tilde{\nabla} \Phi |_{I} \cdot \tilde{\nabla} \Phi |_{J},$$

(4.12)

and

$$T_{Q} = \begin{cases} (\nabla \Phi |_{I} \cdot S_{F})^2 - (\tilde{\nabla} \Phi |_{I} \cdot S_{F} - \frac{\Phi_{J} - \Phi_{I}}{J'F} S_{F})^2 & \text{if } \dot{m}_{F} > 0, \\ (\nabla \Phi |_{J} \cdot S_{F})^2 - (\tilde{\nabla} \Phi |_{J} \cdot S_{F} - \frac{\Phi_{J} - \Phi_{I}}{J'F} S_{F})^2 & \text{if } \dot{m}_{F} \leq 0, \end{cases}$$

(4.13)

where $\nabla \Phi$ is calculated using one of the gradient schemes in Section 4.1.4. If either $T_{Q}$ or $T_{F}$ are negative then an upwind convection scheme is used if the slope test is active.

### 4.1.3 Diffusive terms

The diffusive terms in Equation (4.4) are approximated as

$$\int_{\partial \Omega} \gamma \nabla \Phi \cdot dS \approx \sum_{i=1}^{N_{faces}} \gamma_{i} \frac{\partial \Phi}{\partial n} |_{S_{i}},$$

(4.14)

where $n$ is the normal to the face $i$ and $S_{i}$ is its surface area. Interpolation is necessary to find the values of $\gamma$ and $\partial_{n} \Phi$ at the cell-faces. For the geometry in Figure 4.1a, the gradient is calculated as

$$\frac{\partial \Phi}{\partial n} |_{F} \approx \frac{\Phi_{J} - \Phi_{I}}{|J'F|},$$

(4.15)

which is second order accurate for the special case $J'F = I'F$. In the case of a boundary face (Figure 4.1b), the gradient is calculated as

$$\frac{\partial \Phi}{\partial n} |_{F} \approx \frac{\Phi_{F} - \Phi_{I}}{|I'F|},$$

(4.16)

which is first order accurate.

### 4.1.4 Gradient calculation and reconstruction

The gradient at the cell centre is required in order to calculate the convection terms with the central difference or second order upwind schemes. Therefore gradient calculation is an important element of a CFD solver.

CFD solvers which use unstructured grids need gradient reconstruction schemes to remove
geometrical errors from the gradient calculation at the cell centres. These errors arise from
the interpolation of a function between the cell centres and face centres. The line joining the
cell centres does not necessarily pass through the face centre, as shown with the lines $IJ$ and
$I'J'$ in Figure 4.1a.

There are two distinct methods available for the gradient calculation in Code_Saturne. The
default is an iterative approach and the other is a least squares calculation. In total there
are seven gradient calculation algorithms in Code_Saturne. The default is a purely iterative
approach but there are three least squares approaches with different stencils and three ap-
proaches that use the least squares approach with different stencils to initialise the iterative
approach.

Iterative approach

The iterative approach begins with the Green-Gauss theorem

$$\int_{\Omega} \nabla \Phi \, d^3x = \int_{\partial\Omega} \Phi \, dS,$$  (4.17)

which when discretised becomes

$$\nabla \Phi_I = \frac{1}{\Omega_I} \sum_{i=1}^{N_{\text{faces}}} \Phi_i S_i.$$  (4.18)

This shows that $\Phi_F$ is required in order to calculate $\nabla \Phi_I$, but $\nabla \Phi_I$ is required to calculate $\Phi_F$. Hence an iterative process is started. At each iteration $n$ the approximation of $\nabla \Phi_I$ is improved as

$$\nabla \Phi_I^{(n+1)} = \frac{1}{\Omega_I} \sum_{i=1}^{N_{\text{faces}}} \Phi_i^{(n)} S_i,$$  (4.19)

where

$$\Phi^{(n)} = \alpha \Phi_I + (1 - \alpha) \Phi_J + \frac{1}{2} \left( \nabla \Phi_I^{(n)} \big|_J + \nabla \Phi_J^{(n)} \big|_I \right) \cdot \mathbf{O}_F.$$  (4.20)

The convergence test uses the $\ell^2$ norm of the gradient vector.

Least squares approach

The least squares approach determines the gradient with the expression

$$\Phi_J = \Phi_I + IJ \cdot \nabla \Phi |_J.$$  (4.21)

For a hexahedral cell, this produces six equations for the three components of $\nabla \Phi$. The
equation system is over determined and solved with a least squares sense. At each cell a
matrix equation is written
\[ C_I \nabla \Phi|_I = T_I, \]  
(4.22)
where the elements of the matrix \( C_I \) are
\[ C_{I,pq} = \sum_{i=1}^{N_{\text{faces}}} \frac{I J_p I J_q}{|I J|^2}, \]
(4.23)
and
\[ T_{I,p} = \sum_{i=1}^{N_{\text{faces}}} \frac{(\Phi_J - \Phi_I)}{|I J|^2}. \]
(4.24)

The matrix \( C_I \) is inverted, which allows the gradient to be calculated as
\[ \nabla \Phi|_I = C_I^{-1} T_I. \]
(4.25)

The number of faces included in the sum depends on the stencil used. Three stencils are available: the stencil can include only first cell neighbours; both first and second neighbours; or first neighbours and second neighbours only when the angle between \( I J \) and \( I'J' \) in Figure 4.1a is less than 45°. This removes skewed cells from the stencil.

When the gradient is calculated with the least squares approach, a limiter is applied to the gradient by default. The limiter depends on the \( \ell^2 \) norm of the variation of \( \Phi \) and \( \nabla \Phi \) over the stencil.

### 4.2 Discretisation in time

In Code_Saturne, equations are discretised in time using a \( \theta \)-scheme. The governing equation is written as
\[ \frac{\partial \Phi}{\partial t} = F(t, \Phi), \]
(4.26)
and the equations are advanced in time as
\[ \Phi^{(n+1)} = \Phi^{(n)} + \tau \left( \theta F(t^{(n+1)}, \Phi^{(n+1)}), \Phi^{(n)} \right) + (1 - \theta) F(t^{(n)}), \]
(4.27)
where \( \tau \) is the time step. If \( \theta = 0 \) then the scheme is the first order, explicit forward Euler scheme; if \( \theta = 1 \) then the scheme is the first order, implicit backward Euler scheme. For \( \theta = \frac{1}{2} \) the scheme uses the second order, trapezoidal Crank-Nicolson method.

Physical properties, such as the density or viscosity, mass fluxes and source terms are discretised differently:

- Physical properties, denoted \( \Psi \), are either treated explicitly at time step \( n \) or extrapo-
lated at time step \( n + \theta_P \) with the Adams-Bashforth scheme as

\[
\Psi^{(n+\theta_P)} = (1 + \theta_P) \Psi^{(n)} - \theta_P \Psi^{(n-1)},
\]

(4.28)

with \( \theta_P = \frac{1}{2} \) or \( \theta_P = 1 \).

- Mass fluxes are either treated explicitly at time step \( n \) for both the momentum and scalar equations; explicitly at time step \( n \) for the momentum equations and explicitly at time step \( n + 1 \) for the scalar equations; or taken at time step \( n + \theta_F \) for the momentum equations as

\[
\dot{m}^{n+\theta_F} = 2\dot{m}^{n+\theta_F-1} - \dot{m}^{n+\theta_F-2},
\]

(4.29)

and for the scalar equations as

\[
\dot{m}^{n+\theta_F} = \frac{1}{2 - \theta_F} \dot{m}^{n+1} + \frac{1 - \theta_F}{2 - \theta_F} \dot{m}^{n+\theta_F-1}.
\]

(4.30)

with \( \theta_F = \frac{1}{2} \) or \( \theta_F = 1 \).

- Source terms for a function \( \Phi \) are either taken explicitly as

\[
S^{(n+\theta_S)}(\Phi, \Psi) = \left(\Phi^{(n)}, \Psi^{(n+\theta_S)}\right),
\]

(4.31)

where \( \Psi \) represents the physical properties, or they are taken at time step \( n + \theta_S \) as

\[
S^{(n)}(\Phi, \Psi) = (1 + \theta_S)S(\Phi^{(n)}, \Psi^{(n)}) - \theta_S S(\Phi^{(n-1)}, \Psi^{(n-1)}),
\]

(4.32)

with \( \theta_S = \frac{1}{2} \) or \( \theta_S = 1 \).

When using RANS models only the first order explicit scheme is permitted. For LES only the second order scheme is permitted.

### 4.3 Pressure correction algorithm

*Code_Saturne* uses a projection method (Chorin, 1968) to couple the momentum and continuity equations. The first step is the projection step, in which the solution to the momentum equations at an intermediate time step \( n' \) is calculated as

\[
\frac{\rho \mathbf{U}^{(n')}_t - \rho \mathbf{U}^{(n)}}{\delta t} + \nabla \cdot \left( \rho \mathbf{U}^{(n')} \mathbf{U}^{(n)} - (\mu + \mu_t) \nabla \mathbf{U}^{(n')} \right) = -\nabla P^{(n)} + \mathbf{S}_{\mathbf{U}}^{(n)},
\]

(4.33)

where \( \mathbf{S}_{\mathbf{U}}^{(n)} \) represents any additional source terms. The continuity equation is ignored for this step. Therefore the solution \( \mathbf{U}^{(n')} \) might not obey the continuity equation.
4.4 Solution algorithm and the convergence criteria

In the correction step, the pressure is advanced to time step \( n + 1 \) by using the equation

\[
-\nabla \left( P^{(n+1)} - P^{(n')} \right) = \frac{1}{\delta t} \left( (\rho U)^{(n+1)} - (\rho U)^{(n')} \right),
\]

and requiring that the continuity equation is satisfied at the time step \( n + 1 \), such that

\[
\nabla \cdot (\rho U)^{(n+1)} = \Gamma,
\]

where \( \Gamma \) represents any mass source terms\(^1\). The mass fluxes in Equations (4.34) and (4.35) are calculated using Rhie and Chow interpolation (Rhie and Chow, 1983) to prevent oscillations on structured grids. Equations (4.34) and (4.35) are combined to yield the Poisson equation

\[
\Gamma - \nabla \cdot (\rho U)^{(n')} = -\delta t \nabla^2 \left( P^{(n+1)} - P^{(n')} \right),
\]

which is solved to find the pressure at the time step \( n + 1 \). Then, the velocities are updated by rearranging Equation (4.34) as

\[
U^{(n+1)} = U^{(n')} - \frac{\delta t}{\rho} \nabla \left( P^{(n+1)} - P^{(n')} \right).
\]

4.4 Solution algorithm and the convergence criteria

*Code_Saturne* solves for an increment in \( \Phi \) at each time step, defined as \( \delta \Phi = \Phi^{n+1} - \Phi^n \). Equation (4.1) is re-written as

\[
f_t \delta \Phi + \nabla \cdot (\delta \Phi \rho U - \mu \nabla \delta \Phi) = S'_\Phi,
\]

where \( f_t \) is the discretised time derivative operator and

\[
S'_\Phi = S_\Phi - \nabla \cdot (\Phi^n \rho U - \mu \nabla \Phi^n).
\]

Equation (4.38) is solved iteratively at each time step with the equation

\[
f_t \delta \Phi^k + \nabla \cdot \left( \delta \Phi^k \rho U - \mu \nabla \delta \Phi^k \right) = S^k_\Phi,
\]

with

\[
S^k_\Phi = S_\Phi = f_t \left( \Phi^k - \Phi^n \right) - \nabla \cdot \left( \Phi^k \rho U - \mu \nabla \Phi^k \right).
\]

On convergence, a steady problem has \( \delta \Phi = 0 \) and therefore \( S^k_\Phi = 0 \) since \( \Phi^k \) is the solution to Equation (4.38). Equation (4.40) can be solved more than once at each time step, which would be denoted with \( k > 1 \). The normed residual printed by default is \( ||S^k_\Phi||_2/||S^0_\Phi||_2 \) for \( k \geq 1 \).

\(^1\)With no mass source terms \( \Gamma = 0 \).
Equation (4.40) is solved by writing it as a matrix equation:

$$A_{ij} \Phi_j = b_i.$$ (4.42)

On the right hand side, $b_i = S_{\Phi_i}$ contains all the source terms and on the left hand side, $\Phi_j$ is an array of values of $\Phi$ at each cell $j$ and $A_{ij}$ is the matrix that needs inverting. By default the pressure Poisson equation is solved with the conjugate gradient method. The other convection-diffusion equations are solved using the Jacobi method. The linear system solver exits when either the maximum number of iterations is reached or $\tau < \epsilon \|S^{n}_{\Phi}\|_2$, where $\tau$ is the residual. For the Jacobi solver, $\tau$ is defined as

$$\tau = \sqrt{\sum_{i}^{N} (a_{ii}(\Phi_{i}^{n+1} - \Phi_{i}^{n}))^2},$$ (4.43)

where $a_{ii}$ is the diagonal of the matrix $A$ and there is no implicit sum over $i$.

### 4.5 Boundary conditions

There are two types of face in a mesh: internal faces and boundary faces. Internal faces are shared between two control volumes and do not require boundary conditions. Boundary faces require boundary conditions in order to calculate functions at the neighbouring cell centre. The discretisation of convective and diffusive fluxes must be modified at boundary faces, as must the gradient calculation.

In Code_Saturne, boundary conditions are calculated in terms of coefficients $A_{\Phi}$ and $B_{\Phi}$, for each function $\Phi$, as

$$\Phi_F = A_{\Phi} + B_{\Phi} \Phi_F,$$ (4.44)

where the subscripts refer to the geometry in Figure 4.1b. For a scalar $\Phi$, both $A_{\Phi}$ and $B_{\Phi}$ are scalars. If $\Phi$ is a vector then $A_{\Phi}$ is a vector and $B_{\Phi}$ is a matrix. Expressing the boundary conditions in this way allows at least part of the boundary conditions to be treated implicitly.

Two different types of boundary condition are required for each variable: so-called gradient and flux boundary conditions. Gradient boundary conditions contain the value of a function at the boundary face. These conditions are used when calculating the gradient of a function or when mass fluxes are needed at a boundary face.

Flux boundary conditions contain the diffusive flux of a function at the boundary. The flux boundary conditions are computed in terms of coefficients $A_{\Phi,f}$ and $B_{\Phi,f}$. For example, for the velocity, the diffusive flux boundary at a boundary face is the wall shear stress, which is
written as
\[
(\mu + \mu_t) \frac{\partial U}{\partial n} \bigg|_F = A_{U,f} + B_{U,f} U'.
\] (4.45)

Applying independent Dirichlet and Neumann boundary conditions at the same point on the boundary of an elliptical PDE makes the problem ill posed. Therefore when a Dirichlet boundary condition is applied it is usual to calculate the gradient of the function at the boundary with a discretised gradient operator. The gradient of \( \Phi \) at a boundary face is written
\[
\frac{\partial \Phi}{\partial n} = \frac{(\Phi_{I'} - \Phi_F)}{\Delta},
\] (4.46)
where \( \Delta = |I'F| \) is the distance to the wall. When wall functions are used, the gradient at the wall is not calculated with such a finite difference-type scheme. This explains why the flux and gradient boundary conditions can be specified independently in the wall function implementation in *Code_Saturne*.

Five different types of boundary condition are catered for by default in *Code_Saturne*: inlets, outlets, symmetry boundaries, smooth walls and rough walls. Periodic boundary conditions can also be applied to pairs of boundary faces, which turns them into internal faces.

The implementation of the boundary conditions is expressed in terms of local coordinates in the boundary cell.

### 4.5.1 Global and local coordinates

The global coordinate system is described by the usual Cartesian coordinates \((\hat{e}_x, \hat{e}_y, \hat{e}_z)\), as shown in Figure 4.2a.

The first local coordinate vector \( \mathbf{n} \) is the inward normal to the wall\(^2\) and the second coordinate \( \mathbf{t} \) is defined using \( U_{I'} \), where \( I' \) is defined in Figure 4.2b, as
\[
\mathbf{t} = \frac{U_{I',t}}{|U_{I',t}|},
\] (4.47)
where \( U_{I',t} \) is the velocity component tangential to the plane of the wall, defined by
\[
U_{I',t} = U_{I'} - (U_{I'} \cdot \mathbf{n}) \mathbf{n}.
\] (4.48)
Whenever \( U_{I',t} = 0 \), \( \mathbf{t} \) is defined arbitrarily as
\[
\mathbf{t} = \frac{n_z \hat{e}_y - n_y \hat{e}_z}{\sqrt{n_y^2 + n_z^2}},
\] (4.49)
\(^{2}\)By default \( \mathbf{n} \) is actually stored as \( \tilde{\mathbf{n}} = -\mathbf{n} \)
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(a) The global coordinate system

(b) The local coordinate system

Figure 4.2: The local and global coordinate systems used to determine the boundary conditions in Code_Saturne.

where \( \mathbf{n} = (n_x, n_y, n_z)^T \). If needed, the coordinate system can be completed by defining

\[
\mathbf{b} = \mathbf{t} \times \mathbf{n}. \tag{4.50}
\]

Figure 4.2b shows the vectors \( \mathbf{t} \) and \( \mathbf{n} \) on a diagram.

4.5.2 Inlet boundary conditions

At an inlet boundary the user must specify Dirichlet boundary conditions for all functions apart from the pressure. The pressure is given a homogeneous Neumann boundary condition. Inlet boundary conditions can be challenging to model. For example, at an inlet with LES the user needs to consider how turbulent fluctuations at the inlet are represented.

4.5.3 Outlet boundary conditions

At an outlet all functions apart from the pressure are given homogeneous Neumann boundary conditions, although turbulence model functions can be given Dirichlet boundary conditions. Outlet boundaries should be located in regions of the flow that are approximately one-dimensional. If the velocity at the outlet is calculated to be inwards then it is clipped to zero by the code. As with inlets, with LES the modelling of velocity fluctuations at the outlet can be challenging.
The boundary condition on the pressure is chosen to impose
\[ \frac{\partial^2 P}{\partial n \partial t} \bigg|_F = 0, \]
using a Dirichlet boundary condition. The value of the pressure imposed at the boundary face is computed from the pressure at the cell centre at the previous iteration.

### 4.5.4 Symmetry boundary conditions

Symmetry boundary conditions require no user input. The normal component of the velocity is removed from the velocity at the boundary face, which means that the boundary condition on the velocity is
\[ \mathbf{U}_F = \mathbf{U}_{I'} - (\mathbf{U}_{I'} \cdot \mathbf{n}) \mathbf{n}. \]
Therefore \( \mathbf{U}_F \) can be expressed in matrix form as
\[ \mathbf{U}_F = \mathbf{M} \mathbf{U}_{I'}, \]
with
\[ \mathbf{M} = \begin{pmatrix} 1 - n_x^2 & -n_x n_y & -n_x n_z \\ -n_x n_y & 1 - n_y^2 & -n_y n_z \\ -n_x n_z & -n_y n_z & 1 - n_z^2 \end{pmatrix}, \]
which can be expressed in the form required by Code_Saturne as
\[ \mathbf{A}_U = 0, \quad \mathbf{B}_U = \mathbf{M}. \]

The flux boundary conditions are also determined by \( \mathbf{M} \). The shear stress is
\[ (\mu + \mu_t) \frac{(\mathbf{U}_{I'} - \mathbf{U}_F)}{\Delta} = \chi_U (\mathbf{U}_{I'} - \mathbf{U}_F), \]
\[ = \chi_U (1 - \mathbf{M}) \mathbf{U}_{I'}, \]
where \( \Delta = I'F \) and \( \chi_U = (\mu + \mu_{t,I})/\Delta \). Hence the flux boundary conditions are
\[ \mathbf{A}_{U,f} = 0, \quad \mathbf{B}_{U,f} = \chi_U (I - \mathbf{M}), \]
where \( I \) is the identity matrix.
4.5.5 Wall boundary conditions for LRN models

For LRN turbulence models, the boundary condition on the velocity at a wall boundary face is \( \mathbf{U}_F = 0 \). The gradient boundary conditions are

\[
A_{\mathbf{U}} = 0, \quad B_{\mathbf{U}} = 0, \tag{4.59}
\]

and the flux boundary conditions are

\[
A_{\mathbf{U,f}} = 0, \quad B_{\mathbf{U,f}} = \chi \mathbf{U} I. \tag{4.60}
\]

4.6 Implementation of the scalable wall function

In this section the implementation of the SWF for the \( k - \varepsilon \) model in Code_Saturne is explained.

Unlike some codes, no special numerical discretisation in the near-wall cells is used to implement the SWF in Code_Saturne. However special flux and gradient boundary conditions are calculated for all variables. The purpose of the flux boundary conditions is to determine the diffusive flux at the wall. In the case of the velocity, this means that the flux boundary conditions should determine the wall shear stress according to the SWF. The gradient boundary conditions are used to compute the gradient of the function in the near-wall cell. Thus, the gradient boundary conditions must be such that the discretised gradient operator computes a gradient consistent with the SWF in the near-wall cell. In the case of the velocity, the correct gradient in the near-wall cell is important in order to compute the production term in the \( k \) equation accurately. An effect of this procedure is that the fluid velocity at the wall is stored as a non-zero value. This appears to violate the no slip condition, however the velocity at the boundary face only affects the solution via the gradient operator, so there in no violation in practice.

The SWF can be applied with either a one-scale or a two-scale velocity model. The two-scale velocity model introduces two velocities, \( u_k \) and \( u_\tau \), where

\[
u_k = c_1^{1/4} k_f^{1/2}, \tag{4.61}
\]

and \( u_\tau \) obeys

\[
\frac{U_{\nu,t}}{u_\tau} = \begin{cases} \frac{1}{\kappa} \ln (y_k^+) + 5.2 & \text{if } y_k^+ > y_{\text{lim}}^+ \\ y_k^+ & \text{if } y_k^+ \leq y_{\text{lim}}^+ \end{cases}, \tag{4.62}
\]

where \( U_{\nu,t} = \mathbf{U}_\nu \cdot \mathbf{t} \) and \( y_k^+ = u_k \Delta/\nu \). There is a cut-off distance, \( y_{\text{lim}}^+ = 1/\kappa = 2.38 \) for RANS, which represents the boundary between the log layer and the viscous sublayer. This
value is chosen so that the gradient $\partial_y U^+$ is continuous across the boundary layer\(^3\). For LES the cut-off is $y^+_{\text{lim}} = 10.88$.

The one-scale velocity model defines $u_\tau$ as above and uses $u_k = u_\tau$ so that any dependence on $k$ is removed. This allows the same form of boundary condition to be used consistently for both the one- and two-scale velocity models.

The implementation of the SWF in *Code_Saturne* is outlined below for the $k - \varepsilon$ model.

### 4.6.1 “Flux” boundary conditions

The flux boundary conditions are

$$
A_{U,f} = \chi U V^r_w, \quad B_{U,f} = \chi U M,
$$

(4.63)

where $V^r_w$ is the velocity of the wall with any component normal to the wall removed, $M$ is defined in Equation (4.54) and

$$
\chi U = \frac{1}{U^+ \kappa \Delta} \max (\mu_{t,I}, \rho I \kappa \Delta u_k).
$$

(4.64)

The projection property of $M$ can be used to compute the wall shear stress. For a stationary wall, if $\mu_{t,I} < \rho I \kappa \Delta u_k$ then

$$
(\mu + \mu_t) \partial_n U_F = \chi U U_{F,t} = \frac{U_{t,I} \rho I \kappa \Delta u_k}{U^+} = \rho I u_\tau u_k t,
$$

(4.65)

which is the wall-function value of $\tau_w$ in the correct direction. The last term in Equation (4.64) allows the wall shear stress to be larger than it would be in the logarithmic region if the turbulent viscosity at the near-wall cell centre is large.

### 4.6.2 “Gradient” boundary conditions

The gradient boundary condition ensures that the code calculates the correct velocity gradient at the near-wall cell centre. In turn, this ensures that the production term, which is assumed to be

$$
\rho P_{\text{calc}} = \mu_{t,I} \left( \frac{\partial U_t}{\partial y} \right)^2
$$

(4.66)

is equal to its value from the log law

$$
\rho P_{\text{theo}} = -\rho \mu_t \frac{\partial U}{\partial y} = \mu_t \left( \frac{\partial U}{\partial y} \right)^2 = \rho I u_\tau u_k \left| \frac{\partial U}{\partial y} \right|_I = \rho I u_k u_\tau^2 \frac{\Delta}{\kappa \Delta},
$$

(4.67)

\(^3\)In the logarithmic region $\frac{dt^+}{dy^+} = \frac{1}{n_y}$ and in the viscous sublayer $\frac{dt^+}{dy^+} = 1$.  

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90
where Equation (3.12) has been used to compute the turbulent viscosity and $\tau_w = \rho_l u_\tau u_k$.

This approach is different to the averaging procedure that was used in early wall-function implementations (see Section 3.4) and is used because, in Code_Saturne, it is not possible to compute the average value of a function in the near-wall cell of an unstructured mesh.

It is assumed that Code_Saturne calculates the production as

$$
\rho P_{\text{calc}} = \mu_{l,I} \left( \frac{U_{G,t} - U_{F,t}}{2\Delta} \right)^2 = \mu_{l,I} \left( \frac{U_{I,t} + U_{J,t} - 2U_{F,t}}{4\Delta} \right)^2,
$$

where the locations, $F$, $G$ and $J$ are shown in Figure 4.3, and $U_G = \frac{1}{2} (U_I + U_J)$.

By equating $P_{\text{calc}}$ and $P_{\text{theo}}$ and approximating the velocity at $J$ as

$$
U_{J,t} = U_{I,t} + 2\Delta \frac{\partial U}{\partial y}\bigg|_G = U_{I,t} + \frac{\Delta u_\tau}{\kappa \Delta},
$$

an equation for the velocity at the wall boundary face, $U_{F,t}$, is found

$$
U_{F,t} = U_{I',t} - \frac{u_\tau}{\kappa} \left( 2 \sqrt{\frac{\rho_l k u_k \Delta}{\mu_{l,I}}} - \frac{1}{2} \right),
$$

where it is assumed that $U_{I,t} = U_{I',t}$. An extra condition is imposed on the gradient to ensure that it is at least as steep as the gradient of the log law at $I'$. A further limit is placed on the velocity itself. So long as $y^+_k > y^+_\text{lim}$, the velocity at the wall is not allowed to be smaller than the velocity given by the log law in the near-wall cell. This means that the expression for $U_{F,t}$ becomes

$$
U_{F,t} = \max \left[ u_\tau \left\{ \frac{1}{k} \ln(y^+_\text{lim}) + 5.2 \right\}, U_{I',t} - \frac{u_\tau}{\kappa} \max \left\{ 1, 2 \sqrt{\frac{\rho_l k u_k \Delta}{\mu_{l,I}}} - \frac{1}{2} \right\} \right].
$$
The boundary conditions can be made fully implicit using the definition

$$u_r = \frac{U_{\tau,I}'}{\frac{1}{\varepsilon} \ln (y^+_k) + 5.2},$$

so that the final expression for $U_{F,t}$ is

$$U_{F,t} = U_{I',t} \max \left\{ 0, \max \left[ \frac{1}{\kappa} \ln(y^+_\text{lim}) + 5.2, \frac{1}{\kappa} \ln(y^+_I) + 5.2, 1 - \frac{\max \left(2 \sqrt{\frac{\rho_I \kappa u_k \Delta}{\mu_{t,I}}} - \frac{1}{\tau} \right)}{\kappa (\ln(y^+I) + 5.2)} \right] \right\},$$

$$= CU_{I',t},$$

where the constant $C$ has been introduced for brevity. The gradient boundary conditions on $U$ are

$$A_U = V^T_w, \quad B_U = CM,$$

where $C$ is defined in Equation (4.74) and $M$ is defined in Equation (4.54). If the near-wall cell centre has $y^+_k < y^+_\text{lim}$ then a no-slip condition is applied with $B_U = 0$, as is done for LRN turbulence models.

### 4.6.3 $k$ boundary conditions

A Dirichlet boundary condition is imposed on $k$,

$$k = \frac{u^2_k}{c^4_{\mu}}$$

which is achieved by specifying

$$A_k = \frac{u^2_k}{c^4_{\mu}}, \quad B_k = 0.$$

The flux boundary condition uses a first order finite difference approximation:

$$A_{k,f} = -\chi_k A_k, \quad B_{k,f} = \chi_k,$$

with $\chi_k = (\mu + \mu_{t,I})/\Delta$. This boundary condition assumes that the equilibrium condition $P = \varepsilon$ from Section 3.4 is valid.

### 4.6.4 $\varepsilon$ boundary condition

The boundary condition for the dissipation assumes that the gradient of the dissipation is equal to the gradient of $\varepsilon$ in turbulent equilibrium in Equation (3.47), so that

$$\frac{\partial \varepsilon}{\partial y} = \frac{\partial}{\partial y} \left( \frac{u^3_k}{\kappa y} \right).$$
The gradients of \( \varepsilon \) at \( I' \) and \( F \) are written as Taylor expansions about the midpoint between \( I' \) and \( F \), denoted \( M \). These expansions are used to derive a second order approximation for \( \varepsilon_F \), which is

\[
\varepsilon_F = \varepsilon_{I'} - \Delta \frac{\partial \varepsilon}{\partial y} \bigg|_{M} + O \left( \Delta^3 \right).
\]  

(4.80)

The gradient at \( M \) is calculated with Equation (4.79) by assuming that \( u_k \) is constant, which is implied by the boundary condition for \( k \):

\[
\frac{\partial \varepsilon}{\partial y} \bigg|_{M} = -\frac{u_k^3}{\kappa \left( \frac{\Delta}{2} \right)^2}.
\]  

(4.81)

Therefore

\[
\varepsilon_F = \varepsilon_{I'} + \Delta \frac{u_k^3}{\kappa \left( \frac{\Delta}{2} \right)^2},
\]  

(4.82)

and the gradient boundary condition is identified as:

\[
A_{\varepsilon} = \frac{4u_k^3}{\kappa \Delta}, \quad B_{\varepsilon} = 1.
\]  

(4.83)

The flux boundary condition follows from the gradient in Equation (4.82):

\[
A_{\varepsilon,f} = \chi \frac{4u_k^3}{\kappa \Delta}, \quad B_{\varepsilon,f} = 0,
\]  

(4.84)

with \( \chi \varepsilon = (\mu + \mu t, \sigma_e) / \Delta \).

In the viscous sublayer, where \( y_k^+ \leq y_{\text{lim}}^+ \), \( u_k \) is set to zero. The boundary conditions for \( k \) and \( \varepsilon \) become \( k = 0 \) and \( \varepsilon_F = \varepsilon_I \). There is no correction to any of these equations in the case of a non-orthogonal, irregular mesh.

### 4.6.5 Scalar boundary conditions

The flux of the temperature scalar, \( \Theta \), at the boundary is written using Equation (3.36) with \( \Phi = c_p \Theta \) as

\[
\dot{q}_F'' = c_p \left( \frac{\mu}{\sigma_\Phi} + \frac{\mu_t}{\sigma_{t, \Phi}} \right) \frac{\partial \Theta}{\partial y},
\]  

(4.85)

which is then made dimensionless with the definitions

\[
\Theta^* = \frac{\dot{q}_F''}{\rho_f c_p u_k}, \quad \Theta^+ = \frac{\Theta - \Theta_F}{\Theta^*},
\]  

(4.86)

which turn Equation (4.85) into

\[
1 = \left( \frac{1}{\sigma_\Phi} + \frac{1}{\sigma_{t, \Phi}} \frac{\nu_t}{\nu} \right) \frac{\partial \Theta^+}{\partial y^+}.
\]  

(4.87)
4.6. Implementation of the scalable wall function

Equation (4.87) defines $\Theta^+$ across the near-wall cell, however it must be integrated. The coefficient

$$\mathcal{K} = \left( \frac{1}{\sigma_\Phi} + \frac{1}{\sigma_{t,\Phi}} \nu \right), \quad (4.88)$$

varies significantly over the near-wall region and therefore requires modelling. The model used in Code_Saturne depends on the Prandtl number. A two layer model is used if $\sigma_\Theta < 0.1$ and a three layer model is used if $\sigma_\Theta > 0.1$ (EDF R&D, 2013). In this thesis, all Prandtl numbers are greater than 0.1. In this case, the solution for $\Theta^+$ is

$$\Theta^+ = \begin{cases} 
\sigma_\Phi y_k^+ & \text{if } y_k^+ < y_1^+, \\
 a_2 - \frac{\sigma_\Phi}{2\sigma_{t,\Phi}} y_k^+ & \text{if } y_1^+ \leq y_k^+ < y_2^+, \\
 \frac{\sigma_\Phi}{\kappa} \ln (y_k^+) + a_3 & \text{if } y_2^+ \leq y_k^+, 
\end{cases} \quad (4.89)$$

where the constants $y_1^+, y_2^+, a_1, a_2$ and $a_3$ depend on $\kappa, \sigma_\Theta$ and $\sigma_{t,\Theta}$.

The form of the boundary conditions depends on whether a Dirichlet or Neumann boundary condition is imposed on $\Theta$.

**Dirichlet boundary condition**

In this case, $\Theta_F$ is specified at the wall. From Equation (4.89), $\Theta^+_F$ is known, therefore $\Theta^*$ can be found:

$$\Theta^* = \frac{\Theta_F - \Theta^+_F}{\Theta^+_F} = \frac{q''_F}{\rho Ic_p u_k}, \quad (4.90)$$

which determines the boundary conditions. The gradient boundary condition is

$$A_\Theta = \Theta_F, \quad B_\Theta = 0, \quad (4.91)$$

and the flux boundary condition is

$$A_{\Theta,f} = -\frac{\rho Ic_p u_k \Theta_F}{\Theta^+_F}, \quad B_{\Theta,f} = \frac{\rho Ic_p u_k}{\Theta^+_F}. \quad (4.92)$$

**Neumann boundary condition**

In this case the flux at the wall is known and is imposed with the flux boundary condition

$$A_{\Theta,f} = q''_F, \quad B_{\Theta,f} = 0. \quad (4.93)$$

Since the flux is known, $\Theta^*$ is also known. Therefore $\Theta_F$ can be found from the definition of $\Theta^+_F$ as

$$\Theta_F = \Theta_F - \Theta^* \Theta^+_F = \Theta^+_F - \frac{\Theta^+_F q''_F}{\rho Ic_p u_k}. \quad (4.94)$$
The gradient boundary condition follows as

\[ A_\Theta = -\frac{\Theta_I q''_F}{\rho I c_p u_k}, \quad B_\Theta = 1. \quad (4.95) \]

### 4.7 Implementation of the rough wall function

The rough wall function in *Code_Saturne* is written in terms of the roughness length as (EDF R&D, 2013)

\[ U^+ = \frac{1}{\kappa} \ln \left( y^+_{z_0} + 1 \right), \quad (4.96) \]

which is the form used by Durbin et al. (2001), given in Equation (3.97), and is similar to Equation (3.96).

Equation (4.96) differs from (3.96) because the argument of the logarithm is \( y^+_{z_0} + 1 \). For large \( y^+_{z_0} \) the logarithm varies slowly and the wall function is effectively unchanged. However, for small \( y^+_{z_0} \) the difference is larger. The argument of the logarithm is \( y \) instead of \( y - d \), which it arguably should be (Raupach et al., 1991). Therefore, Equation (4.96) might be invalid at low \( y^+_{z_0} \). However the main advantage of Equation (4.96) is that the wall function remains mathematically defined (and \( U^+ \geq 0 \)) in the limit \( y^+_{z_0} \to 0 \). The trade-off is that the relationship between \( z_0 \) and \( R_h \) is changed, but this relationship is never known a priori in any case.

The boundary conditions for the velocity are computed in a similar way to the smooth wall case (Section 4.6.2). The main differences are that \( u_\tau \) is now computed from Equation (4.96) and \( \kappa (\Delta + z_0) \) is now used as the turbulent velocity length scale instead of \( \kappa \Delta \). The theoretical value of the production is

\[ \rho P_{\text{theo}} = \rho I u_\tau u_k \left| \frac{\partial U}{\partial y} \right|_I = \rho I \frac{u_k u_\tau^2}{\kappa (\Delta + z_0)}, \quad (4.97) \]

hence Equation (4.70) becomes

\[ U_{F,t} = U_I',t - \frac{u_\tau}{\kappa} \left( 2\Delta \sqrt{\frac{\rho_I u_k}{\mu_{I,I}(\Delta + z_0)}} - \frac{1}{2 + z_0/\Delta} \right). \quad (4.98) \]

The velocity is limited so that the production cannot fall below \( P_{\text{theo}} \), which means that the expression for \( U_{F,t} \) becomes

\[ U_{F,t} = U_I',t - \frac{u_\tau}{\kappa} \max \left( 1, \left( 2\Delta \sqrt{\frac{\rho_I u_k}{\mu_{I,I}(\Delta + z_0)}} - \frac{1}{2 + z_0/\Delta} \right) \right). \quad (4.99) \]

Equation (4.99) is used to compute the gradient boundary conditions, which are imposed implicitly with an analogous approach to that used in Section 4.6.2. The flux boundary...
4.7. Implementation of the rough wall function

conditions are computed the same way as in Section 4.6.1, only now with

\[ \chi_U = \frac{1}{U + \kappa(\Delta + z_0)} \max (\mu_{t,1}, \rho_1 \kappa (\Delta + z_0) u_k) . \]  \( \text{(4.100)} \)

The boundary condition for \( k \) is a homogeneous Neumann boundary condition, as it is for the smooth wall case in Section 4.6.3.

Because the roughness length is included in the expression for the production, Equation (4.79) is modified by replacing \( y \) with \( y + z_0 \). The procedure used in Section 4.6.4 is used again for the rough wall function, which leads to

\[ \varepsilon_F = \varepsilon_I + \Delta \frac{u_k^3}{\kappa \left( \frac{\Delta}{2} + z_0 \right)^2} , \]  \( \text{(4.101)} \)

which is analogous to Equation (4.82). Therefore the boundary conditions on \( \varepsilon \) are

\[ A_\varepsilon = \frac{u_k^3 \Delta}{\kappa \left( \frac{\Delta}{2} + z_0 \right)^2} , \quad B_\varepsilon = 1 , \]  \( \text{(4.102)} \)

and

\[ A_{\varepsilon,f} = \chi_\varepsilon \frac{u_k^3 \Delta}{\kappa \left( \frac{\Delta}{2} + z_0 \right)^2} , \quad B_{\varepsilon,f} = 0 , \]  \( \text{(4.103)} \)

with \( \chi_\varepsilon = (\mu + \mu_{t,1}/\sigma_\varepsilon)/\Delta. \)
Chapter 5

Near-wall domain decomposition

This thesis advances the theory and application of the near-wall domain decomposition (NDD) method introduced by Utyuzhnikov (2005a,b, 2006, 2008, 2009, 2012). Previously, the NDD method had only been implemented in an in-house, structured code and applied to either one-dimensional channel flows or a two-dimensional impinging jet flow. This chapter contains details of the developments of the NDD method made during this project and its implementation into Code_Saturne. At the time of writing, two papers on the subject of NDD have been published as part of the work for this project. These are Jones and Utyuzhnikov (2015) and Jones and Utyuzhnikov (2016).

NDD is an alternative to wall function methods for modelling the near-wall regions of turbulent flows. In this sense, there are some similarities between NDD and wall functions, however the implementation of the NDD method is different and it can be implemented for HRN and LRN turbulence models straightforwardly. The method works by splitting the computational domain into an “outer” region and one or more “inner” regions. The inner regions are thin regions that border the wall of a flow and extend a short distance into the computational domain. The mesh covers the outer region of the flow but does not cover the inner regions, as shown in Figure 5.1. Depending on how the inner regions are defined, the walls of the domain can be either partially or completely removed from the outer region. There are surfaces on the boundary between the inner and outer regions, which are called interface boundaries, or simply interfaces.

With NDD, the full RANS\(^1\) equations are solved only in the outer region. This is made possible by special boundary conditions at the interfaces, which are called interface boundary conditions (IBCs). The IBCs are computed by using a boundary layer equation in each inner region to transfer the wall boundary conditions from the wall to the interface. This always

\(^1\)Or LES, however in this thesis NDD is only applied to RANS models.
produces a Robin boundary condition at the interface. Thus, the solution to the RANS
equations can be computed in the outer region without solving for the flow in the inner
regions. This leads to a faster computation because the expense of computing the solution in
the near-wall regions at each iteration is avoided. Once the solution in the outer region has
been obtained, the solution can be computed in the inner region using the boundary layer
equation, if it is required. However this solution in the inner regions is not always needed.
It is possible to compute friction factors, pressure coefficients and skin friction coefficients
without knowing the full solution in the inner regions.

The mesh in the outer region is completely independent of the inner region. Thus the reso-
lution of the mesh of the outer region is independent of the inner region, which may simplify
mesh generation. Additionally, some geometrical features can be completely removed from
the outer region and included only in the inner regions. This means that these features do not
need to appear in the mesh, which might simplify the generation of a suitable mesh for some
problems. For example, the situation where the ribs in a ribbed channel are included entirely
in the inner region is studied in Chapter 7. A one-dimensional mesh may be required in
the inner region to numerically evaluate integrals, however in some cases analytical solutions
exist. The meshes of the inner and outer regions can be refined until a mesh-independent
solution is found. Therefore the NDD solution is mesh-independent, whereas solutions with
wall functions always depend on the mesh to some extent.

The approach is also appealing because IBCs can, in principle, be computed for all quan-
tities with the same set of procedures. This includes velocities, turbulence model functions
and transported scalars. HRN and LRN turbulence models can be handled with the same
procedures, the only difference is that with a HRN model the interface boundary must be
sufficiently far from the wall such that near-wall damping terms are not needed in the outer
region.

If a LRN turbulence model is used, there is no lower limit on the size of the inner region. As the interface boundary moves closer to the wall, the solution in the outer region approaches the LRN solution. However the computation time also increases since the mesh in the outer region must become more refined. Hence there is a clear trade-off between accuracy and computation time with NDD, which is controlled by the location of the interface boundary. The user is in complete control of this trade-off. There is also a trade-off between accuracy and speed with wall functions. However with wall functions the trade-off is not easy to control, and often the wall function solution cannot ever converge to the LRN solution.

The upper limit on the size of the inner region depends on the fidelity of the physics included in the inner region. For the implementation of NDD discussed in Section 5.1, the upper limit is reached when the boundary layer equations become inaccurate, which occurs in the velocity defect layer (see Section 3.2.4). Conventional wall functions also cease to be valid in this region, although not necessarily at the exact same limit due to the different physics that different wall functions include. The upper limit depends on the Reynolds number and cannot be determined a priori. The more accurate approach of non-local NDD discussed in Section 5.9 can be arbitrarily accurate and there is no upper limit on the size of the inner region.

Since the NDD approach requires only the computation of IBCs, which can be computed with an external routine, the approach can be implemented into any code without making significant modifications. In this thesis, for the first time, the NDD approach with IBCs has been implemented into the industrial CFD code, Code_Saturne. Previously, IBCs had only been implemented for a $k-\varepsilon$ model in an in-house code. In this thesis IBCs have been implemented with the Spalart-Allmaras, $k-\omega$ SST and BL-$\nu^2/k$ models. Particular focus is given in this thesis to the application of the NDD method for the $k-\varepsilon$ and Spalart-Allmaras models. The implementation with the $k-\omega$ SST and BL-$\nu^2/k$ models is given in Appendix C.

In order to compute the IBCs, a boundary layer-type equation is assumed to hold in the inner regions. New notation is used to describe the solution in these regions. Many wall functions in the literature can be expressed using the same formalism as the NDD method. Therefore the derivation of IBCs can be used to generalise the concept of a wall function. This allows NDD and wall functions to be compared at a mathematical level.

This chapter begins by showing how the IBCs required for NDD are calculated. The NDD approach is then compared to other advanced wall functions. Details of the implementation of NDD into Code_Saturne are then given. The chapter ends with a discussion of how non-local terms can be included in NDD to increase the accuracy of the method.
5.1 Derivation of interface boundary conditions

The governing RANS equation for a function \( \Phi \) can usually be written in the form
\[
\frac{\partial (\rho \Phi)}{\partial t} + \nabla \cdot (\rho U \Phi) = \nabla \cdot (\Gamma \nabla \Phi) + F, \tag{5.1}
\]
where \( F \) represents any source terms and the coefficient \( \Gamma \) is
\[
\Gamma \equiv \frac{\mu}{\sigma} + \frac{\mu_t}{\sigma_t}, \tag{5.2}
\]
where \( \sigma \) is the Prandtl number for \( \Phi \) and \( \sigma_t \) is the turbulent Prandtl number for \( \Phi \).

When deriving and implementing IBCs it is useful to introduce some locally one-dimensional coordinates, which are shown in Figure 5.1. In the inner regions, the coordinate \( y \) is normal to the interface. On the interface, \( y = y^* \) and at the wall, \( y = 0 \). The definition of \( y \) means that it can point in different directions in different interfaces. The coordinate \( x \) is perpendicular to \( y \) and in the flow direction. As usual, the \( U \) velocity component is parallel to \( x \) and \( V \) is parallel to \( y \). Quantities evaluated at the wall are denoted with a subscript \( w \), and quantities at the interface are denoted with a superscript \( * \).

With this notation, in the near-wall region, \( 0 \leq y \leq y^* \), Equation (5.1) can be written as
\[
\frac{\partial}{\partial y} \left( \Gamma \frac{\partial \Phi}{\partial y} \right) = R_\Phi(y). \tag{5.3}
\]
For now, it is assumed that the Dirichlet boundary condition \( \Phi = \Phi_w \) is imposed at the wall. Equation (5.3) cannot be solved immediately. However it is possible to use Equation (5.3) to transfer the boundary conditions from the wall to \( y^* \). Equation (5.3) can be integrated from the wall to \( y^* \), which yields
\[
\Gamma^* \frac{\partial \Phi}{\partial y} \bigg|_{y^*} - \Gamma(y) \frac{\partial \Phi}{\partial y} = \int_y^{y^*} R_\Phi(\eta) \, d\eta. \tag{5.4}
\]
Although the diffusive flux at \( y^* \) is not known a priori, an approximation is known on an iteration-by-iteration basis as the solution in the outer region converges. The Dirichlet condition at the wall can be used to perform a second integration to find
\[
\Phi^* = \int_0^{y^*} \frac{\Gamma^*}{\Gamma(y)} \frac{\partial \Phi}{\partial y} \bigg|_{y^*} \, dy - \int_y^{y^*} \int_{\eta}^{y^*} \frac{R_\Phi(\eta)}{\Gamma(y)} \, d\eta \, dy + \Phi_w. \tag{5.5}
\]
This is a Robin boundary condition for \( \Phi \) at \( y^* \). The second term on the right-hand side of Equation (5.5) can be re-written as
\[
\int_0^{y^*} \int_{\eta}^{y^*} \frac{R_\Phi(\xi)}{\Gamma(y)} \, d\xi \, dy = \left( \int_0^{y^*} R_\Phi(y) \, dy \right) \int_0^{y^*} \frac{1}{\Gamma(y)} \left( 1 - \frac{\int_0^{y} R_\Phi(\xi) \, d\xi}{\int_0^{y^*} R_\Phi(\xi) \, d\xi} \right) \, dy, \tag{5.6}
\]
so that Equation (5.5) can be expressed in the form used by Utyuzhnikov (2006):

\[
\Phi^* = f_{1,\Phi} \frac{\partial \Phi}{\partial y} \bigg|_{y^*} - \frac{f_{2,\Phi}}{y^*} \int_{0}^{y^*} R_{\Phi}(y) \, dy + \Phi_w,
\]

where

\[
f_{1,\Phi} = \int_{0}^{y^*} \frac{\Gamma_{\Phi}^*}{\Gamma_{\Phi}(y)} \, dy,
\]

and

\[
f_{2,\Phi} = y^* \int_{0}^{y^*} \frac{\Gamma_{\Phi}^*}{\Gamma_{\Phi}(y)} \left( 1 - \frac{\int_{0}^{y} R_{\Phi}(\xi) \, d\xi}{\int_{0}^{y^*} R_{\Phi}(\xi) \, d\xi} \right) \, dy.
\]

For brevity, it is often useful to re-write the Robin boundary condition in Equation (5.7) more compactly as

\[
\Phi^* = f_{1,\Phi} \frac{\partial \Phi}{\partial y} \bigg|_{y^*} + \tilde{f}_{2,\Phi},
\]

with

\[
\tilde{f}_{2,\Phi} = -\frac{f_{2,\Phi}}{y^* \Gamma_{\Phi}^*} \int_{0}^{y^*} R_{\Phi}(y) \, dy + \Phi_w.
\]

Equation (5.10) is the equation that is used to transfer the boundary conditions from the wall to the interface at \( y^* \). A sufficiently accurate profile for \( \mu_t(y) \) in the inner regions is required as well as an approximation of \( R_{\Phi}(y) \). The profiles of \( \mu_t \) used in this project are introduced in Section 5.4. The full form of the right hand side, \( R_{\Phi}(y) \), contains wall-parallel diffusion, the convection terms and any source terms. In many situations, it is sufficiently accurate to ignore wall-parallel diffusion and convection in the inner region (Craft et al., 2002; Knopp et al., 2006; Popovac and Hanjalić, 2007). This approximation is made in this project, which means that the form of \( R_{\Phi} \) for the \( U \) velocity component is \( R_U(y) = \partial_x P \), which is the streamwise pressure gradient. A further approximation is made, which is also made by Utyuzhnikov (2006), which is to assert that \( \partial_x P \) does not vary in the inner region so that the final form of \( R_U(y) \) used in this project, unless stated otherwise, is \( R_U = \partial_x P^* \), which is known on an iteration-by-iteration basis as the solution in the outer region converges. However, convection and wall-parallel diffusion need not be neglected. The reason that these terms are often neglected in this project is that there is no method implemented in \texttt{Code Satanne} to compute them at the required faces on three-dimensional, unstructured meshes. In addition, accurate-enough results were obtained without including these terms, except for some flows in Chapter 7, where these terms are included. Other solvers may have more advanced interpolation techniques already implemented, which will allow convection and wall-parallel diffusion to be included straightforwardly. In contrast, conventional wall functions such as the SWF always require that \( R_{\Phi} = 0 \). For other equations, such as those for turbulence model functions, a more sophisticated treatment of \( R_{\Phi}(y) \) is required. A discussion of how turbulence model functions are treated can be found in Section 5.6.
Information must be sent between the computational mesh and the subroutine that computes $f_1$ and $\tilde{f}_2$. This information exchange is depicted in Figure 5.2 for a case with two inner regions. The Robin boundary condition in Equation (5.10) links the inner and outer regions at every boundary face. For example, for the $U$ velocity component, the inputs from the computational mesh are $U$ at the boundary face and $U$ at the cell centre. Two values of $U$ are required so that the gradient $\partial_y U$ at the interface can be approximated. Values of $f_{1,U}$ and $\tilde{f}_{2,U}$ come from the inner region and are computed using information such as $\nabla P$ and $\mu_t$ from the computational mesh. This allows the boundary condition on $U$ to be determined, as will be explained in Section 5.8.2. At the next iteration, an updated value of $\nabla P$ and $\mu_t$ is sent to the inner region, which allows updated values of $f_{1,U}$ and $\tilde{f}_{2,U}$ to be computed. These are used along with the updated values of $U$ in the computational mesh to advance the solution to the next time step once more.

**Calculation of the wall shear stress**

The wall shear stress is often required as an output from a simulation. It can be calculated immediately from Equation (5.4) as

$$\tau_w = \mu \frac{\partial U}{\partial y} = \Gamma^*_U \left( \frac{U^* - \tilde{f}_2}{f_1} \right) - \int_0^{y^*} R_U(y) dy. \quad (5.12)$$

**Calculation of the bulk velocity or temperature**

Engineering applications often require the mass flow rate, $\dot{m}$, or the bulk temperature, $T_b$. In order to calculate these, the integral of the velocity or temperature across a surface of the flow domain is needed. This surface includes the inner regions. Conventional wall functions often treat the velocity in the near-wall cell as a constant and the mass flow rate is calculated accordingly. This piecewise-constant approximation of the velocity profile is inaccurate and
the error is largest in the near-wall regions, especially on the coarse meshes which must be used with wall functions.

With NDD, the full solution, $\Phi(y)$, from $y = 0$ to $y = y^*$ can be calculated at each iteration as

$$\Phi(y) = \int_y^{y^*} \frac{\Gamma_{\Phi}(\xi)}{\Gamma_{\Phi}(\xi)} \frac{\partial \Phi}{\partial y} \bigg|_{y^*} \, d\xi - \int_0^y \int_y^{y^*} \frac{R_{\Phi}(\eta)}{\Gamma_{\Phi}(\xi)} \, d\eta \, d\xi. \quad (5.13)$$

The gradient $\frac{\partial \Phi}{\partial y} \bigg|_{y^*}$ is computed at each iteration using the boundary conditions at $y^*$:

$$\frac{\partial \Phi}{\partial y} \bigg|_{y^*} = \frac{\Phi^* - \tilde{f}_{1,\Phi}}{f_{1,\Phi}}. \quad (5.14)$$

With this approach, the integral of $\Phi$ across the inner region can be calculated accurately, even when a coarse mesh is used in the outer region. Thus, $\dot{m}$ or $T_b$ can be calculated accurately.

### 5.2 Pressure boundary conditions

Boundary conditions are required for the pressure on the interface in the outer region. The approach taken in this thesis is to impose a homogeneous Neumann condition $\partial_y P^* = 0$. This is the same as the boundary condition that is usually applied at the wall and is often employed with wall function methods. This boundary condition is robust and becomes more accurate as $y^* \to 0$.

### 5.3 The wall-normal velocity boundary conditions

Many conventional wall functions apply the boundary conditions $V = 0$ and $\partial_y V = 0$ at a wall using a first order finite difference approximation. Even on coarse meshes this does not usually lead to serious errors because $V$ is small in the near-wall regions. However the wall-normal velocity $V$ also obeys an equation of the form of Equation (5.1). Therefore, $V$ can be treated in exactly the same way as $U$, and given IBCs.

Utyuzhnikov (2006) studied an impinging jet flow with NDD. The wall-normal velocity was treated in exactly the same way as the wall-parallel velocity and was given a Robin boundary condition of the same form as Equation (5.10). When implemented in Code_Saturne, the Robin boundary condition on $V$ was found to be numerically unstable on the impinging jet and diffuser flows studied in Sections 6.4 and 6.5. With a Robin boundary condition on $V$, large mass fluxes developed across each interface which led to unphysical situations where more fluid left through the interface boundary than entered through the inlet, and eventually...
led to divergence of the simulation. This problem was not encountered by Utyuzhnikov (2006), whose implementation of IBCs is different to the implementation in Code_Saturne. Utyuzhnikov (2006) included an additional half of a control volume on the wall-side of the interface. This provided an extra cell centre in which to store the pressure. The pressure in these additional nodes could be modified by the pressure correction algorithm to account for the mass flux through the interface.

The implementation of Utyuzhnikov (2006) is difficult to apply in Code_Saturne because significant modifications of the code would be required to introduce the extra row of half-cells. Instead, the pressure in the outer region is given a homogeneous Neumann boundary condition at $y^*$, as stated in Section 5.2. It is the change of implementation that led to the instability of the Robin boundary condition on $V$ in Code_Saturne.

Regardless of its stability, the Robin boundary condition might not be the optimal treatment for $V$. One issue is that the continuity equation is never considered in the derivation of IBCs. Another issue is that if the pressure gradient $\partial_y P$ is assumed constant across the inner region and the Robin boundary conditions is used, then the profile of $V$ will be similar to that of $U$. This will give a non-zero shear stress $\mu \partial_y V$ at the wall, in contrast to the real wall boundary condition, $\partial_y V = 0$, which is known from the continuity equation, as shown in Figure 5.3. Therefore $\partial_y P$ should not be treated as a constant over the inner region.

![Figure 5.3: The profile of $V$ when the Robin boundary condition is used with constant $\nabla P$, compared to the theoretically correct form of the profile.](image)

Because of these issues, a different interface boundary condition must be computed for $V$. Many procedures for calculating this IBC were investigated. A full discussion of these methods is given in Appendix B. The most robust and successful method is described below and is used throughout this thesis, except where stated otherwise.
Equation (5.3) can be solved directly for $V$ with the boundary conditions $V = 0$ and $\partial_y V = 0$ at the wall to find

$$V(y) = \int_0^y \frac{d\xi}{\Gamma_V(\xi)} \int_0^\xi R_V(\eta) d\eta. \quad (5.15)$$

It is now assumed that $R_V(y) = \partial_y P(y)$, where the pressure gradient is unknown. A dynamic pressure term is used such that $P \propto V^2 \propto y^4$, which means that $\partial_y P = 4K y^3$, where $K$ is a constant of proportionality that ensures continuity of $V$. In addition, a term is added to Equation (5.15) to ensure mass is conserved across the interface, if this is necessary. This gives the boundary condition

$$V(y^*) = K \int_0^{y^*} \frac{\xi^4 d\xi}{\Gamma_V(\xi)} - \frac{\dot{m}_S}{\rho S}. \quad (5.16)$$

The constant $K$ is chosen to ensure that the near-interface cell-centre value of $V$ in $\Omega_e$ matches the value of $V$ computed by Equation (5.16) when $y^*$ is replaced with $y^* + \Delta$, where $\Delta$ is the distance from the interface boundary to the cell centre. The surface area of the interface boundary is $S$ and $\dot{m}_S$ is the mass flux leaving through the interface boundary before any correction for continuity is applied, which is computed using the first term on the right hand side of Equation (5.16). For the flows studied in this thesis, the mass flux correction is always small compared to the flux through the any inlets, and has a negligible effect on the wall shear stress and pressure coefficient.

In periodic flows it is essential that the net flux leaving through the interfaces is zero. Therefore the second term in Equation (5.16) is essential. However in some flows, such as the impinging jet studied in Section 6.4, some fluid must leave the domain through the interface boundary. In these cases the second term in Equation (5.16) should not be used.

### 5.4 Computation of the turbulent viscosity

In order to calculate the IBCs, the turbulent viscosity across the inner regions of the flow is required. In some cases, for example if a computation has already been performed, the exact form of $\mu_t$ may be known in advance of the simulation. However in general the turbulent viscosity is not known and a flow-dependent profile must be specified. Many wall functions use simple profiles such as a linear profile or a mixing length hypothesis to facilitate analytical integration. However with NDD, any profile of $\mu_t$ can be used. Four turbulent viscosity profiles have been used in this work and are described below. They are general profiles that can be applied in any flow. The four models all require information from the outer region to calculate $\mu_t(y)$ in the inner region. Hence the turbulent viscosity is updated on an iteration-by-iteration basis in the inner region.
5.4. Computation of the turbulent viscosity

In this section, quantities denoted with a subscript \( I' \) are evaluated at the near-interface cell centre, as shown in Figure 4.1b. This location is further from the wall than \( y^* \).

The piecewise linear profile

The piecewise linear profile has been used by Utyuzhnikov (2005a) and is similar to the one used in the AWF (Gerasimov, 2003). The turbulent viscosity varies linearly from \( \mu_{t,I'} \) at the near-interface cell centre, located at \( y_{I'} \), to 0 at a location \( y_v \), which represents the edge of the viscous sublayer. The expression is (Utyuzhnikov, 2005a)

\[
\mu_t(y) = \max \left( 0, \frac{y - y_v}{y_{I'} - y_v} \mu_{t,I'} \right),
\]

with

\[
y_v = \frac{Re_v \mu}{\rho \sqrt{k_{I'}}},
\]

where

\[
Re_v = \frac{\rho \sqrt{k_{I'} y_v}}{\mu} = 10.8.
\]

With this profile, the turbulent viscosity across the inner and outer regions is continuous everywhere. In particular, at \( y^* \) the value of \( \mu_t \) given by Equation (5.17) is guaranteed to match the value of \( \mu_t \) in the outer region, which is given by the turbulence model. In contrast, with many wall functions, such as the AWF, the value of \( \mu_t \) implied by the wall function does not necessarily match the value of \( \mu_t \) returned by the turbulence model at the centre of the near-wall cell, as depicted in Figure 5.4.

![Figure 5.4: Schematic of the turbulent viscosity profile with NDD compared to with the AWF.](image)

The piecewise linear profile has already been tested with NDD on channel and impinging jet flows (Utyuzhnikov, 2008, 2005a) and a similar profile is known to perform well with the
AWF (Gerasimov, 2003). However, since this profile requires $k/v'$ in order to compute $y_d$, it cannot be used with the Spalart-Allmaras model.

The exponential profile

This profile closely resembles the van Driest damping function (Equation (3.21)) and has been used in LES (Cabot and Moin, 1999; Wang and Moin, 2002). In this work it is called the exponential profile, after the exponential term used to smooth the profile as $y \to 0$. The profile is (Utyuzhnikov, 2012)

$$\mu_t = \mu \kappa y_r^+ \left(1 - \exp\left(-y_r^+ / A^+\right)\right)^2,$$

where $A^+ = 19$. The value of $A^+$ is not rigorously fixed. It was set as $A^+ = 19$ by Cabot (1995) so that the LES results obtained with this model coincided with the log law for a channel flow. Other values have been used in other works, for example Johnson and King (1985) used $A^+ = 15$. Utyuzhnikov (2012) used this profile to apply IBCs on a channel flow and used $A^+ = 19$.

Figure 5.5 is a schematic that shows the difference between the exponential and piecewise linear profiles. The exponential profile returns a smooth variation of the turbulent viscosity all the way to the wall. Since this profile depends only on the wall shear stress via the parameter $y_r^+$, it can be used with any turbulence model. A drawback of this profile is that it yields $\mu_t = 0$ whenever the wall shear stress is zero.
5.4. Computation of the turbulent viscosity

The zero pressure gradient (ZPG) Spalart-Allmaras solution

In a zero pressure gradient (ZPG) boundary layer where $R_U = 0$, Equation (5.3) can be solved exactly with the Spalart-Allmaras model (Allmaras et al., 2012). The solution for $\tilde{\nu}$ is

$$\tilde{\nu} = \kappa u_\tau y. \quad (5.21)$$

Equation (5.21) can be used to compute $\mu_t$ throughout the inner region as

$$\mu_t = \rho \tilde{\nu} \frac{\chi}{\chi^3 + c_{e1}^3}, \quad (5.22)$$

where $\chi = \tilde{\nu}/\nu$. This profile is referred to as the ZPG solution and can be used for any turbulence model, since it depends only on the wall shear stress. However in this work it is only used with the Spalart-Allmaras model. If the Spalart-Allmaras model is used and $R_U = 0$, then the solution with NDD will be exact. Like the exponential profile, in cases where the wall shear stress is zero, Equation (5.21) will give $\mu_t = 0$. This profile yields a form of $\mu_t$ similar to the exponential profile, shown schematically in Figure 5.5.

In Allmaras et al. (2012) it is shown how the velocity itself can be computed from Equation (5.21). However the velocity profile would not be accurate in flows where there are pressure gradients and it would always produce logarithmic behaviour, even in flows where this should not be the case. Therefore it is more accurate to use the viscosity profile in Equation (5.21) and use IBCs to include the effect of source terms on the velocity than it is to use the velocity profile in Allmaras et al. (2012) directly. It is found in this thesis that the ZPG profile can be used in flows with pressure gradients without degrading the accuracy of the solution.

The profile of Duprat et al. (2011)

Duprat et al. (2011) modified the van Driest damping function to take into account the stream-wise pressure gradient, in order to improve the accuracy of the profile in regions of flow separation. The profile is (Duprat et al., 2011)

$$\mu_t(\xi) = \mu \kappa \xi^* \left[ \alpha + \xi^* (1 - \alpha)^{3/2} \right] \beta \left( 1 - \exp \left( \frac{-\xi^*}{1 + A\alpha^3} \right) \right)^2. \quad (5.23)$$

where $\xi^* = y u_{\tau p}/\nu$, $u_{\tau p} = \sqrt{u_t^2 + u_p^2}$, $u_\tau = \sqrt{\tau_w/\rho}$, $u_p = |\mu \partial_x P^*/\rho^{1/3}|$ and $\alpha = u_t^2/u_{\tau p}^2$.

To avoid ambiguity, the profile has been written in terms of $\xi$ instead of $y$ to distinguish $\xi^*$ from the NDD parameter $y^*$. The parameter $\alpha$ is zero if the shear stress is locally zero, and unity if the pressure gradient is locally zero. For $\alpha = 1$, the damping terms take the form $1 - e^{-\xi^*/18}$, which is similar to van Driest damping function. The parameters $A$ and $\beta$ come
from consideration of DNS data and the asymptotic behaviour of $\mu_t$ at the wall. They are given the values $A = 17$ and $\beta = 0.78$. Duprat et al. (2011) used this profile in an LES of flow over periodic hills and showed that it is capable of capturing the effects of flow separation.

This profile is useful because it can predict a non-zero turbulent viscosity at separation points, unlike the ZPG and exponential profiles. It can be used with any turbulence model since it depends only on the wall shear stress and the pressure gradient. Due to their similar forms, the Duprat et al. (2011) and exponential profiles yield similar profiles of $\mu_t$.

**Other options**

With any approximation for the turbulent viscosity in the inner region, a full set of boundary conditions can be computed at $y^*$. With these boundary conditions, Equation (5.3) can be solved over the inner region. The solution could then be used to compute the turbulent viscosity in the inner region, using the formula given by the turbulence model. For example, with a $k-\varepsilon$ equation, $k$ and $\varepsilon$ can be computed across the inner region and then the turbulent viscosity could be computed as $\mu_t = f_\mu c_k k^2/\varepsilon$. This approach is similar to that taken with the NWF (Gant, 2002).

This approach has not been taken in this project for two reasons. Firstly, the simpler approach of using an algebraic profile is shown to give accurate enough results in this thesis. Secondly, solving a differential equation (Equation (5.3)) at each boundary face at each iteration would increase the time taken per time step to close to that of a LRN computation (Gant, 2002). It would also increase the storage requirements of the method. As discussed in Gant (2002), if a differential equation were solved for each boundary face at each iteration in a steady state calculation, then the total computation time would still be lower than a LRN computation because the independence of the inner and outer regions means the overall solution converges more quickly. However, implementation of this approach would be complex in an unstructured code for only a small improvement in accuracy and possible reductions in numerical stability.

**5.5 IBCs for passive scalars**

In the inner regions, passive scalars obey governing equations with the same form as Equation (5.3). In this thesis, passive scalars obey either Dirichlet or Neumann boundary conditions at the wall. The treatment of these two types of boundary conditions with NDD is outlined in this section.
5.5.1 Dirichlet boundary condition at the wall

If the scalar obeys a Dirichlet boundary condition at the wall, then the situation is analogous to the velocity boundary conditions. The same procedure is followed and the appropriate boundary condition is

\[ \Phi^* = f_{1,\Phi} \frac{\partial \Phi}{\partial y} \bigg|_{y^*} + f_{2,\Phi}, \]  

(5.24)

where \( f_{1,\Phi} \) and \( f_{2,\Phi} \) are calculated as in Equations (5.8) and (5.9), with the appropriate Prandtl number and source term. The profile of the scalar across the inner region can be calculated using Equation (5.13).

5.5.2 Neumann condition at the wall

With a Neumann boundary condition at the wall, Equation (5.3) can be integrated and the diffusive flux at the wall, \( \dot{q}''_{w} \), can be used to find

\[ \Gamma_{\Phi} \frac{\partial \Phi}{\partial y} \bigg|_{y^*} = \dot{q}''_{w} + \int_{0}^{y^*} R_{\Phi}(\xi) d\xi. \]  

(5.25)

This Neumann condition is the boundary condition that is applied at \( y^* \) with NDD.

The value of the scalar itself can be calculated in the inner region by integrating Equation (5.25) once more to find

\[ \Phi(y) = \Phi^* - \int_{y}^{y^*} \frac{\dot{q}''_{w}}{\Gamma_{\Phi}(\xi)} d\xi - \int_{y}^{y^*} \frac{\int_{0}^{y} R_{\Phi}(\eta) d\eta}{\Gamma_{\Phi}(\xi)} d\xi. \]  

(5.26)

5.6 IBCs for turbulence models

Turbulence model equations often contain non-linear terms which are important in the inner regions. These must be included in the computation of IBCs for turbulence model functions. IBCs have been applied to four turbulence models in this project. The implementation for the \( k - \varepsilon \) and Spalart-Allmaras models is given below. The implementation for the \( k - \omega \) SST and BL-\( \nu^2/k \) models is given in Appendix C.

In this thesis NDD has only been implemented for the HRN \( k - \varepsilon \) model, since there is no LRN \( k - \varepsilon \) model available in Code_Saturne version 3.0.5. The LRN \( k - \varepsilon \) model of Chien (1982) was implemented as part of the project, however it suffered from numerical instabilities in two-dimensional flows and consequently was not taken forward for development.
5.6.1 IBCs for the $k - \varepsilon$ model

In the boundary layer, where convection and wall-parallel diffusion are ignored, the $k$ equation can be written in the form of Equation (5.3) as

$$\frac{\partial}{\partial y} \left( \Gamma_k \frac{\partial k}{\partial y} \right) = -\rho P + \rho \varepsilon. \quad (5.27)$$

Therefore all the results of Section 5.1 can be used with

$$R_k = -\rho P + \rho \varepsilon. \quad (5.28)$$

Figure 5.6 shows $P$ and $\varepsilon$ in a channel flow with half-height $h$ at $Re_\tau = 590$ according to the DNS data of Moser et al. (1999). Both vary significantly for $y^+ < 50$, which is the region over which a wall function would normally be applied. Hence, $R_k$ is expected to vary significantly in the inner region.

![Figure 5.6: $P$ and $\varepsilon$ in a channel flow with half-height $h$ at $Re_\tau = 590$, according to the DNS data of Moser et al. (1999).](image)

In the inner region, the production is calculated as

$$\rho P = -\rho \mu \frac{\partial U}{\partial y} = \mu_t \left( \frac{\partial U}{\partial y} \right)^2. \quad (5.29)$$

The velocity derivative can be computed with Equation (5.4) by taking $\partial_y U^*$ from the Robin boundary condition:

$$\frac{\partial U}{\partial y} = \frac{\Gamma_U^*}{\Gamma_U(y) f_{1,U}} \left( U^* - \tilde{f}_{2,U} \right) - \int_{y^*}^{y} \frac{R_U(x) d\xi}{\Gamma_U(y)}. \quad (5.30)$$

The dissipation is computed as it is in the AWF (Gerasimov, 2003; Utyuzhnikov, 2006), with
the expression
\[ \varepsilon(y) = \frac{(k_I')^{3/2}}{c_1 \max(y, y_d)}, \tag{5.31} \]
where \( y_d = 2c_\mu/(\rho \sqrt{k_I'}) \). Equation (5.31) is used to impose a Dirichlet boundary condition on \( \varepsilon \) at the interface. For \( y^* > y_d \) and \( y > y_d \) the dissipation varies inversely with distance from the wall, which is consistent with many wall functions in the logarithmic region of the boundary layer (Craft et al., 2002). For \( y^* > y_d \) and \( y < y_d \) the dissipation is constant and equal to the wall-limiting value \( 2\mu k_I'/(\rho y_d^2) \). The location \( y_d \) is in the viscous sublayer (Craft et al., 2002), which means that if \( y^* < y_d \) then the interface is located in the viscous sublayer and a LRN turbulence model should be used with a modified profile of \( \varepsilon \) (Utyuzhnikov, 2012).

However for every flow in this thesis, the condition \( y^* > y_d \) is always satisfied.

In principle IBCs could also be calculated for \( \varepsilon \), however this reduces the numerical stability of the approach. In addition, Equation (5.31) is a well-established and widely used formula that eliminates the need to couple the \( k \) and \( \varepsilon \) equations. It has also been shown to be reliable and sufficiently accurate for use in a near-wall model (Craft et al., 2002; Utyuzhnikov, 2006).

The IBCs for \( k \) and \( \varepsilon \) do not guarantee that the implied value of the turbulent viscosity in the inner region, \( c_\mu k^2/\varepsilon \), matches that predicted by the turbulent viscosity profile. The piecewise linear viscosity profile is scaled such that it is always continuous at \( y^* \), however the exponential and Duprat et al. (2011) profiles may not yield a continuous turbulent viscosity at the interface. Hence there is a potential inconsistency in the interface boundary conditions. This inconsistency could be removed by modifying one of \( k \), \( \varepsilon \) or \( \mu_t \). For example, Utyuzhnikov (2012), computed the boundary conditions on \( k \) at the interface as \( k^* = (\mu_t^* \varepsilon^*/c_\mu)^{1/2} \). However the inconsistency is intentionally included in this thesis because it has been observed to improve the results. Many of the profiles used in this thesis have been taken from academic literature and have been refined over a number of years to yield accurate results on a number of flows. Therefore it is not surprising that they yield accurate results in this thesis. In addition, similar inconsistencies exist in many wall functions, including those of Craft et al. (2002), Gant (2002), Popovac and Hanjalić (2007) and wall functions based on the log law. Thus, the inconsistency is neither unusual nor problematic and does not pose any particular problem because the profiles for \( \mu_t(y) \) and \( \varepsilon(y) \) are only models.

5.6.2 IBCs for the Spalart-Allmaras model

The definition of \( \mu_t \) for the Spalart-Allmaras model is \( \mu_t = \rho \bar{\nu} f_{\mu_1} \). Hence \( \bar{\nu} \) can be computed from the profile of \( \mu_t \) and imposed with a Dirichlet boundary condition at the interface.
writing $\mu_t$ explicitly in terms of $\tilde{\nu}$

$$\mu_t = \frac{\rho \tilde{\nu}}{\left( \frac{\rho}{\tilde{\nu}} \right)^3 + c_{\nu1}^3}, \quad (5.32)$$

it is clear that the process of calculating $\mu_t$ from $\tilde{\nu}$ must be iterative. A fixed point iteration method is used in which successive values of $\tilde{\nu}$ are generated by the function

$$\tilde{\nu}_{i+1} = A(\tilde{\nu}_i) = \frac{\mu}{\rho} \left( \frac{\mu_t}{\rho} \frac{\tilde{\nu}_i^3}{\rho} + c_{\nu1}^3 \right)^{1/3}. \quad (5.33)$$

The procedure is initialised with $\tilde{\nu}_0 = \mu_t / \rho$. The function $A(\tilde{\nu}_i)$ is plotted in Figure 5.7 for $\mu = 0.01$, $\mu_t = 0.2$ and $\rho = 1$.

![Figure 5.7: A plot of $A(\tilde{\nu}_i)$, for $\mu = 0.01$, $\mu_t = 0.2$ and $\rho = 1.$](image)

Since $\tilde{\nu}$ is computed from the turbulent viscosity profile, there will never be any inconsistency between the value of $\mu_t$ implied by the turbulence model and the value of $\mu_t$ given by the turbulent viscosity profile.

**Modification of the wall distance calculation**

The Spalart-Allmaras model equations depend on the distance from the wall, $d$. The computation of this distance must be modified with NDD in order to account for the offset between the wall and the interface boundary. By default *Code_Saturne* computes $d$ as (Tucker, 1998)

$$d = -|\nabla \Psi| + (\nabla \Psi \cdot \nabla \Psi + 2\Psi)^{1/2}, \quad (5.34)$$
where $\Psi$ obeys the Poisson equation
\[ \nabla^2 \Psi = -1, \quad (5.35) \]
with $\Psi = 0$ at the walls and $\partial_n \Psi = 0$ at every other boundary face.

The most accurate way to compute $d$ for a simulation with NDD is to compute it using the above procedure on a mesh of the entire computational domain and then interpolate the solution onto the mesh of the outer domain. However this process would require generating another mesh and is therefore undesirable. It is more appealing to compute $d$ with a mesh of the outer region only, which can be done with the following procedure.

From Equation (5.34) it follows that
\[ \nabla \Psi \cdot \nabla \Psi + 2\Psi = d^2 + 2|\nabla \Psi| d + |\nabla \Psi|^2. \quad (5.36) \]
It is then assumed that near the wall, $\Psi$ is one-dimensional so that $\nabla \Psi = \partial_n \Psi > 0$, and hence the gradient of $\Psi$ is
\[ \nabla \Psi = \frac{\Psi}{d} - \frac{d}{2}. \quad (5.37) \]
As explained in Section 4.5, the gradient is approximated as $\partial_n \Psi = (\Psi_{I'} - \Psi^*)/\Delta$ at the interface boundary. This allows the following Dirichlet boundary condition to be imposed on $\Psi$ at $y^*$:
\[ \Psi^* = \frac{y^*}{2(1 + y^*/\Delta)} + \frac{\Psi_{I'} y^*}{\Delta (1 + y^*/\Delta)}, \quad (5.38) \]
which means that $d$ can be computed using Equation (5.34) even in computations with NDD.

### 5.7 Comparison of NDD with wall functions

The approach outlined above is a non-overlapping domain decomposition method and is different to conventional wall functions. Conventional wall functions usually calculate average quantities at the centre of the near-wall cell of a coarse mesh. This means that not only must the mesh extend to the wall, but it must also be coarse over multiple cells extending from the wall. Normally the cell size expansion ratio should be limited to approximately 1.2 to ensure that the interpolation of functions between cells is accurate. Although this limitation is still present when NDD is used, the mesh in the outer region is independent of the mesh in the inner region. This means that there can be an effective jump in cell size at the interface boundary.

The NDD method also allows a more sophisticated treatment of turbulence model functions than conventional wall functions. For example, the full variation of the production and dissipation...
pation in the inner region can be included in the computation of the $k$ boundary conditions. Few wall functions are able to incorporate this information.

Many of the assumptions that are used to derive IBCs are also used to derive the AWF and NWF. The similarities and differences between the methods are discussed below.

1. In order to allow analytical integration with the AWF, the pressure gradient and convection terms are assumed to be constant over the near-wall cell (Gerasimov, 2003). These restrictions are unnecessary with NDD. In theory, any variation can be accounted for in the form of $R_U$. However in this project the pressure gradient is assumed constant in the near-wall region for the wall-parallel velocity component, except when non-local NDD is used (see Section 5.9).

2. The piecewise linear turbulent viscosity profile in Equation (3.73) is necessary with the AWF to facilitate analytical integration. However, any profile of $\mu_t(y)$ can be used with NDD because numerical integration is used. There is no need to specify a turbulent viscosity profile with the NWF; the turbulent viscosity is computed from the RANS governing equations in the wall function mesh. In principle this approach could be taken with NDD, however it has not been taken in this work because it would increase the complexity of the approach and the computation time (Gant, 2002). In addition, the results with a profile of $\mu_t$ have been found in this project to be accurate enough. The different turbulent viscosity profiles are compared in Chapter 6 to assess their performance.

3. IBCs can be extended to finite difference or finite element schemes without any modification of their calculation. In fact, they can be computed by a separate routine, which makes it straightforward to transfer the routines for calculating IBCs between different CFD codes. Implementation of IBCs amounts to merely modifying the boundary conditions at the interface boundaries in a mesh. In contrast, the implementation of many wall functions, including the AWF or NWF, affects the discretisation in the near-wall cell, which must be modified to suit the particular code that they are implemented into (Utyuzhnikov, 2008).

4. Unlike the AWF and NWF, the steps required to extend NDD to any turbulence model are clear. In particular, it is possible to apply the NDD method to LES.

5. The NWF treats all functions in the same manner in the near-wall cell, with the exception of the wall-normal velocity. In contrast, while the AWF computes an analytical profile for $U$, the $k$ equation is not integrated; instead cell-average values of the production and dissipation term are computed. With NDD, the same approach can be applied to most unknown functions, including both $U$ and $k$, with the same procedure.
The exceptions are the wall-normal velocity and some turbulence model functions.

6. For buoyant flows, the variation of molecular viscosity with temperature in the viscous sublayer can significantly affect a flow. The developers of the AWF initially sought to model the variation of $\mu$ across the sublayer with a linear profile. However such a profile introduces a singularity into the equations, and stable numerical solutions cannot be obtained (Craft et al., 2002). Instead, a parabolic or hyperbolic variation is used (Gerasimov, 2003). Thus, the AWF does not always accommodate linear interpolation of fluid properties. Such a problem would not be encountered with NDD because no differentiation is performed in the sublayer. Lack of smoothness of $\mu$ would pose no problems (Utyuzhnikov, 2008).

7. Because they are based on similar mathematical equations, there is an analogous expression for Equation (5.10) for the AWF at the centre of the first near-wall cell. This expression can be written heuristically for $U$ as

$$U^{*(n+1)} = f_{1,U} \left. \frac{\partial U}{\partial y} \right|_{y^*}^{(n)} + \tilde{f}_{2,U}, \quad (5.39)$$

where the superscript refers to the time step. The AWF updates the velocity using the derivative from the previous iteration. With the Robin boundary condition used in NDD, the velocity and its derivative can be evaluated at the same time step. This leads to faster convergence since the leading term in Equation (5.39) is the derivative (Utyuzhnikov, 2008).

8. The solution obtained with either the AWF, NWF or NDD will inevitably have some sensitivity to $y^*$ (either the near-wall cell size or location of the interface boundary). However with NDD the meshes in the inner and outer regions can be arbitrarily fine, which means that the solution can be made independent of the mesh, such that it depends exclusively on $y^*$. Mesh independence is attained regardless of the accuracy of the solution. In contrast, with the NWF and AWF, due to constraints on the cell size expansion ratio, it is not always possible to refine the mesh in the outer region (here defined as the cells beyond the near-wall cell), without modifying the size of the near-wall cell itself. Thus with the AWF or NWF, the solution depends on both $y^*$ and the mesh of the outer region.

9. With NDD, $y^*$ is a parameter and can be varied independently of the mesh of the outer region. Thus, in serial calculations, which may be performed as part of a design optimisation, simulations can be performed for different $y^*$ and different input data on the same mesh. In such a situation a solution for a previous design can be used as an initial approximation for the next design. With wall functions, any change of geometry
analogous to changing $y^*$ inevitably requires a change of the mesh. Previous solutions could still be used to initialise the next design, but this would require interpolation.

5.8 Numerical implementation

Some notes on the implementation of NDD are given in this section. The implementation of NDD in Code_Saturne is also outlined.

5.8.1 Maintaining stability of $k$

1. In poorly initialised simulations, $k$ can be slow to converge or even become negative at some iterations. One way to ameliorate this issue is to impose a Dirichlet boundary condition on $k$ at the beginning of a simulation. A suitable Dirichlet boundary condition can be calculated from the turbulent viscosity profile as

$$k^* = \sqrt{\frac{\mu^t \varepsilon^*}{\rho c\mu}}. \quad (5.40)$$

This boundary condition can be changed to the Robin boundary condition after a few iterations.

2. To reduce the likelihood of divergence of the simulation, it is sometimes useful to introduce $\tilde{f}_{2,k}$ slowly, over a few iterations, for the $k$ boundary conditions. A variable $\alpha$ can be introduced, which is zero at the beginning of a simulation and tends to unity after a few iterations, such that the boundary condition in Equation (5.10) for $k$ becomes

$$k^* = f_{1,k} \frac{\partial k}{\partial y} \bigg|_{y^*} + \alpha \tilde{f}_{2,k}. \quad (5.41)$$

3. Whereas $f_{1,k}$ is always positive, $\tilde{f}_{2,k}$ can become negative in regions where $\varepsilon > \mathcal{P}$. The gradient of $k$ itself varies significantly in the near-wall region and is often negative. Hence Equation (5.10) can sometimes imply a negative value of $k$ if the solution is far from convergence. This is most likely to occur at the beginning of a poorly initialised simulation. When this happens, Equation (5.10) can be rewritten in a way that ensures positivity of $k$ by using the value of $k$ from the previous iteration, $k^{(n)}$ as (Utyuzhnikov, 2008).

$$k^{(n+1)} = f_{1,k} \frac{\partial k^{(n+1)}}{\partial y} + \tilde{f}_{2,k} \frac{k^{(n+1)}}{k^{(n)}}, \quad (5.42)$$

which rearranges to

$$k^{(n+1)} = \frac{f_{1,k}}{1 - \tilde{f}_{2,k}/k^{(n)} \frac{\partial k^{(n+1)}}{\partial y}} > 0. \quad (5.43)$$
5.8. Numerical implementation

This correction is only required if Equation (5.10) yields $k^{(n+1)} < 0$.

5.8.2 Implementation of NDD into CodeSaturne

There are many possible ways to implement the Robin boundary conditions used in NDD in CodeSaturne. The most suitable method should be accurate and convergent and require a minimum of superfluous calculations. The method used in this thesis to implement Robin type boundary conditions is described in detail below for the velocity, $U$. Other variables, such as turbulence model functions, are scalars and therefore the treatment is simpler since no coordinate transformation is required. The geometry referred to is shown in Figure 5.8a and the local coordinates used are shown in Figure 5.8b.

Although the velocity is three-dimensional, the treatment of the near-wall velocity requires only a two-dimensional treatment. The velocity at $I'$ is split into interface-parallel and interface-normal components using the interface-parallel vector, $t$, and the interface-normal vector, $n$, defined in Section 4.5.1. For convenience, the interface-parallel velocity is referred to as $U$ and the interface-normal velocity is referred to as $V$. The Cartesian velocity components in the global coordinate system are written in this section as $U' = (U', V', W')^T$.

The velocity in the local coordinate system is

$$U = U' \cdot t, \quad V = U' \cdot n. \quad (5.44)$$

and the pressure gradient is also split into interface-parallel and interface-normal components

$$\partial_t P = t \cdot \nabla P = t_{x'} \partial_{x'} P, \quad \partial_n P = n \cdot \nabla P = n_{x'} \partial_{x'} P, \quad (5.45)$$

so that $\partial_t P$ applies to the $U$ equation, and $\partial_n P$ applies to the $V$ equation.

The gradient of $U$ at the interface boundary is written with a first order finite difference approximation,

$$\left. \frac{\partial U}{\partial n} \right|_{\ast} = \frac{U'_{\ast} - U_{\ast}}{\Delta}, \quad (5.46)$$

which allows Equation (5.10) to be approximated for $U$ as

$$U_{\ast} = f_{1, U} \frac{U'_{\ast} - U_{\ast}}{\Delta} + \tilde{f}_{2, U}, \quad (5.47)$$

which rearranges to

$$U_{\ast} = \frac{f_{1, U} U'}{\Delta} + \frac{\Delta \tilde{f}_{2, U}}{f_{1, U}}. \quad (5.48)$$

The interface-normal velocity is given a Dirichlet boundary condition from Equation (5.16).
Chapter 5. Near-wall domain decomposition

Figure 5.8: The geometry and coordinates used to impose IBCs.

Thus, the boundary conditions for the velocity in the form required by Code_Saturne are

\[ A_U = \frac{\hat{f}_{2,U} t}{1 + \hat{f}_{1,U}/\Delta} + V_F n, \quad B_U = \frac{1}{1 + \Delta/\hat{f}_{1,U}} M, \]

for the gradient boundary conditions, where \( M \) is defined in Equation (4.54), and

\[ A_{U,f} = -\chi_U (U^* t + V^* n), \quad B_{U,f} = \chi_U (M + nn^T), \]

for the flux boundary conditions.

5.9 NDD with non-local IBCs

The formulation of NDD using Equation (5.3) assumes that in the inner region, the governing RANS equation is one-dimensional so that direct integration with respect to \( y \) is possible. In many boundary layers this is a good approximation, since the boundary layer is dominated by the shear in the wall-normal direction. However, this approximation is not accurate in every case. Sometimes it may be necessary to use a multidimensional governing equation in the inner region. It is possible to compute interface boundary conditions using a multidimensional equation with the approach of Utyuzhnikov (2009). The resulting IBCs include non-local effects, hence the approach is referred to as NDD with non-local IBCs (NLIBCs). In this thesis, any non-local IBCs are always referred to as NLIBCs so that the term IBCs refers exclusively to boundary conditions computed with the one-dimensional governing equation in Equation (5.3). Only Section 7.3.3 and Appendix D contain results with NLIBCs. All other results with NDD in this thesis have been computed using the one-dimensional formulation.
of NDD, with the boundary condition in Equation (5.10).

The approach of Utyuzhnikov (2009) involves the calculation of a set of auxiliary functions. These auxiliary functions are the solutions to partial differential equations with special source terms and special boundary conditions at the interface. They can be computed in advance of the solution in the outer region, or simultaneously with it. If the auxiliary functions are computed simultaneously with the outer region, the convergence and stability of computations with NLIBCs are similar to those with IBCs. If the auxiliary functions are computed in advance of the solution in the outer region, then the convergence is enhanced and NLIBCs are more stable than IBCs.

In one-dimensional flows, IBCs and NLIBCs are the same. However in a multidimensional case, NLIBCs are more accurate. In this section, the underlying theory of NDD with NLIBCs and the procedure used to compute NLIBCs are explained.

5.9.1 Notation

New notation is introduced for this section since the geometry of the inner region has more relevance than before. The full computational domain is referred to as $\Omega$ and its boundary is $\gamma \equiv \partial \Omega$. Domain walls are denoted $\gamma_w$ and are the parts of the boundary of $\Omega$ where wall boundary conditions are required. The domain is split into $N$ inner regions, each denoted $\Omega_i$ with $i = 1, \ldots, N$, and a single outer region, $\Omega_e$ such that

$$\Omega = \bigcup_{i=1}^{N} \Omega_i \cup \Omega_e \quad (5.51)$$

The equation to be solved in $\Omega$ for each function $\Phi$ is Equation (5.1) with $\Phi = \Phi_w$ on $\gamma_w$.

The governing equation can be written more concisely in terms of a non-linear operator $L$ as

$$L\Phi = \tilde{f}, \quad (5.52)$$

where $\tilde{f}$ contains any source terms (for the velocity, $\tilde{f}$ is a vector with $\tilde{f}_i = -\partial_i P$), and

$$L\Phi \equiv \frac{\partial (\rho \Phi)}{\partial t} + \nabla \cdot (\rho U \Phi) - \nabla \cdot (\Gamma \nabla \Phi). \quad (5.53)$$

To proceed with the derivation of NLIBCs, the governing equation is written again in terms of a linear operator $L$

$$L\Phi = f, \quad (5.54)$$

where

$$L\Phi \equiv \nabla \cdot (\Gamma \Phi \nabla \Phi), \quad (5.55)$$
and \( f \) is a new source term which comprises \( \tilde{f} \), the time derivative and the convection terms:

\[
f = \frac{\partial (\rho \Phi)}{\partial t} + \nabla \cdot (\rho U \Phi) - \tilde{f}.
\]  

(5.56)

The interface between \( \Omega_e \) and \( \Omega_i \) is denoted \( \Upsilon_i \):

\[
\Upsilon_i = \partial \Omega_e \cap \partial \Omega_i,
\]  

(5.57)

and the full interface, denoted \( \Upsilon \), is the union of the \( \Upsilon_i \),

\[
\Upsilon = \bigcup_{i=1}^{N} \Upsilon_i = \partial \Omega_e \cap \bigcup_{i=1}^{N} \partial \Omega_i.
\]  

(5.58)

It is \( \Upsilon \) upon which NLIBCs are imposed. The rest of the boundary of \( \Omega_e \) is denoted, \( \gamma_e \), where \( \gamma_e = \partial \Omega_e \setminus \Upsilon \). The boundary conditions on \( \gamma_e \) are unaffected by NDD. The parts of the boundary of each \( \Omega_i \) that are walls are denoted \( \gamma_{w,i} \), where

\[
\gamma_{w,i} = \gamma_w \cap \partial \Omega_i.
\]  

(5.59)

The remaining part of the boundary of each \( \Omega_i \) that is neither the wall nor an interface is denoted \( \gamma_{o,i} \), where

\[
\gamma_{o,i} = \partial \Omega_i \setminus (\Upsilon_i \cup \gamma_{w,i}).
\]  

(5.60)

These could be, for example, symmetry, periodic, inlet or outlet boundaries. The meanings of the definitions in this section are shown for an example geometry in Figure 5.9. The coordinates \( y \) and \( x \) within each inner region are defined with respect to the interface boundary in the same way as in Section 5.1.

![Figure 5.9: The notation used with NDD for NLIBCs on an example geometry.](image-url)
5.9. NDD with non-local IBCs

5.9.2 Computation of NLIBCs

Equation (5.54) cannot be solved immediately because the boundary conditions at the interface are not known in advance of the simulation. However, because the operator $L$ is linear, the principle of superposition can be used to build the solution to a general problem in terms of solutions to a set of simplified problems. Hence to proceed, a set of auxiliary problems are solved in each $\Omega_i$. Two sets of functions are obtained, $W_{i,\alpha}(x)$ and $W^e_{i,\alpha}(x)$, which obey the equations (Utyuzhnikov, 2009)

\[
LW_{i,\alpha} = 0, \quad (5.61) \\
LW^e_{i,\alpha} = v_{i,\alpha}(x), \quad (5.65)
\]

\[
l_y W_{i,\alpha} \mid_{\gamma_{w,i}} = 0, \quad (5.62) \\
l_y W^e_{i,\alpha} \mid_{\gamma_{w,i}} = 0, \quad (5.66)
\]

\[
l_x W_{i,\alpha} \mid_{\gamma_{o,i}} = 0, \quad (5.63) \\
l_x W^e_{i,\alpha} \mid_{\gamma_{o,i}} = 0, \quad (5.67)
\]

\[
W_{i,\alpha} \mid_{\gamma_i} = u_{i,\alpha}(x'), \quad (5.64) \\
W^e_{i,\alpha} \mid_{\gamma_i} = 0, \quad (5.68)
\]

where $x \in \Omega_i \subset \mathbb{R}^m$, $m \in \mathbb{N}$, $x' \in \gamma_i \subset \mathbb{R}^n$, $n = m - 1$ and $\alpha$ is a counting variable.

The boundary conditions on $\gamma_{w,i}$ and $\gamma_{o,i}$ are determined by the linear operators $l_y$ and $l_x$, respectively. The basis functions $u_{i,\alpha}$ are defined on the interface. They are chosen such that, in $\Omega_i$, the restriction of $\Phi$ to $\gamma_i$ can be written

\[
\Phi(x) \mid_{\gamma_i} = \sum_{\alpha=0}^{N} u_{\alpha} u_{i,\alpha}(x'), \quad (5.69)
\]

for some coefficients $u_{\alpha}$. The other basis functions, $v_{i,\alpha}$, are defined throughout $\Omega_i$ and are chosen such that, in $\Omega_i$, $f(x)$ can be written

\[
f(x) = \sum_{\alpha=0}^{N} r_{\alpha} v_{i,\alpha}(x), \quad (5.70)
\]

for some coefficients $r_{\alpha}$.

Equations (5.69) and (5.70) indicate that the set of functions $\{W_{i,\alpha}\}$ ensures continuity of $\Phi$ at the interface and the set $\{W^e_{i,\alpha}\}$ ensures that the source terms in $\Omega_i$ are equal to $f$. The functions $\{W_{i,\alpha}\}$ and $\{W^e_{i,\alpha}\}$ depend only on the geometry of $\Omega_i$ and $\mu_t$.

If the dependence on $\mu_t$ is weak enough that $\{W_{i,\alpha}\}$ and $\{W^e_{i,\alpha}\}$ can be treated as purely geometrical functions then $\{W_{i,\alpha}\}$ and $\{W^e_{i,\alpha}\}$ can be calculated once and re-used wherever the geometry of the inner region is the same. This would be useful in the study of an AGR fuel assembly, shown in Figure 1.1, where the fuel pins form a repeated geometry.

With the auxiliary functions $\{W_{i,\alpha}\}$ and $\{W^e_{i,\alpha}\}$, the solution to Equation (5.54) can be built.
using the principle of superposition. The solution, restricted to \( \Upsilon_i \), is (Utyuzhnikov, 2009)

\[
\Phi (x)|_{\Upsilon_i} = \sum_{\alpha=0}^{N_u} u_{\alpha} W_{i,\alpha} (x)|_{\Upsilon_i} + \sum_{\alpha=0}^{N_r} r_{\alpha} W_{i,\alpha}^e (x)|_{\Upsilon_i} . \tag{5.71}
\]

This ensures continuity of \( \Phi \) on \( \Upsilon_i \). The gradient of \( \Phi \) on the interface can be found using the Poincaré-Steklov operator for the boundary value problem in Equation (5.54) in each \( \Omega_i \), denoted \( \mathcal{R}_{\Omega_i} \), which is given by the expression (Utyuzhnikov, 2009)

\[
\mathcal{R}_{\Omega_i} \Phi (x)|_{\gamma} = \nabla \Phi (x)|_{\gamma} = \sum_{\alpha=0}^{N_u} u_{\alpha} \nabla W_{i,\alpha} (x)|_{\gamma} + \sum_{\alpha=0}^{N_r} r_{\alpha} \nabla W_{i,\alpha}^e (x)|_{\gamma} , \tag{5.72}
\]

for any boundary \( \gamma \). Smoothness of \( \Phi \) is ensured if the derivatives of \( \Phi \) on \( \Upsilon_i \) are the same in \( \Omega _e \) and \( \Omega _i \), which is the case if

\[
\nabla \Phi|_{\Upsilon_i} = \sum_{\alpha=0}^{N_u} u_{\alpha} \nabla W_{i,\alpha}|_{\Upsilon_i} + \sum_{\alpha=0}^{N_r} r_{\alpha} \nabla W_{i,\alpha}^e|_{\Upsilon_i} . \tag{5.73}
\]

Equation (5.73) is the boundary condition for \( \Phi \) that should be imposed on \( \Upsilon_i \) in order to solve Equation (5.1) in \( \Omega_e \).

The full solution to Equation (5.54) in \( \Omega_i \) has been obtained and can be expressed as

\[
\Phi (x) = \sum_{\alpha=0}^{N_u} u_{\alpha} W_{i,\alpha} (x) + \sum_{\alpha=0}^{N_r} r_{\alpha} W_{i,\alpha}^e (x) , \tag{5.74}
\]

and

\[
\nabla \Phi (x) = \sum_{\alpha=0}^{N_u} u_{\alpha} \nabla W_{i,\alpha} (x) + \sum_{\alpha=0}^{N_r} r_{\alpha} \nabla W_{i,\alpha}^e (x) . \tag{5.75}
\]

The gradient of \( \Phi \) at the boundary \( \gamma_{w,i} \) can be calculated with the Poincaré-Steklov operator as

\[
\partial_n \Phi (x)|_{\gamma_{w,i}} = \mathcal{R}_{\Omega_i} \Phi (x)|_{\gamma_{w,i}} \cdot n = \sum_{\alpha=0}^{N_u} u_{\alpha} \partial_n W_{i,\alpha}|_{\gamma_{w,i}} + \sum_{\alpha=0}^{N_r} r_{\alpha} \partial_n W_{i,\alpha}^e|_{\gamma_{w,i}} , \tag{5.76}
\]

where \( n \) is the normal to \( \gamma_{w,i} \). This can be used to compute the wall shear stress, for example.

The coefficients \( u_{\alpha} \) and \( r_{\alpha} \) can be found by solving the variational problems (Utyuzhnikov, 2009)

\[
\min_{u_{\alpha}} \left\| \Phi (x)|_{\Upsilon} - \sum_{0}^{N_u} u_{\alpha} u_{i,\alpha} (x') \right\|_{L^2} , \tag{5.77}
\]

and

\[
\min_{r_{\alpha}} \left\| f (x) - \sum_{\alpha=0}^{N_r} r_{\alpha} v_{i,\alpha} (x) \right\|_{L^2} . \tag{5.78}
\]

Thus the boundary condition in Equation (5.73) is computed by solving a variational problem at each iteration in \( \Omega_e \). A computational mesh with \( M \) boundary faces along \( \Upsilon_i \) would require
5.9. NDD with non-local IBCs

$N_u = M - 1$ in Equation (5.69) to guarantee that the function, $\Phi$, in $\Omega_i$ and in $\Omega_e$ matches everywhere on $\Upsilon$. Any $N_u < M - 1$ will lead to some inaccuracy in the matching of $\Phi$ on $\Upsilon$. However, the variational problem grows in complexity as $N_u$ increases, which increases the computation time. The approach taken by Utyuzhnikov (2009) and used in this thesis is to compute only two auxiliary functions which obey the equations

\begin{align*}
L W_{i,0} &= 0, \\ l_y W_{i,0} |_{\gamma_w,i} &= 0, \\ l_x W_{i,0} |_{\gamma_o,i} &= 0, \\ W_{i,0} |_{\Upsilon_i} &= 1,
\end{align*}

\begin{align*}
L W_{e,0} &= f, \\ l_y W_{e,0} |_{\gamma_w,i} &= 0, \\ l_x W_{e,0} |_{\gamma_o,i} &= 0, \\ W_{e,0} |_{\Upsilon_i} &= 0,
\end{align*}

in each inner region. Then Equation (5.71) is written locally, at each boundary face, as

$$
\Phi (x) |_{\Upsilon_i} = \Phi |_{\Upsilon} W_{i,0} (x) |_{\Upsilon_i} + W_{e,0} (x) |_{\Upsilon_i},
$$

and Equation (5.73) is also written locally, at each boundary face, as

$$
\nabla \Phi |_{\Upsilon_i} = \nabla \Phi |_{\Upsilon} W_{i,0} |_{\Upsilon_i} + \nabla W_{e,0} |_{\Upsilon_i},
$$

which is a Robin boundary condition that can be imposed on $\Upsilon$ in $\Omega_e$ and guarantees that there is no inconsistency in the value of $\Phi$ on $\Upsilon_i$ in $\Omega_i$ and $\Omega_e$. In a case where the governing equation is one-dimensional or there is only one boundary face on $\Upsilon_i$, Equation (5.88) is the same as Equation (5.10). When the governing equation is multidimensional, Equation (5.88) is more accurate because it includes non-local effects through $W_{i,0}$ and $W_{e,0}$.

Applying Equation (5.88) locally at each boundary face introduces an error into the method. However if the variation of $\Phi$ on $\Upsilon_i$ is sufficiently small, then using Equation (5.88) leads to good enough accuracy in the solution, as shown in Utyuzhnikov (2009).

So far it has been assumed that a sufficiently accurate profile of $\mu_t$ is available so that the auxiliary functions can be computed. If such a profile is known a priori, say, from a prior calculation, possibly on a coarser mesh, then this profile can be used. However, when such a profile is not known a priori, $\mu_t$ can be computed using one of the profiles in Section 5.4. In order to do this, information such as $k$ or the wall shear stress, must be exchanged between $\Omega_e$ and $\Omega_i$ at each iteration, so that the auxiliary functions converge concurrently with the solution in $\Omega_e$. An example of using this coupled approach is given in Appendix D. However, exchanging information in this way is not computationally efficient. The original objective is to solve Equation (5.52) in $\Omega$. Therefore, if the domain is split into $\Omega_e$ and $\Omega_i$, then the most useful information to exchange between the two regions is the value of $\Phi$ on $\Upsilon$. This is what is done in the normal parallelisation procedure in Code_Saturne. With the NDD approach however, it would be necessary to couple not only the information required to compute $\mu_t$ but
also the information required to compute $f$ (in the case of IBCs for $U$, $f = \partial_x P^*$). Thus, the amount of information that must be exchanged between $\Omega_e$ and $\Omega_i$ is similar to that which must be exchanged in a normal parallel computation. Hence there would be no decrease in computation time unless other simplifications were possible. This might be the case if there are many repeated sections of a geometry near the wall, so that a single set of auxiliary functions in $\Omega_i$ could be used to provide interface boundary conditions on multiple interface boundaries, such as for the AGR fuel assembly pictured in Figure 1.1. However, it will be seen in Chapter 7 that a more accurate form of $f$ is required than can be computed using only information from $\Omega_e$. Therefore this coupled approach is not explored in detail in this thesis.

Instead, the NDD approach with NLIBCs computed using a form of $\mu_t$ and $f$ computed in advance is used in Chapter 7 to assess the feasibility of relegating a region of the flow between two ribs to an inner region. Section 7.3.3 and Appendix D are the only parts of this thesis that contain results with NLIBCs. All other applications of NDD in this thesis use the one-dimensional formulation with the boundary condition given in Equation (5.10).
This chapter presents the results of using the NDD method on five test cases. During the
EngD, the results of this chapter were published in two journal articles. These are Jones and
Utyuzhnikov (2015) and Jones and Utyuzhnikov (2016).

The purpose of these test cases is to assess which of the turbulent viscosity profiles discussed
in Section 5.4 performs best and to assess the accuracy of the NDD method compared to
LRN and HRN approaches.

In this chapter results with NDD are presented using the HRN $k - \varepsilon$ model and the LRN
Spalart-Allmaras model in \textit{CodeSaturne} version 3.0.5. There is no LRN $k - \varepsilon$ model in
\textit{CodeSaturne} version 3.0.5. The LRN model of Chien (1982) was implemented as part of the
project, however it suffered from numerical instabilities on two-dimensional flows and so was
not taken forward for development. Therefore the NDD results with the $k - \varepsilon$ model should
be compared to the HRN $k - \varepsilon$ results with the SWF. On the one-dimensional flows in this
chapter, LRN $k - \varepsilon$ results using the model of Chien (1982) are presented for comparison.
However there is no particular relationship between the LRN and HRN $k - \varepsilon$ results, since
the turbulence model equations are different. The Spalart-Allmaras results with NDD should
be compared with the LRN Spalart-Allmaras results.

The turbulence models used in this chapter are summarised in Table 6.1, which also indicates
which turbulent viscosity profiles have been used with the turbulence models.

When simulations are performed using the HRN $k - \varepsilon$ model, the near-wall cell centres always
lie in the same location as the interface boundaries in an NDD simulation. For example, if
for $y^*/h = 0.2$ with NDD then in the corresponding HRN calculation, the near-wall cell
extends up to $y^*/h = 0.4$ so that its centre is at $y^*/h = 0.2$. This is approach is used because
in \textit{CodeSaturne} the log law is evaluated at the centre of the near-wall cell to compute the
boundary conditions. Thus the region between the wall and the cell centre is the area over
Table 6.1: The turbulence models used in this chapter and the turbulent viscosity profiles used with them for NDD.

<table>
<thead>
<tr>
<th></th>
<th>LRN</th>
<th>Spalart-Allmaras</th>
</tr>
</thead>
<tbody>
<tr>
<td>k-ε model</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Spalart-Allmaras</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>LRN</td>
<td>Yes</td>
<td>Exponential</td>
</tr>
<tr>
<td>HRN</td>
<td>Yes</td>
<td>Exponential</td>
</tr>
<tr>
<td>NDD</td>
<td>Piecewise linear</td>
<td>Duprat et al. (2011)</td>
</tr>
<tr>
<td>µt profile</td>
<td>Exponential</td>
<td>Duprat et al. (2011)</td>
</tr>
<tr>
<td>ZPG</td>
<td>Duprat et al. (2011)</td>
<td></td>
</tr>
</tbody>
</table>

which the wall function applies. This approach means that the NDD and HRN results are directly comparable and that for each NDD result there is a corresponding result with the SWF. However, the situation where the inner region of an NDD calculation corresponds to the full height of the near wall cell of the HRN mesh could also be studied. This would be more natural in codes that store variables at nodes rather than cell centres.

The five test cases in this chapter are:

1. The flow in a plane channel at a Reynolds number based on the friction velocity of $Re_\tau = 590$.
2. The flow in a plane channel at a bulk Reynolds number $Re = 1.1 \times 10^4$, which, according to the DNS data of Moser et al. (1999), is actually the same as the channel flow at $Re_\tau = 590$.
3. The flow through a heated annulus at a bulk Reynolds number of $Re = 8.9 \times 10^3$.
4. The flow in a jet impinging on a wall, with three different Reynolds numbers and two wall locations.
5. The flow in a two-dimensional, asymmetric diffuser at $Re = 1.8 \times 10^4$.

After presenting the results of these test cases, the computation time with NDD is discussed before the conclusions that can be drawn from all five test cases are summarised at the end of the chapter.

### 6.1 Channel flow at $Re_\tau = 590$

A plane channel flow is one of the simplest flows that can be performed with CFD and there is a wealth of DNS and experimental data available to compare results to. The simplicity of the problem also means that simulations run very quickly and it is possible to find analytical solutions of some turbulence model functions. For these reasons, plane channel flows are often used as test cases for CFD models. In addition, when using NDD on a channel flow,
Equation (5.3) is exact since the convection terms are identically zero and there is no streamwise diffusion.

In a plane channel flow with channel half-height $h$, there is an algebraic relationship between the friction velocity and the pressure gradient:

$$u_\tau = \sqrt{h |\partial_x P| / \rho}.$$  \hfill (6.1)

This result can be used to specify the flow conditions in terms of the friction Reynolds number, which for this channel flow is

$$Re_\tau = \frac{hu_\tau \rho}{\mu} = 590.$$  \hfill (6.2)

DNS data for this $Re_\tau$ is available from the work of Moser et al. (1999). The Reynolds number is achieved in the simulations by introducing a constant source term into the RANS equations, which performs the same function as an imposed pressure gradient.

A schematic of the mesh is shown in Figure 6.1. The flow moves in the $x$ direction and the wall-normal is in the $y$ direction. The mesh width in the $x$ direction is $h/10$ and its width in the $z$ direction is $h/100$.

LRN results for the channel are computed using the Spalart-Allmaras model and the LRN $k-\varepsilon$ model of Chien (1982). The LRN mesh has 255 cells, and the results were found to be mesh independent by comparing the solution to that obtained with a finer mesh.

The range of $y^*$ and the corresponding values of $y^*_\tau$ that are studied with NDD are shown in Table 6.2. The NDD meshes were generated by removing near-wall cells from the LRN mesh.

<table>
<thead>
<tr>
<th>$y^*/h$</th>
<th>0.01</th>
<th>0.03</th>
<th>0.05</th>
<th>0.1</th>
<th>0.15</th>
<th>0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y^*_\tau$</td>
<td>5.9</td>
<td>17.7</td>
<td>29.5</td>
<td>59</td>
<td>88.5</td>
<td>118</td>
</tr>
</tbody>
</table>

Table 6.2: The range of $y^*$ studied for the channel flows. The case with $y^*/h = 0.01$ is not studied with the HRN $k-\varepsilon$ model because the value of $y^*_\tau$ is too small.

Since the pressure gradient is fixed by the friction Reynolds number, the bulk Reynolds
Chapter 6. Test cases of the NDD method

number,

\[ Re = \frac{hU_b \rho}{\mu}, \]  

(6.3)

is not determined a priori. Hence \( Re \) is an output of the simulations and can be used to assess the accuracy of the result.

6.1.1 Results and discussion

In each simulation the wall shear stress agrees with the theoretical value to at least five decimal places. This validates the implementation of the NDD method in Code_Saturne.

Profiles of \( U^+ = U/u_+ \) with \( y^*/h = 0.05 \) for the different turbulent viscosity profiles are shown in Figures 6.2a and 6.2b for the \( k - \varepsilon \) and Spalart-Allmaras models, respectively. The solution is plotted in both the inner and outer regions. For the Spalart-Allmaras model with NDD, with all three turbulent viscosity profiles, the velocity is consistent with the LRN and DNS data. With the \( k - \varepsilon \) model the velocity with NDD is also in agreement, although there is more variation in the centre of the channel, at \( y_+^+ = 590 \), between the turbulent viscosity profiles. For \( y^*/h = 0.05 \) there is less spread in the velocity computed using NDD with the Spalart-Allmaras model than there is with the \( k - \varepsilon \) model. Note however that the lowest peak velocity with the \( k - \varepsilon \) model is given by the piecewise linear profile, which cannot be used with the Spalart-Allmaras model. The velocity computed with the exponential and Duprat et al. (2011) profiles is similar for the \( k - \varepsilon \) and Spalart-Allmaras models. The change in the peak velocity affects the bulk velocity, and so the bulk Reynolds number. This can be seen in Figure 6.3, which shows the bulk Reynolds numbers for each \( y^* \) and viscosity profile, where there is a greater spread in \( Re \) in the \( k - \varepsilon \) results than there is in the Spalart-Allmaras results.

The smallest \( y^*_+ \) used with the \( k - \varepsilon \) model is 17.7, which is below the logarithmic layer. At this \( y_+^+ \), the damping terms in the LRN \( k - \varepsilon \) model are active. However, the NDD and SWF results use the \( k - \varepsilon \) model in Code_Saturne which is a HRN model and contains no damping functions. Therefore the model is strictly not valid. This explains the large change in \( Re \) with NDD between \( y^*_+ = 17.7 \) and \( y^*_+ = 29.5 \). Note that although all NDD Reynolds numbers are lower than the LRN value, different LRN \( k - \varepsilon \) models would produce different Reynolds numbers, which may agree more closely with the NDD results. Since NDD is used with the HRN form of the \( k - \varepsilon \) model, there is no particular reason why the NDD results should match the LRN \( k - \varepsilon \) results, because different model equations are used. The constants in the SWF are tuned so that the model produces accurate results in a channel flow. Therefore it is not surprising that the SWF results show little sensitivity to \( y^* \) (except for \( y^*_+ = 17.7 \), where the model equations are invalid). The variation in the NDD predictions of \( Re \) over the
6.1. Channel flow at $Re_{\tau} = 590$

Figure 6.2: Velocity in the channel at $Re_{\tau} = 590$ compared to the DNS of Moser et al. (1999). The NDD results have $y^*/h = 0.05$, which corresponds to $y^+_\tau = 29.5$.

Figure 6.3: Bulk Reynolds number in the channel at $Re_{\tau} = 590$ for different $y^*$ compared to the DNS of Moser et al. (1999)

range of $y^*_\tau$ shown in Figure 6.3a is always less than 11 % as a fraction of the DNS result.

The Spalart-Allmaras model is a LRN model, the equations for which are valid to the wall. Consequently in Figure 6.3b the computed Reynolds number converges to the LRN result as $y^* \to 0$. The convergence is especially apparent for the ZPG profile. The variation in the NDD predictions of $Re$ over the range of $y^*$ tested is always less than 10 % as a fraction of the DNS result.

In both Figures 6.3a and 6.3b the exponential and Duprat et al. (2011) profiles yield the largest values of $Re$ for $y^*_\tau = 29.5$, which is near to the boundary between the buffer and logarithmic regions of the boundary layer. This indicates that the turbulent viscosity profiles are less accurate in this region, since $Re$ is approximately the same for larger or smaller $y^*$ with
these two viscosity profiles. In Figure 6.3a, the piecewise linear profile yields approximately
constant values of $Re$ across the range of $y^*$. In this sense it is competitive with the SWF. The
Reynolds number obtained with the ZPG profile decreases as $y^*$ increases in Figure 6.3b. The
ZPG profile is an exact solution to the $\hat{\nu}$ equation in one-dimensional flows with no pressure
gradient. The only difference between such a flow and the channel flow in this section is the
pressure gradient, which is imposed to drive the flow. In the outer region, the flow responds
accurately to the pressure gradient because the full model equations are solved there. Thus
the difference between the LRN and NDD results with the ZPG profile is caused entirely
by the error in the ZPG profile due to the pressure gradient in the inner region. This error
grows as the size of the inner region grows. Hence the deviation of $Re$ from the LRN value
is approximately proportional to the size of the inner region.

With both models the velocity is continuous and smooth at the interface. At small $y^+_f$, in the
viscous sub layer, the velocity is appropriately damped and agrees well with the DNS and
LRN profiles.

The turbulent viscosity in the near-wall region is plotted as $\mu^+_t = \mu_t/\mu$, for the same flows
in Figure 6.4. The Duprat et al. (2011) profile always yields a larger $\mu_t$ than the exponential
profile, which is expected from their governing equations because the pressure gradient in this
flow is non-zero. The effect of this is that the shear stress in the inner region is larger with the
Duprat et al. (2011) profile. Since the wall shear stress is fixed in this case, an increase the
turbulent viscosity causes a decrease in the velocity gradient, which in turn causes a decrease
in the velocity. Therefore, at constant $Re$, the Duprat et al. (2011) profile produces a lower
bulk velocity. This can be seen in Figures 6.2 and 6.3.

Figure 6.4: Turbulent viscosity in the near-wall regions of the channel at $Re = 590$. The
NDD results have $y^*/h = 0.05$, which corresponds to $y^+_f = 29.5$. 
There is a discontinuity in the turbulent viscosity at $y^*$ in Figure 6.4a for the exponential and Duprat et al. (2011) profiles. The reason for this is that the implied value of the turbulent viscosity, $c_* u^+ \kappa^2 / \varepsilon^*$, does not match the value given by the turbulent viscosity profile, as discussed in Section 5.6.1. This discontinuity is implicitly present in any results obtained with the AWF (Craft et al., 2002). Note that although the piecewise linear viscosity profile has no discontinuity at $y^*$, it actually produces the least accurate velocity in Figure 6.2a. Thus, continuity of $\mu_t$ is not always beneficial for the results.

The turbulent viscosity is continuous in all cases with the Spalart-Allmaras model. The differences in $\mu_t^+$ with the three profiles are greatest at $y^*$. The difference in $\mu_t^+$ computed by the different profiles decreases with increasing distance away from $y^*$.

Figure 6.3 shows that although all the flows in this section have the same value of $Re_\tau$, they do not have the same value of $Re$. It is common in engineering for flows to be specified in terms of $Re$. Therefore it is instructive to study a channel flow in terms of a bulk Reynolds number as this yields more insight into practical applications of NDD.

### 6.2 Channel flow at $Re = 1.1 \times 10^4$

The DNS data of Moser et al. (1999) can be used to compute the bulk Reynolds number for the channel flow at $Re_\tau = 590$. This reveals that the channel flow in Section 6.1 has

$$Re = 1.1 \times 10^4.$$  \hfill (6.4)

In this section, the channel flow is studied at this bulk Reynolds number. A constant bulk Reynolds number is obtained by introducing a momentum source term into the RANS equations. The value of the source term is updated at each iteration by a factor proportional to the difference between the current bulk velocity and the target bulk velocity, until convergence to the target is achieved. Hence the procedure is significantly different to the flow at $Re_\tau = 590$. The output of the simulation is the source term, which is effectively the pressure gradient and is reported in terms of a friction factor

$$f = \frac{h |\partial_x P|}{2 \rho U^2_b}.$$  \hfill (6.5)

The simulations are run on the same meshes used in Section 6.1 and NDD simulations are performed with the same range of $y^*$, as shown in Table 6.2.
6.2.1 Results and discussion

The velocity in the channel for \( y^*/h = 0.05 \) is plotted as \( U/U_b \) in Figure 6.5a and 6.5b for the \( k - \varepsilon \) and Spalart-Allmaras turbulence models respectively, for different viscosity profiles. The velocity profiles in Figure 6.5 are in closer agreement with each other in the centre of the channel than they were at \( Re_\tau = 590 \) in Figure 6.2. This is because the constant bulk Reynolds number restricts the possible values that \( U \) can take near the centre of the channel, so that the integral of the velocity is correct. With the HRN \( k - \varepsilon \) model, the integral of the velocity near to the wall is computed using the finite volume method by assuming that \( U \) is constant over the near-wall cell. In contrast, with NDD the full variation of \( U \) in the near-wall region is integrated. Therefore the contribution of the near-wall region to the bulk velocity is over-predicted in the HRN \( k - \varepsilon \) model. Consequently, towards the centre of the channel the HRN model must under-predict the velocity in order to return the specified bulk velocity. In addition, a finer mesh can be used with NDD than with the SWF, which allows \( U \) to vary more smoothly between adjacent cells. This leads to even greater accuracy in the bulk velocity with NDD.

![Graphs showing velocity profiles](image)

Figure 6.5: Velocity in the channel at \( Re = 1.1 \times 10^4 \) compared to the DNS of Moser et al. (1999). The NDD results have \( y^*/h = 0.05 \), which corresponds approximately to \( y_+^* = 29.5 \).

However, the agreement between the velocity profiles near the channel wall between the different viscosity profiles is poorer than at \( Re_\tau = 590 \). This implies that the different profiles yield different wall shear stresses, which manifests as different friction factors, as seen in Figure 6.6. The friction factor depends on both the wall shear stress (which is related to the pressure gradient) and the bulk velocity. A larger friction factor in Figure 6.6 corresponds to a smaller bulk Reynolds number in Figure 6.3. Consequently, the variation in the friction factors in Figure 6.6 is similar to the variation of \( Re \) in Figure 6.3, and the same behaviour is seen. That is: the piecewise linear viscosity profile produces approximately
constant friction factors; the exponential and Duprat et al. (2011) profiles yield lower values of \( f \) for \( y^*/h \approx 0.05 \) than for larger or smaller values of \( y^* \); the friction factor found with the ZPG profile increases with \( y^* \); and the Duprat et al. (2011) always produces a larger friction factor than the exponential profile because it always yields a larger turbulent viscosity. The errors in \( f \) with \( y^* \) at constant Re are inverted compared to the errors in Re with \( y^* \). Thus, with NDD similar results are found for a channel flow at constant bulk Reynolds number to the results at the corresponding friction Reynolds number.

6.3 Annular flow at \( Re = 8.9 \times 10^3 \)

Annular flows are characterised by the inner and outer radii, denoted \( R_1 \) and \( R_2 \), respectively. Flow parameters are often computed in terms of the equivalent diameter

\[
d_e = \frac{4A}{P_w} = \frac{4\pi(R_2^2 - R_1^2)}{2\pi(R_1 + R_2)} = 2(R_2 - R_1),
\]

where \( A \) is the flow cross-sectional area and \( P_w \) is the wetted perimeter. Like a channel flow, flows in annuli are statistically one-dimensional. Annular flows occur in engineering applications such as pipeline flows or heat exchangers. In these applications it is common for the thermal boundary conditions to be different on the inner and outer walls of the annulus. Pressure drops are typically reported in terms of the friction factor. The heat transfer coefficient is often reported in terms of the Nusselt number, \( Nu \), or the Stanton number, \( St \), which are defined respectively as

\[
Nu = \frac{hd_e}{\lambda},
\]

Figure 6.6: Friction factor in the channel at \( Re = 1.1 \times 10^4 \) for different \( y^* \) compared to the DNS of Moser et al. (1999).
Chapter 6. Test cases of the NDD method

and

\[ St = \frac{h}{\rho U_b c_p} = \frac{Nu}{Re \sigma} \tag{6.8} \]

where \( h \) is the heat transfer coefficient, \( \lambda \) is the thermal conductivity of the fluid and \( c_p \) is the specific heat capacity.

Over many years, many experiments have been performed to calculate the pressure drop and heat transfer coefficient in annular passages. For example, Davis (1943) developed a numerical correlation for a range of Reynolds numbers, radius ratios and Prandtl numbers, whereas Kays and Leung (1963) produced tabulated data for a range of Reynolds numbers and radius ratios. Considerable effort is still going into developing useful correlations. For example, Yu et al. (2005) developed more accurate correlations for the Nusselt number than early experimental studies for the case of a heated inner wall and an adiabatic outer wall. A numerical correlation was built by integrating the energy equation, using an accurate model for the turbulent stresses. In recent years it has become possible to perform DNS studies of annular flows. Examples include the study of Chung et al. (2002), who studied the effect of the radius ratio and the study of Ould-Rouiss et al. (2009), who studied the effect of the ratio of the heat fluxes at the two walls.

It is well-known (Maubach, 1972; Churchill and Chan, 1995) that the position of maximum velocity in a turbulent annular flow does not coincide with the position of zero shear stress. Therefore any turbulence model based on the Boussinesq hypothesis (Equation (2.55)) will always produce inaccurate velocity profiles in annular flows. Despite this deficiency, eddy viscosity models still yield accurate friction factors. The friction factor depends on the shear stresses at both the inner and outer walls, denoted \( \tau_1 \) and \( \tau_2 \), respectively. A relationship between these two stresses can be found from a force balance in the annulus, since the wall shear stresses balance the pressure gradient:

\[ 2\pi R_2 \tau_2 + 2\pi R_1 \tau_1 = -\partial_z P \pi (R_2^2 - R_1^2) . \tag{6.9} \]

Equation (6.9) has been used to validate the simulation results.

The annular flow studied in this section is that of Chung and Sung (2003), which has

\[ Re = \frac{d_e U_b \rho}{\mu} = 8.9 \times 10^3 . \tag{6.10} \]

Both the inner and outer walls are heated with the same heat flux, \( q''_{w} \). Skin friction and heat transfer data is reported on both walls via the skin friction coefficient,

\[ C_{f,i} = \frac{2\tau_i}{\rho U_b^2} , \tag{6.11} \]
6.3. Annular flow at \( Re = 8.9 \times 10^3 \)

and Nusselt number, which is computed as

\[
Nu_i = \frac{q''_w d_e \sigma}{\mu c_p (T_{w,i} - T_b)},
\]

(6.12)

where \( T_{w,i} \) is the wall temperature on wall \( i \). The subscript \( i \) is either 1, when it refers to the inner wall, or 2, when it refers to the outer wall. The bulk temperature, \( T_b \) is defined as

\[
T_b = \frac{\oint \rho c_p T U \cdot dS}{\oint \rho c_p U \cdot dS},
\]

(6.13)

where the integrals are over a single plane at a constant axial location.

For every simulation, the mesh contains a 1° sector of the annulus and is one cell thick in the flow direction, which defines the \( z \) axis. The mesh also contains one cell in the azimuthal direction, \( \phi \). A schematic of the geometry of the mesh is shown in Figure 6.7. LRN simulations are performed with the LRN \( k - \varepsilon \) model of Chien (1982) and the Spalart-Allmaras model.

The mesh used for the LRN simulations has 500 cells in the radial direction and the largest value of \( y^*+ \) at either wall is always less than unity.

![Figure 6.7: The geometry of the mesh of the annulus.](image)

In the NDD simulations, both walls are replaced by interface boundaries. The distance between the interface boundary and the corresponding wall is the same for both the inner and outer walls, and is equal to \( y^* \). Simulations are performed with the range of \( y^* \) in Table 6.3. The outer wall has the smallest wall shear stress and therefore gives the smallest values of \( y^*+ \). This range of \( y^*+ \) means that the HRN \( k - \varepsilon \) model in CodeSaturne is strictly not valid at any of these wall distances. Regardless, simulations are run with the HRN \( k - \varepsilon \) model for all \( y^*/d_e \geq 0.02 \) because this gives an indication of how NDD and the SWF compare on cases at small Reynolds numbers. In every simulation, the LRN and NDD results have been verified as mesh independent by performing the same study on a mesh with double the number of cells.

In a physical experiment, a flow with a small Reynolds number such as this one would be affected by buoyancy forces. However in this work the temperature is treated as a passive scalar and the effects of buoyancy are ignored, since this is the case in the DNS.
Table 6.3: The range of $y^*$ studied for the annular flow and the corresponding value of $y^* + \tau_2$, which applies to the outer wall. The cases with $y^*/d_e = 0.005$ and $y^*/d_e = 0.01$ are not studied with the HRN $k-\varepsilon$ model because the value of $y^* + \tau_2$ is too small.

and Sung, 2003). Because the walls of the annulus are heated and the computations assume periodicity in the axial direction, a scalar source term is introduced into the temperature equation so that the computations converge to a constant bulk temperature. The form of this source term is $-S_TW$, where $S_T$ can be calculated algebraically as

$$S_T = -\frac{2\dot{q'}_w R_1}{\rho c_p U_b (R_2 - R_1)}. \quad (6.14)$$

However, geometric errors due to the mesh having flat, instead of curved, faces mean that the algebraic expression is not exactly correct for use in CFD. Instead the value $S_T$ is updated at each iteration using the value of $T_b$ at the previous iteration, until convergence is achieved. The source term is included in the calculation of the interface boundary conditions for the temperature. The Prandtl number is $\sigma_T = 0.7$ and the turbulent Prandtl number is $\sigma_{t,T} = 1$.

6.3.1 Results and discussion

The velocity in the annulus for the $k-\varepsilon$ and Spalart-Allmaras models is shown in Figures 6.8a and 6.8b, respectively, with $y^*/d_e = 0.02$ for the NDD cases. All cases return a similar velocity profile, which is a result of specifying the flow in terms of the bulk Reynolds number, as discussed in Section 6.2. The shear stress on the inner wall is greater than on the outer wall, which manifests as a steeper slope in the velocity profile in Figure 6.8. The shear stresses on the two walls are consistent with Equation (6.9), which validates the implementation of the NDD method into Code_Saturne.

The skin friction coefficient for different $y^*$ is shown for the inner wall in Figure 6.9 and for the outer wall in Figure 6.10. Likewise, the Nusselt number for different $y^*$ is shown for the inner wall in Figure 6.11 and for the outer wall in Figure 6.12.

For the $k-\varepsilon$ model, the values of $C_{f,1}$ obtained with NDD are always larger than those found with the SWF or the LRN models. The same result is seen for $C_{f,2}$, $Nu_1$ and $Nu_2$. This means that the skin friction coefficient found with NDD often agrees more closely with the DNS than the other $k-\varepsilon$ models, however the Nusselt numbers are less accurate. The piecewise linear and Duprat et al. (2011) profiles show little variation in $C_f$ and $Nu$ with $y^*$, as do the SWF results. The exponential profile always returns lower values of $C_f$ and $Nu$ and shows more variation with $y^*$, however the variation is less than 10% over the range of
6.3. Annular flow at \( Re = 8.9 \times 10^3 \)

Figure 6.8: The velocity in the annulus at \( Re = 8.9 \times 10^3 \) compared to the DNS of Chung and Sung (2003). The NDD results have \( y^*/d_e = 0.02 \), which corresponds to \( y^+_r = 12 \).

Figure 6.9: The skin friction coefficient on the inner wall of the annulus at \( Re = 8.9 \times 10^3 \) compared to the DNS of Chung and Sung (2003).

Figure 6.10: The skin friction coefficient on the outer wall of the annulus at \( Re = 8.9 \times 10^3 \) compared to the DNS of Chung and Sung (2003).
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Figure 6.11: Nusselt number on the inner wall of the annulus at $Re = 8.9 \times 10^3$ compared to the DNS of Chung and Sung (2003).

Figure 6.12: Nusselt number on the outer wall of the annulus at $Re = 8.9 \times 10^3$ compared to the DNS of Chung and Sung (2003).

$y^*$ studied.

On both walls, $C_f$ and $Nu$ vary more with the Spalart-Allmaras model than the $k - \varepsilon$ model when NDD is used, although the exponential viscosity profile shows less variation in $C_f$ and $Nu$ on the inner wall with the Spalart-Allmaras model than it did with the $k - \varepsilon$ model. The Spalart-Allmaras results show that as $y^*$ reduces the NDD solution approaches the LRN solution. As with the $k - \varepsilon$ results, the Duprat et al. (2011) profile always yields larger values of $C_f$ and $Nu$ than the exponential profile. The same behaviour is seen for the channel flow in Section 6.2 and is caused by the Duprat et al. (2011) profile always returning a larger turbulent viscosity than the exponential profile.

For quantities plotted on the inner wall with the Spalart-Allmaras model (Figures 6.9b and
6.11b), the exponential profile produces results in close agreement with the LRN and DNS results for all $y^*$. This indicates that the exponential profile is accurate on the inner wall of this flow.

The Reynolds number of this flow is relatively small for a turbulent flow which means that the assumption of a fully turbulent region in the boundary layer may be invalid. The maximum $y_+^*$ that could be attained, computed at the midpoint between the inner and outer walls is 310. This makes it challenging to create a HRN mesh with enough cells to resolve the flow but with large enough cells to have an acceptable $y_+^*$ in the near-wall cell. Thus, HRN models should not be used on this flow. LRN models should be used instead.

### 6.4 Axisymmetric impinging jet at three different Reynolds numbers

The impinging jet studied in this section is a well-established test case and has been used to develop many turbulence models and wall functions including the NWF (Craft et al., 2001). It has been studied in two ERCOFTAC/IAHR workshops on turbulence modelling (Pironneau et al., 1991; Leschziner and Launder, 1993) and has already been studied with NDD by Utyuzhnikov (2008), who reported encouraging results. This is the first time NDD has been used on this case with an unstructured code, the first time the wall-normal boundary conditions of Section 5.3 have been used, the first time the Spalart-Allmaras model has been used and the first time turbulent viscosity profiles other than the piecewise linear profile have been used.

The geometry is shown in Figure 6.13. A fully-developed pipe flow with diameter $D$ enters

![Figure 6.13: Impinging jet geometry, with the interface boundary at $z = y^*$ shown.](image-url)
Chapter 6. Test cases of the NDD method

the flow domain in thermal equilibrium and impinges on a flat, heated wall a distance $H$ from the pipe exit. The wall is supposedly infinite in extent, however the computational domain terminates at a radius $L$ large enough that the flow is approximately constant with the radial distance. All simulations in this section have $L = 13D$. In this thesis $H = 2D$ or $6D$ and the Reynolds number based on the pipe diameter and the bulk velocity in the pipe is either $Re = 2.3 \times 10^4$, $7 \times 10^4$ or $9 \times 10^4$.

A discussion of different impinging jet implementations can be found in Pattamatta et al. (2011). Along the entrainment boundary at $z = H$, the flow can be either confined, such that no fluid passes the boundary, or unconfined, with entrainment of ambient fluid possible. These boundary conditions have been studied by Behnia et al. (1999), who used a $\nu^2 - f$ model and found that for $H > 0.5D$ the boundary condition on the entrainment boundary has no significant effect on the results at the wall. In this work, an outlet boundary condition is applied on the entrainment boundary, which confines the flow.

The inlet conditions are calculated using a fine, fully-resolved turbulent pipe flow with the corresponding LRN turbulence model. For the $k - \varepsilon$ model, the LRN model of Chien (1982) is used, which solves for $\tilde{\varepsilon}$, to which a factor of $2\mu_k/(\rho y^2)$ is added to convert it into $\varepsilon$, which is used in the inlet conditions for the HRN $k - \varepsilon$ model. A uniform temperature distribution is imposed at the inlet. The fluid Prandtl number is $\sigma_T = 0.7$ and the turbulent Prandtl number is $\sigma_{t, T} = 1$.

The mesh domain is a $1^\circ$ sector of a cylinder with one cell in the azimuthal direction. Outlet boundary conditions are applied at $r = L$, and $z = H$ for $r > D/2$. Because the mesh is three-dimensional and Cartesian, there is no boundary face on the axis of symmetry, therefore no boundary condition is required there. The wall is located at $z = 0$ and has a constant temperature. The interface boundary is placed at $y^*$, above the wall, as shown in Figure 6.13, with $y^* = 0.02D$ for $H = 2D$ and $y^* = 0.04D$ for $H = 6D$. Only one position of the interface boundary is tested for each geometry with this flow, in order to reduce the parameter space.

The number of cells in the axial direction is 170 for the LRN results and 120 for the HRN and NDD results. All meshes have 149 cells in the radial direction and the distribution of cells in this direction is the same for each mesh such that only the axial resolution is different. All results have been verified as mesh-independent by comparing the solutions to those obtained on a mesh with double the number of cells in each direction (with the exception of the HRN $k - \varepsilon$ results, where the mesh was not refined in the axial direction to avoid changing $y^*$).

The different pipe outlet heights and Reynolds numbers in this section have been studied experimentally by Baughn et al. (1992), Cooper et al. (1993) and Knowles and Myszko (1998). For the flows at $Re = 2.3 \times 10^4$ and $7 \times 10^4$, experimental measurements of the fluid
6.4. Axisymmetric impinging jet at three different Reynolds numbers

Figure 6.14: Streamlines for the flow, superimposed on the speed of the fluid for the case with $H = 2D$ and $Re = 9 \times 10^4$ with the LRN Spalart-Allmaras model.

Streamlines for the flow, superimposed on the speed of the fluid, are shown for the case with $H = 2D$ and $Re = 9 \times 10^4$ with the LRN Spalart-Allmaras model in Figure 6.14. The flow exits the pipe at the point marked A, and impinges on the wall. The flow stagnates at the point marked B, and moves along the wall in the direction BC. The outlet boundary condition on the upper boundary prevents entrainment of any fluid. This conserves fluid mass within the computational mesh and leads to the generation of a large recirculation region, which is consistent with the findings of Behnia et al. (1999) and does not affect quantities computed at the wall.

The speed of the fluid against $z$ at $r/D = 0, 1, 2$ and $3$ is shown for both turbulence models in Figure 6.15 for $H = 2D$ and $Re = 7 \times 10^4$. The speeds computed with NDD show little sensitivity to the turbulent viscosity profile and are in close agreement with the LRN and

$$C_f = \frac{\tau_w}{\frac{1}{2} \rho U_b^2}$$

and the Nusselt number is

$$Nu = \frac{h d}{\lambda} = \frac{q''_w D \sigma}{\mu c_p(T_w - T_i)}$$

where $T_w$ is the temperature of the wall and $T_i$ is the temperature of the pipe outlet.

6.4.1 Results and discussion

Streamlines for the flow, superimposed on the speed of the fluid, are shown for the case with $H = 2D$ and $Re = 9 \times 10^4$ with the LRN Spalart-Allmaras model in Figure 6.14. The flow exits the pipe at the point marked A, and impinges on the wall. The flow stagnates at the point marked B, and moves along the wall in the direction BC. The outlet boundary condition on the upper boundary prevents entrainment of any fluid. This conserves fluid mass within the computational mesh and leads to the generation of a large recirculation region, which is consistent with the findings of Behnia et al. (1999) and does not affect quantities computed at the wall.

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SWF results. At $r = 0$, on the axis, the wall-parallel velocity is zero. Hence near the interface the NDD results depend primarily on the wall-normal velocity boundary conditions used in NDD. No flux correction term is included in this case, since some fluid must pass through the interface. The close agreement between the LRN and SWF results on the axis indicates that Equation (5.16) is an accurate boundary condition and justifies the use of $\partial_y P = 4K_y^3$ to compute the wall-normal boundary conditions in Section 5.3.

Figure 6.15: The speed of the fluid at $r/D = 0, 1, 2$ and 3 for $H = 2D$ and $Re = 7 \times 10^4$. The Nusselt number on the wall for $Re = 2.3 \times 10^4$ is shown for $H = 2D$ in Figure 6.16 and for $H = 6D$ in Figure 6.17. For cases with $H = 6D$, the Spalart-Allmaras model performs poorly, as can be seen in Figure 6.17b. The poor performance occurs only for the larger value of $H$ and is caused by the model over-predicting the spreading rate of the jet. Thus the jet is spread over too large an area at the wall, which reduces the heat transfer coefficient and so the Nusselt number, as can be seen in Figure 6.17b. The poor performance affects
both the LRN and NDD results by different amounts. While the NDD solutions returned
approximately the same peak value of $\Nu$ as the LRN solution for $H = 2D$, at $H = 6D$ the
peak value of $\Nu$ is approximately half its LRN value. This is caused by the change in $y^*$ for
$H = 6D$. For the purposes of the discussion, the Spalart-Allmaras results with $H = 6D$ are
ignored.

Figure 6.16: Nusselt number on the wall for $H = 2D$ and $Re = 2.3 \times 10^4$.

Figure 6.17: Nusselt number on the wall for $H = 6D$ and $Re = 2.3 \times 10^4$.

In Figure 6.16 a peak in $\Nu$ at $r = 0$ is predicted by the $k – \varepsilon$ model with NDD with the
piecewise linear viscosity profile. This behaviour is consistent with the SWF and experimental
results. In contrast, the exponential, Duprat et al. (2011) and ZPG profiles return relatively
low values of $\Nu$ at the impingement point.

The exponential and ZPG profiles depend only on the wall shear stress. This is plotted as $C_f$
for both turbulence models for $H = 2D$, $Re = 9 \times 10^4$ in Figure 6.18. At the impingement
point, the wall shear stress is zero and the exponential viscosity profile returns $\mu_t = 0$, which implies a low turbulence intensity. The Nusselt number depends on the heat flux at the wall, which, with NDD, is calculated as

$$\dot{q}''_w = c_p \left( \frac{\mu}{\sigma} + \frac{\mu^*}{\sigma_t} \right) \frac{\partial T}{\partial z} \bigg|_* .$$

(6.17)

If $\mu^*_t$ is zero, the heat flux at the wall is under-estimated. This leads to a lower heat transfer coefficient, and hence a lower Nusselt number. The Duprat et al. (2011) profile depends on the wall shear stress and also the pressure gradient. However the pressure gradient has a similar profile to $C_f$ and is also zero at the impingement point. Therefore the Duprat et al. (2011) profile also predicts a small Nusselt number at the impingement point. In contrast, the piecewise linear profile uses $k_I'$ and $\mu_{t,I}'$ to determine the turbulent viscosity. The turbulent kinetic energy peaks at the impingement point. Therefore the Nusselt number is also a maximum at the impingement point with the piecewise linear profile. The value of $k$ is given implicitly in Table 6.4, which shows the non-dimensional distance $Re_{\eta^*} = \rho k_{I'}^{1/2} y^*/\mu$ at the impingement point for $H = 2D$ and $H = 6D$ for $Re = 2.3 \times 10^4$.

<table>
<thead>
<tr>
<th></th>
<th>$H = 2D$</th>
<th>$H = 6D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>$y^*/D$</td>
<td>$Re_{\eta^*}$</td>
</tr>
<tr>
<td></td>
<td>0.02</td>
<td>209</td>
</tr>
<tr>
<td>Duprat</td>
<td>0.02</td>
<td>187</td>
</tr>
<tr>
<td>Exponential</td>
<td>0.02</td>
<td>147</td>
</tr>
</tbody>
</table>

Table 6.4: Values of $y^*$ and $Re_{\eta^*}$ at the impingement point for $Re = 2.3 \times 10^4$ for the NDD simulations with the $k - \varepsilon$ model.

LRN LEVMs typically over-predict heat transfer at the stagnation point because the production term is predicted to be large and positive (Craft et al., 1993). However a theoretical analysis suggests that the production should be small, and possibly negative at the impinge-
6.5 Asymmetric diffuser at \( Re = 1.8 \times 10^4 \)

In this section the flow in an asymmetric diffuser is studied. The flow exhibits separation caused by an adverse pressure gradient on the inclined wall and reattachment on the wall of the outlet channel. Accurately determining the location of separation and reattachment is a challenge for many turbulence models. This makes a useful test case for NDD.

The geometry of the diffuser is shown in Figure 6.19. The corners are smoothed with a radius of curvature \( 9.7H \). This case is the first in which NDD is applied to a separated flow and to a geometry that contains a corner. This is non-trivial because the governing equations of the NDD method should ideally be modified to account for the curvature, as is done in the NWF (Gant, 2002). However, no such modification is made in this case. The Cartesian formulation is retained.

Experimental data is available for this flow from the work of Buice and Eaton (1995). The
Chapter 6. Test cases of the NDD method

Figure 6.19: The geometry of the diffuser. The corners are smoothed with a radius of curvature $9.7H$.

flow was first studied experimentally by Obi et al. (1993), who found that the flow separated at a distance $11H$ along the inclined wall after the diffuser entrance and reattached after a distance of $26H$. An LES of the same flow was performed as part of the work of Kaltenbach et al. (1999). Early in the course of the work of Kaltenbach et al. (1999) it was found that the results of Obi et al. (1993) did not obey mass and momentum conservation and that this was caused by three-dimensional effects in the diffuser (Buice and Eaton, 1995). This prompted Buice and Eaton (1995) to set up another experiment to improve the experimental data by ensuring that the flow was statistically two-dimensional before the final LES results of Kaltenbach et al. (1999) were published. The results of Buice and Eaton (1995) are more detailed than those of Obi et al. (1993) and include measurements of the skin friction coefficient along the inclined wall. Separation occurs after a distance of $7.5H$ from the diffuser entrance and reattachment occurs at $29H$ (Buice and Eaton, 1995).

The diffuser was studied numerically as part of the 8th ERCOFTAC/IAHR workshop (Hellsten and Rautaheimo, 1999) with a number of RANS turbulence models. Of particular note are the results with the LRN $k - \varepsilon$ model of (Launder and Sharma, 1974), which have no recirculation region at all.

Apsley and Leschziner (2000) studied this diffuser with a range of turbulence models including linear EVMs, non-linear EVMs and RSMs. All of the models they used had problems resolving the region just after the diffuser entrance on the inclined wall. They suggested that unsteady reattachment and separation occurs repeatedly in this region and is caused by deceleration of the fluid in the diffuser entrance.

The diffuser has also been studied by Durbin (1995) with a $v^2 - f$ model. The results were in agreement with the experimental data, however they were less accurate than the LES results of Kaltenbach et al. (1999). The recirculation region was predicted to be larger than in the experiment, with the flow separating at $4H$ and reattaching at $35H$. The pressure was actually closer to the experimental data than the LES.

Uribe (2006) studied this diffuser using *Code_Saturne* and a range of LRN turbulence models
and found that the assumptions of the scalable wall function are not valid for this flow. Thus, any model that uses the scalable wall function will produce inaccurate results. That makes this a particularly interesting test case to assess the effect of the additional physics included in NDD.

Simulations are performed with the HRN $k-\varepsilon$ and LRN Spalart-Allmaras models with NDD. A LRN computation with the Spalart-Allmaras model is also performed, as are computations with the HRN $k-\varepsilon$ model with the SWF and different near-wall cell sizes. The implementation of the LRN $k-\varepsilon$ model of Chien (1982) did not converge on this flow. Since there is no LRN $k-\varepsilon$ model in Code_Saturne version 3.0.5, there are no LRN $k-\varepsilon$ results for this flow. Results are reported in terms of the skin friction coefficient

$$C_f = \frac{\tau_w}{\frac{1}{2} \rho U_b^2},$$

(6.19)

and the pressure coefficient

$$C_p = \frac{P - P_{ref}}{\frac{1}{2} \rho U_b^2},$$

(6.20)

along both walls of the diffuser. The reference pressure, $P_{ref}$, is the pressure in the mid-point of the inlet channel at $x/H = -1.7$.

The Reynolds number, based on the bulk velocity and channel height at the inlet, is $Re = 1.8 \times 10^4$. The flow inlet conditions are those of a fully developed plane channel flow and are implemented by running a separate simulation and then imposing the results as boundary conditions at $x/H = -10$. For the $k-\varepsilon$ calculations, the LRN model of Chien (1982) was used to calculate the inlet conditions. As in Section 6.4, $\tilde{\varepsilon}$ was converted into $\varepsilon$ by adding $2\mu k/(\rho y^2)$ to it. The flow exits the diffuser at $x/H = 75$, where outlet boundary conditions are imposed.

With NDD, the interface boundaries have heights equal to either 1\%, 3\%, 5\% or 8\% of the local height of the diffuser in the $y$ direction. The local height of the diffuser is denoted $h$. This is used to name each mesh. For example, the mesh called $y^*/h = 0.05$ has a height of $0.9H$ at the inlet and $4.23H$ at the outlet, since the two interface boundaries always remove 5\% of the diffuser height. The range of $y^*/h$ and the corresponding $y^*_+$ on the inlet channel wall are shown in Table 6.5. With NDD, when $y^*$ increases, the minimum cell size in the mesh increases, since the smallest cells are found near to the wall. Therefore it is possible to increase the pseudo time step used in the computations each time the mesh is changed and maintain the same maximum Courant number. This has been done in the simulations in this section.

The LRN simulation is performed on a mesh that contains 140 cells in the $y$ direction and 398 cells in the $x$ direction. Cells are clustered towards the wall so that the maximum $y^*_+$ of
Table 6.5: The range of \( y^*/h \) studied for the diffuser flow and the corresponding value of \( y^*_τ \), on the inlet channel wall.

<table>
<thead>
<tr>
<th>( y^*/h )</th>
<th>0.01</th>
<th>0.03</th>
<th>0.05</th>
<th>0.08</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y^*_τ )</td>
<td>10</td>
<td>30</td>
<td>50</td>
<td>81</td>
</tr>
</tbody>
</table>

any near-wall cell is less than 0.5. The NDD meshes are created by removing cells from the LRN mesh. For example, the mesh with \( y^*/h = 0.05 \) is created by removing any cells that lie at \( y > 0.95h \) or \( y < 0.05h \). What remains in the mesh is identical to the LRN mesh. HRN simulations are performed on meshes with an identical cell distribution in the \( x \) direction and either 50, 16 or 10 cells in the \( y \) direction. These correspond to the NDD meshes \( y^*/h = 0.01, 0.03 \) and 0.05, respectively. The cell sizes are such that the near-wall cell centres lie exactly where the interface boundary is in the corresponding NDD mesh.

Many \( k-\varepsilon \) simulations, including that with the SWF, did not converge for \( y^*/h = 0.08 \). Therefore results are only presented for this \( y^* \) with the Spalart-Allmaras model.

### 6.5.1 Results and discussion

The boundary conditions at the inlet and outlet imply that the flow is supposed to be one-dimensional in these sections. Hence the net mass flux leaving through the interfaces in the NDD simulations is zero. Therefore the flux correction, discussed in Section 5.3 in Equation (5.16), is used. If no correction is applied, the flux through the interfaces is always less than 3% of the total mass flow rate. When the correction is included, the velocity correction is approximately \( 10^{-4}U_b \). The effect on the results of the flux correction is negligible.

Simulations with the exponential viscosity profile took over twice as long to converge as simulations with the other profiles. This is due to the small values of \( τ_w \) on both walls of the diffuser. The wall shear stress is used in the definition of \( y^+ \), which is exponentiated in the exponential profile. Thus any error in \( τ_w \) leads to a large difference in the turbulent viscosity predicted by the exponential profile. To speed up convergence, the value of \( τ_w \) is updated at each iteration when the exponential profile is used with the relaxation procedure

\[
τ_w^{(n+1)} = ατ_w^{NDD} + (1−α)τ_w^{(n)},
\]

where \( τ_w^{NDD} \) is computed using the NDD method (Equation (5.12)) and \( α = 0.5 \).

Streamlines, superimposed on the speed of the fluid, calculated from the LRN Spalart-Allmaras results are shown in Figure 6.20. The results are consistent with previous studies. The flow enters from the channel on the left, where the flow is a one-dimensional shear flow. After the corner marked \( A \), which is at \( x/H = 0 \), the flow remains attached on the upper
6.5. Asymmetric diffuser at \( Re = 1.8 \times 10^4 \)

wall for a short distance downstream. A recirculation region is present near the upper wall of the diffuser between the points \( A \) and \( C \). The recirculation region extends downstream of the corner marked \( B \), and reattaches a distance down the outlet channel at \( C \). After point \( C \), the flow gradually returns to an attached, one-dimensional shear flow.

![Streamlines](image)

Figure 6.20: Streamlines, superimposed on the speed of the fluid, in the diffuser calculated with the LRN Spalart-Allmaras results.

The velocity component \( U \) from the LRN and NDD simulations with the Spalart-Allmaras model is shown up to \( x/H = 25 \) in Figure 6.21, where the Duprat et al. (2011) turbulent viscosity profile has been used. The locations of the profiles are \( x/H = -5.87, 2.59, 5.98, 13.56, 16.93, 20.32 \) and 23.71. The convergence of the NDD solution to the LRN solution as \( y^* \to 0 \) is visible. The thickness of the inner regions can be seen in this plot and it is clear that the viscous sublayer, where the velocity gradient is large, is in the inner region for the NDD simulations. It can also be seen that \( U \) becomes noticeably different to the other results when \( y^*/h = 0.08 \), and no recirculation region is predicted. In this case the mesh covers only 84\% of the diffuser and, on the upper wall, the interface is well within the recirculation region in the experimental results.

For \( y^*/h = 0.03 \), the skin friction coefficient on the inclined wall is shown in Figure 6.22. A recirculation region is predicted on the inclined wall with NDD with the Spalart-Allmaras model for every viscosity profile. This is consistent with the LRN and experimental results. For the \( k - \varepsilon \) model the exponential and piecewise linear profiles predict a recirculation region but the Duprat et al. (2011) profile does not, although the skin friction factor does become small. In contrast, the SWF predicts no recirculation region at all. In the outlet region of the diffuser, for \( x/H \gg 21 \), the three profiles and the SWF tend to the same value of \( C_f \). For the \( k - \varepsilon \) model, the exponential profile predicts the most accurate reattachment point and the piecewise linear profile predicts the most accurate separation point. For the Spalart-Allmaras model, the skin friction coefficient from the Duprat et al. (2011) profile agrees most closely with the LRN result and predicts similar separation and reattachment points.

The skin friction coefficient on the straight wall for \( y^*/h = 0.03 \) is shown in Figure 6.23.
Figure 6.21: $U$ in the diffuser from the inlet up to $x/H = 25$ from the Spalart-Allmaras model. The Duprat et al. (2011) turbulent viscosity profile is used for the NDD simulations.
6.5. Asymmetric diffuser at $Re = 1.8 \times 10^4$

On both the straight and inclined walls, with the Spalart-Allmaras model, the results with the Duprat et al. (2011) profile agree most closely with the LRN results. Only the Spalart-Allmaras model captures the local peak in $C_f$ on the straight wall in the region $10 < x/H < 21$. With the piecewise linear and Duprat et al. (2011) profiles, the $k - \varepsilon$ NDD results are close to the SWF result on the straight wall.

With the $k - \varepsilon$ model, the exponential viscosity profile erroneously predicts a recirculation region on the straight wall of the diffuser. With the Spalart-Allmaras model, the exponential and ZPG profiles actually predict two recirculation regions on the straight wall. These two profiles use only $\tau_w$ to determine the turbulent viscosity, which is small in the region $0 < x/H < 30$. Therefore in this region, the exponential and ZPG profiles both predict $\mu_t^* \approx 0$. With $\mu_t^* = 0$, the wall shear stress is computed in the NDD method as

$$\tau_w = \mu \frac{\partial U}{\partial y} \mid_{y^*} - y^* \partial_z P.$$

(6.22)
Figures 6.25 and 6.24, show the pressure coefficient on the straight and inclined walls of the diffuser, respectively. The figures show that the pressure gradient is positive in the region $0 \leq x/H \leq 30$ and largest near to $x/H = 0$. Thus the pressure gradient dominates Equation 6.22 and $\tau_w$ becomes negative. In contrast, the Duprat et al. (2011) and piecewise linear profiles, which depend on $\nabla P$ and $k$, respectively, predict no recirculation region on the straight wall because they return a relatively large turbulent viscosity near to the wall. This result highlights the importance of using more than one parameter to compute the turbulent viscosity for this case.

For the Spalart-Allmaras model, with the exponential and ZPG profiles, $C_f$ briefly becomes positive on the straight wall for $15 \leq x/H \leq 21$. This is because the pressure gradient reduces as $x$ increases and the flow accelerates. Thus, the flow is more strongly attached and the wall shear stress grows, which leads to a larger value of $\mu_t$. With a large magnitude of $\mu_t$,
the pressure gradient, which is falling with increasing \( x \), no longer dominates the calculation of \( \tau_w \) and \( C_f \) becomes positive. Whereas the ZPG solution shows a smooth variation of \( \tau_w \), the exponential profile shows a sudden jump. This is because \( y^+ \) is exponentiated in the exponential profile, which makes the profile sensitive to \( \tau_w \). In this region, the exponential profile yields an accurate value of \( C_f \) that is similar to the Duprat et al. (2011) profile.

Around \( x/H = 21 \), \( C_f \) becomes negative again on the straight wall with the Spalart-Allmaras model, and there is another jump in the case of the exponential viscosity profile. The wall shear stress on the inclined wall begins to decrease around this point, as demonstrated in the LRN results in Figure 6.23, where there is a peak in \( C_f \) around \( x/H = 21 \). Along with this, the flow begins to decelerate. Thus, downstream of this point, the wall shear stress decreases, and becomes comparable to the pressure gradient. This leads to another collapse in the value of \( \tau_w \) predicted by NDD through Equation (6.22). As before, the exponential viscosity profile is sensitive to this change due to the exponentiation of \( y^+ \).

There is a final jump in \( C_f \) with both the ZPG and exponential profiles at \( x/H \approx 30 \) for the Spalart-Allmaras model and at \( x/H \approx 25 \) with the \( k-\varepsilon \) model. These are the locations at which the pressure gradient stops being positive for the two turbulence models. Thus, downstream of these points the flow is stable. Results with the exponential and ZPG profiles agree well with the LRN results after these points.

Figures 6.24 and 6.25 show that, of the two turbulence models tested, only the Spalart-Allmaras model is able to capture the curvature in \( C_P \) that occurs near to the diffuser outlet entrance at \( x/H = 21 \) in the experimental results. However the Spalart-Allmaras model with NDD tends to under-predict \( C_P \) near to the diffuser outlet compared to the LRN result. This actually improves the agreement with the experimental data. The value of \( C_P \) shows little sensitivity to the turbulent viscosity profile, in contrast to \( C_f \). This is because the pressure is computed only in the outer region and so the form of \( C_P \) is similar between the NDD, SWF and LRN results.

As discussed in Section 5.6.1, with the \( k-\varepsilon \) model, a Dirichlet boundary condition could be imposed on \( k \) at the interface boundary instead of the Robin boundary condition in Equation (5.10). The effect of doing this is shown in Figure 6.26, which shows the skin friction coefficient on the inclined wall for \( y^*/h = 0.03 \) with the piecewise linear viscosity profile. The figure shows that the Robin boundary condition on \( k \) is essential in order to predict the recirculation region on the inclined wall. This is because the Robin boundary condition captures the flow physics that affect \( k \) in the inner region. In contrast, the Dirichlet boundary condition and the SWF both assume that the turbulence is in local equilibrium in the near-wall region, which is not the case for this flow. Thus, the Dirichlet boundary
Chapter 6. Test cases of the NDD method

condition leads to results more similar to the SWF result and the results are less accurate.

Figure 6.26: $C_f$ on the inclined wall of the diffuser with the HRN $k-\varepsilon$ model for $y^*/h = 0.03$, with either a Robin or Dirichlet boundary condition on $k$ at the interface boundary. The piecewise linear viscosity profile is used.

In Figures 6.22 and 6.23, the piecewise linear profile performs best with the $k-\varepsilon$ model since it correctly predicts a recirculation region on the inclined wall but not on the straight wall. For the same reasons, the Duprat et al. (2011) profile performs best for the Spalart-Allmaras model. The behaviour of these turbulence models with these profiles for different $y^*$ is shown in Figure 6.27, which shows the skin friction coefficient on the inclined wall.

The SWF never predicts a recirculation region on the inclined wall. The implementation of the SWF in Code_Saturne computes the wall shear stress as $\tau_w = \rho u_k u_{\tau}$. Since both $\rho$ and $u_k = c_{\mu}^{1/4} k^{1/2}$ are positive, $\tau_w$ can only be negative if $u_{\tau}$ is negative. This requires a negative wall-parallel velocity at the near-wall cell centre. Figure 6.22 indicates that this does not happen for $y^*/h = 0.01, 0.03$ or $0.05$. Thus, with almost any reasonable size of near-wall cell, $u_{\tau} > 0$, and there is no recirculation region with the SWF. In contrast the near-wall pressure gradient is taken into account with NDD. This enables the NDD results to capture the recirculation region, which is always present except for $y^*/h = 0.01$. For this mesh, the maximum $y^+_c$ on the inclined wall is 4.4, which is low too low for the HRN $k-\varepsilon$ model to be applicable. Therefore, the failure of the NDD simulations to predict a recirculation region with this mesh is due to the underlying turbulence model. Thus, while the SWF and NDD method are roughly as accurate as each other in the outlet region, NDD is more accurate in the diffuser region $0 < x/H < 21$. Since there is a recirculation region, it is impossible to
create a mesh that has $y^+ > 30$ everywhere. This highlights a limitation of HRN models and the advantage of having a near-wall modelling strategy that can accommodate low values of $y^+$.

![Graphs showing $C_f$ on inclined wall for different $y^*/h$.](image)

Figure 6.27: $C_f$ on the inclined wall of the diffuser for different $y^*/h$.

Figure 6.27b shows that with the Spalart-Allmaras model, the NDD solution correctly con-
verges to the LRN solution as $y^* \to 0$. The profile of $C_f$ is insensitive to $y^*$ until $y^*/h = 0.08$, where the recirculation region disappears\(^1\). Thus for $y^*/h = 0.08$ the upper limit on $y^*$ for this flow has been exceeded and the assumptions of the NDD method are no longer valid.

### 6.6 Comparison of computation time

Until now this chapter has focussed on assessing the accuracy of NDD for both LRN and HRN turbulence models. However another advantage that HRN models have over LRN models is that computations take significantly less time to converge. Therefore it is necessary to compare the computation time of LRN, HRN and NDD computations.

The LRN solution will always be the most accurate solution possible, subject to the limitations of the turbulence model. In contrast, HRN models are the fastest way to obtain a solution using RANS but the solution is often less accurate. In the trade-off between accuracy and speed, HRN and LRN models are anchor points on the Pareto curve. NDD solutions lie on the Pareto frontier between these anchor points. For a large $y^*$, a HRN model emerges naturally with NDD. As $y^* \to 0$ the NDD solution has been shown to approach the LRN solution. The computation time with NDD is also affected by $y^*$. For large values of $y^*$, the computation time is similar to that of a HRN calculation. As $y^* \to 0$ the computation time approaches that of the LRN computation.

All computations, including the LRN computations, in Sections 6.1, 6.2 and 6.3 are all one-dimensional and converge quickly. Therefore the computation times are unimportant, and there is no industrial motivation for a faster method to compute these flows using RANS. The simulations were set up in order to compare the accuracy of the various methods rather than their speed, therefore the computation time for the flows in these sections is not discussed.

In contrast, the two-dimensional impinging jet and diffuser flows take longer to converge, and a comparison of the computation times is useful and revealing. In all results presented below, simulations with the same turbulence model are initialised with identical initial conditions, which are the default initial conditions in Code_Saturne.

Convergence is assessed through a convergence parameter, $D$, which can be calculated for

\(^1\)A calculation with $y^*/H = 0.07$, not shown in this chapter, still predicts a recirculation region on the inclined wall, with a reduced magnitude of $C_f$ in the recirculation region. The transition from predicting a recirculation region to not predicting a recirculation region occurs smoothly with $y^*$.  

Comparison of computation time

every non-zero variable, \( \Phi \), at every iteration, \( n \), with the expression

\[
D(\Phi) = \frac{1}{\Delta t} \sqrt{\sum_{i=1}^{N} (\Phi_i^n - \Phi_i^{n-1})^2 \Omega_i}.
\] (6.23)

In Equation (6.23), \( \Delta t \) is the time step, \( \Omega_i \) is the volume of the \( i \)th control volume and the sums are over the total number of cells, \( N \). The solution is considered converged when \( D < \epsilon = 10^{-7} \) for every non-zero variable \( \Phi \).

The sum of \( D(\Phi) \) for every \( \Phi \), where \( \Phi \in \{ P, U, V, W, k, \varepsilon \} \) for the \( k - \varepsilon \) model or \( \Phi \in \{ P, U, V, W, \tilde{\nu} \} \) for the Spalart-Allmaras model, can be plotted to assess the convergence of a simulation. This sum is plotted for the diffuser flows of Section 6.5 for different \( y^* \) in Figure 6.28 for both turbulence models. The piecewise linear profile has been used with the \( k - \varepsilon \) model and the Duprat et al. (2011) profile with the Spalart-Allmaras model. Note that these simulations were run for 3000 time steps to allow a comparison of the limiting value of \( D \), even though the convergence criterion was met in a smaller number of time steps.

Both figures show that with NDD, the residuals decrease to a similar order of magnitude as the LRN computation or the HRN computation with the SWF. Figure 6.28a shows that for \( y^*/h = 0.03 \) or 0.05, the value of \( D \) for the NDD solution is smaller than it is for the solution with the SWF. However for \( y^*/h = 0.01 \), which is small for the HRN \( k - \varepsilon \) model in Code_Saturne, the SWF achieves a smaller value of \( D \).

The relative computation times for the NDD, SWF and LRN simulations for the impinging jet are shown in Figure 6.29. The computation times are the mean of all computations performed across the range of \( H \) and \( Re \) studied, and are normalised such that the fastest computation has a relative computation time of unity. The NDD results were obtained with the piecewise linear profile for the \( k - \varepsilon \) model and the Duprat et al. (2011) profile for the Spalart-Allmaras model. The relative computation times show the expected pattern: the LRN computation takes the most time, the NDD computations take less time and the SWF computations are the fastest. NDD leads to a decrease in the computation time of approximately two thirds compared to the LRN computation. NDD computations take around 2 times as long as the HRN computation, whereas the LRN computation takes approximately 7.5 times as long. NDD simulations with the Spalart-Allmaras model are seen to be slightly faster than they are with the \( k - \varepsilon \) model. One cause of this is that the \( k - \varepsilon \) model has one more function to solve for \( (k \text{ and } \varepsilon \text{ instead of just } \tilde{\nu}) \), which requires more computation.

The relative computation times for the diffuser are shown in Figure 6.30, where they are plotted for different \( y^* \). Again, the NDD results were obtained with the piecewise linear
Figure 6.28: The sum of $D$ for every variable for the diffuser flows. For the NDD simulations, the piecewise linear profile was used with the $k-\varepsilon$ model and the Duprat et al. (2011) profile was used with the Spalart-Allmaras model.
6.6. Comparison of computation time

![Figure 6.29: Mean relative computation time for every impinging jet flow studied in Section 6.4, normalised such that the fastest computation time is unity. For the NDD simulations, the piecewise linear profile was used with the $k-\varepsilon$ model and the Duprat et al. (2011) profile was used with the Spalart-Allmaras model.](image)

The relative computation times follow the same pattern as they do for the impinging jet, the only exception being that in this case with NDD the Spalart-Allmaras calculations take slightly longer than the $k-\varepsilon$ calculations. This is because the location of recirculation region on the diffuser flow depends on the IBCs, and converge along with the rest of the solution. However, since the Duprat et al. (2011) profile is used with the Spalart-Allmaras model. Thus, the IBCs and recirculation region are coupled via the wall shear stress, and take longer to converge. In contrast, the $k-\varepsilon$ results use the piecewise linear profile, which does not couple the wall shear stress to the IBCs. Therefore the recirculation region and the IBCs are uncoupled, and the solution converges more quickly. On the impinging jet flow, the profile of $k$ is similar to the profile of $\tau_w$ and $\nabla P$, which means that the coupling of IBCs and flow physics affects all results approximately equally.

In Figure 6.30, the change in computation time with $y^*$ can be seen. Both the $k-\varepsilon$ and Spalart-Allmaras computations require less time for larger $y^*$, although the effect is more pronounced in the $k-\varepsilon$ results. The LRN computation takes approximately 56 times as long as the fastest computation with the SWF, whereas the NDD computations typically take around 10 times as long. However, as can be seen in Figure 6.27a, for any $y^*$, the
computations with NDD are more accurate than the SWF. Also shown in Figure 6.30 is the maximum error in $C_f$ on the inclined wall for the Spalart-Allmaras simulations with NDD. The error, $e$, is computed in terms of the LRN solution as
\[
e = \frac{\max \left( C_{f \text{LRN}}(x) - C_{f \text{NDD}}(x) \right)}{C_{f0}},
\]
where $C_{f0}$ is the skin friction coefficient of the inlet channel. This figure is not reported for the $k - \varepsilon$ solutions because no LRN results are available to compare $C_f$ against. It is observed that $e$ decreases as $y^*$ does, which is the expected behaviour as the NDD solution converges to the LRN solution. For every $y^*$ the NDD computation takes longer than the HRN computation. This is because more computations are required in order to calculate the IBCs than are required with the SWF. However these extra computations lead to more accurate boundary conditions so the extra time requirement is justified. Thus, the trade-off between accuracy and computation time is clear.

The reason the fastest HRN computation is so much faster on the diffuser than it is on the impinging jet is due to the cell distribution in the meshes. In the mesh of the impinging jet, cells are clustered around the pipe outlet, in order to adequately resolve the inlet region.
Even when the SWF is used, the mesh resolution in the inlet region is still fine, and the flow in these cells must still be resolved. Hence the computation with the SWF takes relatively longer for the impinging jet than it does for the diffuser.

6.7 Conclusions

The results of applications of the NDD method to five distinct test cases were shown in this chapter. These applications were a plane channel flow with a constant pressure gradient, a plane channel flow with a constant bulk Reynolds number, an annular flow, an impinging jet flow and an asymmetric diffuser flow.

The two aims of the chapter were to assess the accuracy of the NDD method compared to the LRN and SWF approaches; and to compare the different turbulent viscosity profiles in Section 5.4.

The conclusions from this chapter are grouped by the test case.

Conclusions from the channel flow at \( Re_\tau = 590 \) (Section 6.1)

1. The wall shear stress computed in the NDD solution matches the theoretical value to at least five decimal places, which validates the implementation of NDD into Code_Saturne.

2. The bulk Reynolds number found with NDD varies by less than 10% for different \( y^* \) for both turbulence models. This compares to less than 5% for the SWF. Thus, at least for the HRN \( k-\varepsilon \) model, the SWF performs slightly better than NDD on this flow. However, this is because the constants for the SWF are tuned to data from channel flows. In addition, the SWF is only applicable at large enough \( y^*_\tau \), whereas the NDD method is applicable for both large and small \( y^*_\tau \) and converges to the LRN result as \( y^* \rightarrow 0 \) with the Spalart-Allmaras model.

3. The bulk Reynolds number varies by approximately 12% for the different NDD viscosity profiles and \( y^* \). This causes the mean velocity to look considerably different near the centre of the channel for different turbulent viscosity profiles.

Conclusions from the channel flow at \( Re = 1.1 \times 10^4 \) (Section 6.2)

4. Friction factors computed with NDD for this flow show the same trend with \( y^* \) and the viscosity profile as the bulk Reynolds does for the flow at \( Re_\tau = 590 \). However
the variation in the velocity with the turbulent viscosity profile is much smaller; the variation is instead transferred to the pressure gradient required to drive the flow.

5. NDD allows more accurate values of $U_b$ to be calculated than the SWF does because the full variation of $U$ in the inner region can be integrated, instead of treating $U$ as a constant over the near-wall cell.

6. Velocities predicted for flows at a constant bulk Reynolds number are more accurate than they are for flows at constant $Re_\tau$, however the accuracy of the wall shear stress is compromised.

Conclusions from the annular flow (Section 6.3)

7. The variation in $C_f$ and $Nu$ with a given viscosity profile depends on the turbulence model. Hence there is no universally best profile to choose.

8. As was found for the channel flows, the SWF produces skin friction coefficients and Nusselt numbers closer to the LRN $k - \varepsilon$ model of Chien (1982) than NDD does. However, the HRN $k - \varepsilon$ model used with NDD and the SWF is strictly invalid in the range of $y^\tau$ studied on this flow.

9. The Reynolds number of this flow is relatively small, consequently so is the maximum value of $y^\tau$. It is challenging to make a suitable mesh for the SWF that gives a sufficiently large $y^\tau$ and also allows the flow to be accurately resolved. In contrast, NDD can still be used at lower $y^\tau$. NDD is accurate for small $y^\tau$ if a LRN turbulence model is used.

Conclusions from the impinging jet (Section 6.4)

10. Although the exponential and Duprat et al. (2011) profiles perform well in one-dimensional flows, these profiles break down at the impingement point of the jet, where both predict no turbulent viscosity when it should be at a maximum. This leads to poor predictions of the heat transfer coefficient at impingement points. Therefore it is beneficial to use another parameter such as $k$ to calculate the turbulent viscosity, as is done by the piecewise linear profile.

11. The wall-normal boundary condition based on $\partial_y P \propto y^3$ is accurate and produces accurate enough results for the velocity on the axis of symmetry.
**Conclusions from the diffuser flow (Section 6.5)**

12. NDD can predict a recirculation region on the inclined wall of the diffuser, whereas the SWF fails to.

13. It is beneficial to use $\nabla P$ or $k$ to compute the turbulent viscosity; if only $\tau_w$ is used then simulations can be unstable where $\tau_w$ is near to zero. The exponential viscosity profile performs particularly poorly in regions of separation and can give rise to sudden jumps in the wall shear stress.

14. With the $k - \varepsilon$ model, a recirculation region on the inclined wall of the diffuser is only predicted when a Robin boundary condition is used on $k$. This demonstrates the theoretical superiority of NDD over the SWF.

15. It is possible to apply NDD to a curved geometry without any modification of the boundary layer equations and obtain accurate enough results.

16. It is impossible to make a suitable HRN mesh for this flow because of the small values of $\tau_w$. This highlights the advantages of LRN turbulence models over HRN models. The LRN Spalart-Allmaras model is seen to perform well on this flow and the NDD results converge to the LRN results as $y^* \to 0$.

As a consequence of the break down of the exponential turbulent viscosity profile on the diffuser and impinging jet flow, it was decided not to use this profile in future studies, other than for testing purposes. The piecewise linear profile consistently yields the most physically accurate results on the more challenging test cases of the impinging jet and the diffuser. Therefore when the $k - \varepsilon$ model is used, it is recommended to use the piecewise linear viscosity profile. However the Spalart-Allmaras model does not solve for $k$, and therefore this profile cannot be used. If the exponential profile is discounted, the Duprat et al. (2011) profile and the ZPG profile are the remaining choices. Although the Duprat et al. (2011) profile performed better on the diffuser, the ZPG profile is recommended. This is because it was more accurate in the one-dimensional flows and the Duprat et al. (2011) profile breaks down at impingement points anyway. The ZPG profile also has the advantage of being exact in one-dimensional regions where there are no momentum source terms.

There may be other turbulent viscosity profiles that are more accurate for a particular flow. It may even be that the exact solution is known. In such cases the most accurate turbulent viscosity profile should be used.

A drawback of the simulations performed in this chapter is that there is no LRN $k - \varepsilon$ model in Code_Saturne, so it has not been possible to compare LRN, NDD and SWF results with the same turbulence model. This would have been possible with the $k - \omega$ SST model,
which is a LRN turbulence model implemented in Code_Saturne with a wall function already implemented by default. Some results with the $k - \omega$ SST model with NDD are given in Appendix C and in Jones and Utyuzhnikov (2015). However the $k - \omega$ SST model has not been widely used in this thesis because its predictions of the friction factor for the flows in Chapters 7 and 8 were significantly lower than the predictions of other models used in this work. Instead, in this chapter, the NDD method can be compared to the SWF for the $k - \varepsilon$ model, and to LRN results with the Spalart-Allmaras model. This emphasises how flexible NDD is, because it can be implemented for any turbulence model. This is important for engineering purposes because not all CFD codes have every turbulence model implemented in them.
Chapter 7

Ribbed channel flow

In this chapter, a ribbed channel flow is studied using NDD. The purpose of the chapter is to assess how much of the rib profile can be relegated to the inner region in an NDD computation, and what shape of interface boundary is most appropriate.

The test case is also relevant for the industrial aspect of the project, since AGR fuel pins typically contain ribs on their surfaces. The flows over transverse pins studied in Chapter 8 are conceptually similar to the plane ribbed channel flow studied in this chapter. In addition, the flow studied in this chapter has been extensively studied experimentally by Rau et al. (1998). Thus, more data is available from these experiments than is reported in the industrial reports related to AGR fuel pins. Therefore it is instructive to study this test case and assess the performance of NDD before moving onto fuel pin flows.

The chapter ends with an example of how NDD can be used for efficient parametric design optimisation studies. In such cases it is possible to vary the rib height by changing $y^*$, instead of making a new mesh. This would lead to significant time savings in CFD models of complex systems where the aim is to optimise a rib height based on the friction factor.

7.1 Introduction

Flows through ribbed channels have been extensively studied over many years. The separation and reattachment caused by the ribs enhance heat transfer, which is useful for industrial applications such as turbine blade cooling and industrial heat exchangers. However, the increase in heat transfer must be balanced against the increase in pressure drop also caused by the ribs.

An important feature of ribbed channels is the arrangement of the ribs. In most studies the
ribs are aligned normal to the bulk flow velocity and on either one or two opposite walls of a square channel. When there are ribs on two opposite walls, the ribs can be either in-line or staggered. Different rib shapes, and channel heights have also been studied. Numerous studies have also considered rotating ribbed channels for turbine blade cooling applications. This chapter is concerned with non-rotating ribbed channels, which are relevant to nuclear reactor heat transfer problems. The flow studied with NDD in this chapter has square ribs on one wall of a square channel. However, a review of more general cases leads to useful insight.

Rau et al. (1998) studied the flow of air through a heated square channel with square ribs arranged normal to the flow on either one wall or two opposite walls of the channel. The height of each rib, $h$, was ten percent of the channel height, $H$. The time-averaged wall shear stress, heat transfer coefficient and velocity were measured for different rib pitch to height ratios. The ratio of the rib pitch, $W$, to rib width, $w$, was varied and it was found that the friction factor and heat transfer enhancement caused by the ribs peaks at $W/w \approx 9$. The same result was found by Okamoto et al. (1993), who found additionally that the optimum rib pitch to width ratio is approximately independent of Reynolds number. In the rough wall terminology introduced in Section 3.6, small $W/w$ corresponds to $d$-type roughness, and large $W/w$ corresponds to $k$-type roughness. A rib pitch to width ratio of 9 corresponds to $k$-type roughness.

In an experimental study, Iacovides et al. (1998) measured the flow and heat transfer in a U-bend with square cross-section with ribs on opposite walls. Iacovides and Raisee (1999) then studied these U-bend flows and flow through straight ribbed passages, with a LRN $k-\varepsilon$ model and a RSM. The straight channel had ribs on two opposite walls, with a rib pitch to height ratio of 10, and a rib height to channel height ratio of either 0.0675 or 0.1. They concluded that LRN turbulence models are essential in order to predict accurate levels of heat transfer, and suggested a modified lengthscale correction term for the $\varepsilon$ equation of the LRN $k-\varepsilon$ model, based on the Yap term (Yap, 1987). LRN RSMs were found to make superior heat transfer predictions compared to LRN LEVMs.

Iacovides et al. (2003) then studied ribs in a square channel at 45° to the bulk flow velocity using a two-layer modelling approach for the near-wall region with either a $k-\varepsilon$ model or a RSM. They found that if the ribs are at an angle to the mean flow then the secondary motion reduces the differences in heat transfer predictions between the two models compared to when the ribs are normal to the mean flow direction.

Ooi et al. (2002) studied the ribbed channel of Rau et al. (1998) using a $\sqrt{\nu^2 - f}$ model, a two-layer $k-\varepsilon$ model and the Spalart-Allmaras model. They found that the $\sqrt{\nu^2 - f}$ model makes the most accurate predictions of the heat transfer coefficient, the $k-\varepsilon$ model severely
under-predicts the levels of heat transfer between the ribs and the Spalart-Allmaras model results are in between the two, but the heat transfer coefficients are significantly different to the experimental results. They report that none of the models capture the secondary flows seen in experimental data, which limits their ability to accurately predict the heat transfer on the side walls of the channel where there are no ribs.

Raisee et al. (2008) studied both rotating and non-rotating ribbed channels with ribs in an in-line or staggered arrangement on opposite walls with a linear and non-linear $k-\varepsilon$ model. They found that with the original lengthscale correction in the $\varepsilon$ equation (Yap, 1987), both models over-predict the heat transfer level. However, with an improved lengthscale correction term, the NLEVM yields heat transfer coefficients similar to those of a RSM.

The ribbed channel of Rau et al. (1998) has been extensively studied by Keshmiri (2010), Keshmiri (2011), Keshmiri and Gotts (2011), Keshmiri (2012) and Keshmiri et al. (2012) with many RANS models, including a LRN $k-\varepsilon$ model, a non-linear $k-\varepsilon$ model, the $k-\omega$ SST model and a $\nu^2 - f$ model. The effects of changing the rib height, pitch and width were studied. In particular, non-square ribs with a profile similar to that of the ribs on an AGR fuel pin were studied and it was found that there was no significant difference in thermal performance compared to a square profile. The LRN $k-\varepsilon$ model was seen to dramatically over-predict the heat transfer coefficient, whereas the $\nu^2 - f$ model produced the most accurate values.

Further experimental studies of rotating ribbed passages include those by Iacovides et al. (1998), who used laser Doppler-anemometry, Casarsa and Arts (2002), who used PIV and Arts et al. (2007), who also used PIV. Further numerical studies include those by Narasimhamurthy and Andersson (2015), who used DNS and Arts et al. (2007), who used LES. A review of heat transfer for turbine blade cooling purposes can be found in Iacovides and Launder (2007).

DNS studies have been performed on ribbed channels up to Reynolds numbers of approximately $1.5 \times 10^4$ (Narasimhamurthy and Andersson, 2015), which is half of the Reynolds number studied in this chapter. However, RANS studies are still useful, particularly for high Reynolds numbers, and NDD would also be useful for efficient parametric studies of different rib heights.

A conclusion from previous numerical studies is that, while the flow velocity field is often accurately captured with RANS models, heat transfer predictions are more challenging, and higher fidelity models tend to perform better (Ooi et al., 2002; Raisee et al., 2008). Ribbed channels are challenging flows and many HRN treatments fail to accurately capture the flow separation that occurs between the ribs (Ooi et al., 2002). This makes the ribbed channel an interesting test case for NDD.
The geometry of the ribbed channel in this section is chosen to match the experimental set up of Rau et al. (1998) with ribs on one wall of a square channel. It is shown in Figure 7.1, which also shows the definitions of the rib height $h$, rib width, $w$, channel height, $H$, and rib pitch, $W$. The channel studied in this chapter has $H/h = 10$, $w/h = 1$ and $W/H = 0.9$. The walls of the channel, including the rib, are heated with a constant heat flux, which is the same on every part of both walls. While the experiment of Rau et al. (1998) was performed in a three-dimensional channel with square cross-section, the mesh used in this study is two-dimensional, with symmetry boundary conditions applied in the span-wise $z$ direction. This geometry is taken to be a model of the centreline of the experimental channel with ribs on one wall. However, the three-dimensional flow field observed by Rau et al. (1998) cannot be captured. In addition, since the side walls of the channel are missing from the simulations presented here, the total friction factor for the channel cannot be computed. However, the approach taken here is the same as the approach taken by Keshmiri (2012), Billard et al. (2015) and Cui et al. (2003), who found that a two-dimensional mesh is sufficient to represent the flow properties on the centreline of the experimental channel.

![Figure 7.1: The geometry used to study the ribbed channel in this chapter.](image)

The three-dimensional channel has an equivalent diameter of $d_e = H$, since the area of the side walls is included in the computation of the wetted perimeter. In contrast, the two-dimensional mesh would have an equivalent diameter of $d_e = 2H$, since there are no side walls. However, for the simulations performed in this chapter, the equivalent diameter is taken as $d_e = H$, in an attempt to correspond to the experimental setup of Rau et al. (1998). The Reynolds number is

$$Re = \frac{Ub pd_e}{\mu} = 3 \times 10^4.$$

(7.1)
With NDD, interface boundaries are placed variously above the smooth and ribbed walls of the channel. The smooth interface is always straight, however different shapes of the interface boundary are tested on the ribbed wall. These interfaces are given names, which are indicated in Figure 7.2. Interface A is straight, and lies above the rib tops. Interface B is rectilinear and follows the contour of the rib around its corners. With both interfaces A and B, the outer region does not contain any part of the rib wall. Interface C is straight like interface A, but lies in between the top of the ribs, such that some of the rib wall is located within the outer region.

![Figure 7.2: The different interface boundaries tested on the ribbed wall of the channel. Each interface is given a name, A, B or C. The arrows show how $y^*$ is defined in different portions of the inner regions.](image)

The method used to calculate $y^*$ for each interface is indicated by the arrows in Figure 7.2. In particular the computation of $y^*$ at the corners of interface B is shown. The interfaces can be characterised by a cut height, expressed in terms of the rib height. Interface A corresponds to $y^*/h > 1$, whereas interface C corresponds to $y^*/h \leq 1$.

With NDD, the LRN Spalart-Allmaras model is used with all interface boundaries in Figure 7.2, however the HRN $k-\varepsilon$ model is only used with interfaces A and B. This is because with interface C a portion of the rib is included in the outer region. Resolving the flow in this region would require using both the SWF and NDD in the same simulation. In such a case, little accuracy would be gained using NDD since the SWF would still be used in part of the flow. It would also be impossible to separate the effects of NDD from the effects of the SWF. Thus, there is no benefit from mixing both the SWF and NDD methods in a single computation.

The mesh for the wall-resolved LRN simulation has 53,630 hexahedral cells in a structured arrangement with refinement near to the walls. There are 62 cells along the top of a rib, and 60 cells along the height of a rib. This mesh was verified as sufficient to produce mesh independent results by comparing the solution to that obtained on a similar, but finer, mesh with 204,880 cells. As usual, meshes for NDD are created by removing cells from the LRN
mesh that lie fully or partially within the inner region. The mesh used with the SWF has 2724 cells in a structured arrangement with 18 cells covering the width of a rib and 3 cells covering the height of a rib.

The effects of convection around the upper corners of the ribs are significant in this flow. Despite this, IBCs are usually calculated by ignoring convection. The extent to which this omission affects the results of the simulation is unknown. Hence one purpose of this test case is to investigate how accurate NDD can be on flows where the inner region contains non-linear effects.

The main parameter used to assess the NDD method in this chapter is the friction factor for the two-dimensional channel, which is computed as

$$f = \frac{d_e |\Delta P|}{2W \rho U_b^2},$$  \hfill (7.2)

where $\Delta P$ is the pressure drop over the periodic section. Note that since the simulations are two-dimensional, and the side-walls of the channel studied by Rau et al. (1998) are not included in the simulation, the friction factors computed in this chapter are not comparable to those reported by Rau et al. (1998). Since the purpose of a simulation with NDD is to replicate the LRN solution as accurately as possible, the LRN value of $f$, $f_{LRN}$ is used for comparison. The error in the friction factor is defined as

$$E = 100 \% \times \frac{f_{NDD} - f_{LRN}}{f_{LRN}}.$$  

Since there is no LRN $k - \varepsilon$ model in Code_Saturne, $E$ is not calculated for the $k - \varepsilon$ results.

The following experimental data of Rau et al. (1998) are also available, and are used for comparison against NDD results:

1. The Nusselt number along the wall between the ribs;

$$Nu = \frac{q''_{w} d_e \sigma}{\mu_c p (T_w - T_b)},$$  \hfill (7.3)

2. The pressure coefficient along the wall between the ribs,

$$C_P = \frac{P - P_{ref}}{\frac{1}{2} \rho U_b^2},$$  \hfill (7.4)

where $P_{ref}$ is the pressure at the wall immediately downstream of the rib;

3. The velocity component $U$ at $y/h = 0.1$,

4. The velocity component $V$ at $y/h = 1$.

The skin friction coefficient

$$C_f = \frac{\tau_w}{\frac{1}{2} \rho U_b^2},$$  \hfill (7.5)

is plotted on the wall between the ribs for some simulations, although no experimental data
is available for comparison.

7.2 Overview of the LRN solution with the Spalart-Allmaras model

Streamlines, superimposed on the velocity, computed from the LRN Spalart-Allmaras solution are shown in Figure 7.3. The flow moves from left to right and is essentially one-dimensional above the top of the rib. Thus, on the upper wall, NDD will be accurate for small enough $y^*$. There is a large recirculation region on the bottom wall immediately downstream of the rib, and a smaller recirculation region near to the upstream face of the rib. The wall shear stress is negative over much of the region between the ribs.

Figure 7.3: Streamlines, superimposed on the velocity, computed with the LRN Spalart-Allmaras model.

7.3 Simulations with interface A

NDD simulations were performed with interface $A$, with the $k - \varepsilon$ model using the Duprat et al. (2011) and piecewise linear viscosity profiles and with the Spalart-Allmaras model using the Duprat et al. (2011) and ZPG viscosity profiles. The meshes have $y^*/h = 1.1$ and 1.2 on
the ribbed wall. On the smooth wall \( y^*/h = 0.2 \) in every case. The overall friction factors from the LRN, HRN and NDD solutions are shown in Table 7.1.

<table>
<thead>
<tr>
<th></th>
<th>SA ( 10^3 f )</th>
<th>( k - \varepsilon ) ( 10^3 f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>LRN</td>
<td>9.97</td>
<td>—</td>
</tr>
<tr>
<td>HRN</td>
<td>—</td>
<td>14.0</td>
</tr>
<tr>
<td>NDD Linear</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>( y^*/h = 1.1 ) Duprat</td>
<td>3.46</td>
<td>-65% 3.32</td>
</tr>
<tr>
<td>ZPG</td>
<td>3.26</td>
<td>-67%</td>
</tr>
<tr>
<td>NDD Linear</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>( y^*/h = 1.2 ) Duprat</td>
<td>3.13</td>
<td>-69% 3.13</td>
</tr>
<tr>
<td>ZPG</td>
<td>3.12</td>
<td>-69%</td>
</tr>
</tbody>
</table>

Table 7.1: Friction factors with interface \( A \).

Friction factors from the NDD simulations are always lower than the LRN or HRN values. For the Spalart-Allmaras model, \( f \) is under-predicted by around 70%. Although there is no LRN value of \( f \) for the \( k - \varepsilon \) model, all friction factors found with NDD are significantly below either the HRN \( k - \varepsilon \) or LRN Spalart-Allmaras results, which indicates that the NDD results are inaccurate.

Changing the turbulent viscosity profile has little effect on \( \varepsilon \). Friction factors for \( y^*/h = 1.2 \) are around 10% lower than those for \( y^*/h = 1.1 \) for both turbulence models and all viscosity profiles.

The low accuracy of the friction factors with NDD is caused by the low accuracy of the IBCs imposed at the interface. Near to the smooth wall of the channel, the flow is approximately one-dimensional, and resembles a channel flow. It is known from Section 6.2 that NDD performs well in such regions, and the error on the IBCs in a channel flow would not cause the 70% errors seen in Table 7.1. Hence the large errors in the friction factor are caused by inaccurate boundary conditions on the interface above the ribbed wall.

The effect that inaccurate boundary conditions on the interface have on the friction factor can be elucidated by analysing how the friction factor is related to the fluid momentum equations.

**Analysis of the pressure drop calculation**

For a steady simulation, the RANS momentum equations (Equation (2.31)) can be integrated over a volume \( \Omega \) with surface \( S \) to yield the equation

\[
\int P dS_i = \int (\mu + \mu_t) \nabla U_i \cdot dS - \int \rho U_i U \cdot dS. \tag{7.6}
\]

On the symmetry faces of the ribbed channel flow in this section, the integrals in Equa-
tion (7.6) cancel exactly. The integrals also balance exactly on the periodic boundary, except for the contribution of the pressure gradient imposed to drive the flow. At the wall, the final integral on the right hand side of Equation (7.6) is zero because of the no slip boundary condition.

The pressure gradient can be decomposed into its periodic part, \( p \), and its constant part \( s_U \) as

\[
\nabla P = \nabla p + s_U \hat{e}_x,
\]

where \( \hat{e}_x \) is a unit vector in the \( x \) direction. Because the simulations in this chapter are periodic, the total pressure drop over the domain comes entirely from \( s_U \), which applies only in the \( x \) direction. Its value can be calculated from

\[
s_U V_\Omega = \int_{\text{walls}} (\mu + \mu_t) \nabla U \cdot dS - \int_{\text{walls}} p dS_x,
\]

where \( V_\Omega \) is the volume of \( \Omega \), which in this case is the whole of the channel. The square profile of the ribs means that only the vertical walls of the ribs contribute to the last integral in Equation (7.8).

When the integrals in Equation (7.8) are computed using the LRN Spalart-Allmaras solution, they reveal that the total pressure force on the walls of the ribs is approximately five times greater than the friction at the walls. That means that only approximately one sixth of the pressure drop goes towards balancing the wall shear stress; the rest is so-called “form drag”. Hence capturing the pressure on the rib walls accurately is essential in order to calculate an accurate friction factor. If the friction factor were computed using only the contribution from the wall shear stress, the friction factor would be under-predicted by around 85%. This error is of a similar order of magnitude to the errors in the NDD friction factors in Table 7.1 and suggests that the NDD solutions significantly under-estimate the form drag in the channel.

With interface \( A \) the ribs are no longer included in the mesh of the outer domain. However, the RANS momentum equations can be integrated over the outer domain, \( \Omega_e \). Since the interfaces are planes with normals in the \( y \) direction, the pressure surface integral vanishes on the interfaces for the \( U \) equation. However, the convection term does not vanish and the integrated RANS equations become

\[
s_U V_{\Omega_e} = \int_{\text{interfaces}} (\mu + \mu_t) \nabla U \cdot dS + \int_{\text{interfaces}} \rho U U \cdot dS,
\]

where \( V_{\Omega_e} \) is the volume of the outer domain. The velocity gradient at the interface can be computed using the Robin boundary condition, and the convection term can be expanded to give

\[
s_U V_{\Omega_e} = \int_{\text{interfaces}} \left( \frac{(\mu + \mu_t)U}{f_1} - \frac{(\mu + \mu_t)f_2 U}{f_1} + \rho UV \right) dS_y.
\]
Equation (7.10) shows that with NDD, the pressure drop is determined entirely by the boundary conditions at the interfaces. More specifically, with NDD there are four separate factors that affect the friction factor:

1. The turbulent viscosity profile, which directly affects \( f_1 \).

2. The source terms used in the NDD governing equation, which directly affect \( \tilde{f}_{2,U} \). The source terms are expressed as \( R_U \) in Equation (5.3). The exact form of the source terms is
   \[
   R_U = \nabla P + \rho \mathbf{U} \cdot \nabla \mathbf{U}.
   \]

3. The solution for \( V \) at \( y^* \), which is computed using NDD.

4. The methodology used to compute \( f_1 \) and \( \tilde{f}_{2,U} \).

Thus, it should be possible to improve the friction factor predicted with NDD by improving the treatment of these factors.

Figure 7.4 shows \( \mu_t \), the components of \( R_U \) and \( V \) in the inner region, computed from the LRN Spalart-Allmaras solution over the whole domain.

Figure 7.4a shows that \( \mu_t \) varies smoothly throughout the inner region and that \( \mu_t \) increases with distance from the wall, which is consistent with the turbulent viscosity profiles used with NDD. However, just upstream and downstream of the rib, on the lines \( AA' \) and \( BB' \) in Figure 7.4a, the turbulent viscosity is small. This blocking effect is not included in any of the turbulent viscosity profiles used with NDD.

Figure 7.4b shows that the pressure gradient is constant with \( y \) across much of the region between the ribs, but varies significantly in the regions around the top corners of the rib. Note that the scale in the figure has been clipped to \( \pm 0.25 \) so that the variation between the ribs can be seen clearly; the dimensionless pressure gradient actually varies from \(-27\) to \(8.6\) in the regions circled in the figure. Hence the assumption of a constant pressure gradient is a poor one in these regions, and will reduce the accuracy of the IBCs.

So far in this thesis, the functional form of \( R_U \) used to compute IBCs ignores the convection terms. However, Figure 7.4c shows that the convection terms that affect \( U \) in the inner region are of a similar magnitude to the pressure gradient shown in Figure 7.4b. Therefore, if convection is ignored in the calculation of the IBCs, the accuracy of the NDD solution will be poor. Note that, as with the dimensionless pressure gradient, the dimensionless convection term has been clipped to \( \pm 0.25 \); whereas in reality it varies from \(-1.3\) to 31 in the regions circled in the figure.

Figure 7.4d shows that \( V \) is small over much of the region in between the ribs and on the interface. However, in the region near the upstream corner of the rib, circled in the figure, \( V \)
7.3. Simulations with interface $A$

(a) Dimensionless turbulent viscosity

(b) Dimensionless pressure gradient in the $x$ direction (clipped to $\pm 0.25$)

(c) Dimensionless convection terms affecting $U$ (clipped to $\pm 0.25$)

(d) Dimensionless wall-normal velocity

Figure 7.4: Parameters that affect the friction factor computed by NDD, shown in the inner region of the domain and calculated from the LRN Spalart-Allmaras solution.

can be non-zero and will affect the friction factor. Hence it is important to use an accurate profile of $V$ to compute the IBCs.

7.3.1 Simulations of smaller ribs with interface $A$

Figure 7.4 shows that since $R_U$ is assumed constant with $y$, it is impossible for NDD to give correct results in the flow over large ribs. However, it is anticipated that if the height of the rib is reduced, the variation of $R_U$ with $x$ will reduce until eventually a smooth channel solution is found with a rib height of zero. Therefore it may be possible to compute more accurate friction factors using NDD on a case with smaller ribs. In addition, the maximum $y^*$ with $y^* > h$ can be reduced when the ribs are smaller.
Chapter 7. Ribbed channel flow

For the NDD simulations in Table 7.1, the only difference between a simulation of a ribbed and smooth channel is the definition of $y^*$. Therefore, a further set of computations is performed where the rib height is reduced to one tenth of its original size, so that $h/H = 0.01$. The width of the rib is kept constant with $W/w = 9$. The equivalent diameter of the channel is unaffected by this modification, and the Reynolds number remains $Re = 3 \times 10^4$.

NDD simulations are performed with $y^* = 1.5h$ on the ribbed interface and $y^* = 0.5h$ on the smooth interface using the Spalart-Allmaras model with the ZPG turbulent viscosity profile.

Simulations of both a ribbed channel and a smooth channel are performed, in order to assess how the friction factor changes with NDD. The resulting friction factors are shown in Table 7.2.

<table>
<thead>
<tr>
<th>Case</th>
<th>$10^3 f$</th>
<th>$\xi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small ribbed channel</td>
<td>LRN 3.00</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>NDD 2.78</td>
<td>$-7%$</td>
</tr>
<tr>
<td>Smooth channel</td>
<td>LRN 2.79</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>NDD 2.77</td>
<td>$-1%$</td>
</tr>
</tbody>
</table>

Table 7.2: Friction factors for the ribbed channel with the Spalart-Allmaras model for a case with small ribs ($h/H = 0.01$) and a no rib (smooth channel). The NDD simulations use the ZPG turbulent viscosity profile.

The LRN results show that the friction factor for $h/H = 0.01$ is smaller than that for $h/H = 0.1$, shown in Table 7.1. The friction factor decreases further when the rib is removed and the channel is smooth. The NDD solution accurately reproduces the friction factor for the smooth channel, with an error in the friction factor of only $1\%$. However, when the rib is included the friction factor increases by only $0.5\%$ compared to the smooth channel case. In contrast, the friction factor of the channel computed with the LRN simulation increases by $7\%$ when the rib is introduced. Hence the application of NDD using the method tested in Chapter 6 does not capture the effect of the rib when the rib is included entirely within the inner region, even if the rib is small compared to the height of the channel.

7.3.2 Simulations with interface $A$ using more accurate forms of $\mu_t$ and $R_U$

The most direct way to improve the accuracy of the IBCs is to use a more accurate profile for either $\mu_t$ and/or $R_U$. The easiest way to do this is to compute the exact form of $\mu_t$ or $R_U$ from a LRN solution and use it to compute the IBCs in a simulation with NDD. With this approach, it is anticipated that the friction factors computed with NDD will be closer to the LRN values.

At first, this process appears to defeat the purpose of using NDD. If the LRN solution is
known, then there is no need to use NDD. However, the procedure outlined here may be useful in some circumstances. For example if a solution for a periodic case is known but a simulation of a larger section of the geometry must be performed, then the solution in the inner regions from the periodic case can be used to compute IBCs for a study of a larger geometry with NDD. In other situations, a solution might already be known, either from experimental data or from previous studies, and NDD can be used in parts of a study to reduce the computation time in areas of less interest. For example, if the ribbed channel of this section served as an inlet pipe to another geometry, then NDD could be used to simplify the mesh of the inlet pipe. In industrial applications it may be necessary to study the same system multiple times with similar conditions. In such cases, NDD could be used to dramatically reduce the computation time. The results of this section also perform a useful test of the implementation of NDD in Code_Saturne, since the theoretical behaviour that the friction factor becomes more accurate as $\mu_t$ and $R_U$ become more accurate can be tested.

Simulations are performed using the LRN Spalart-Allmaras model with NDD on the ribbed channel with $h/H = 0.1$. To ensure that only the treatment of the ribbed wall affects the results, the flow near the smooth wall is fully resolved, without using NDD. The inner region has $y^*/h = 1.2$ such that the inner region is the space shown in Figure 7.4. NDD simulations were run with either the ZPG turbulent viscosity profile, or the exact turbulent viscosity, taken from the LRN solution in the inner region. In this section, simulations are performed for three different forms of $R_U$, which are given codes. The first form, given the code “C”, is $R_U = \partial_x \tilde{P}$, which is the case for all the flows with IBCs in Chapter 6. The second form, given the code “P”, is $R_U = \nabla \tilde{P}$, where $\nabla \tilde{P}$ is taken from the LRN solution. The final form, given the code “F”, includes the effects of convection and is $R_U = \nabla \tilde{P} + \rho U \cdot \nabla U$, where both terms are computed from the LRN solution. In each case, the $V$ boundary conditions are computed using the usual procedure with a correction to ensure that no net flux leaves through the interface boundary.

The resulting friction factors are shown in Table 7.3. Each simulation in the table is given a name in order to facilitate the discussion of the results.

As was the case in Table 7.1, the friction factor computed with the ZPG profile with constant $R_U$ (simulation I) is smaller than the LRN value by approximately 70%. Using the exact turbulent viscosity does not lead to a significant increase in $f$ if $R_U$ is still treated as a constant, as is seen for simulation IV. Therefore the only way to improve the prediction of the friction factor is to use a more accurate form of $R_U$.

Simulations II and V, which use $R_U = \nabla \tilde{P}$ to compute $\tilde{f}_{2,U}$, yield larger friction factors than simulations I and IV. This brings the friction factor closer to the LRN value and reduces the
error, although the friction factor is now over-predicted. It is counterintuitive that the LRN form of $\mu_t$ should lead to a larger error than the ZPG profile. However, since simulations II and V ignore convection, there are multiple sources of error and it cannot be determined a priori which simulation is more accurate.

Simulations III and VI include the full effects of convection in the calculation of $\tilde{f}_2$, $U$. It is seen that this leads to a small decrease in $f$ compared to the cases with $R_U = \nabla P$, which further reduces the error in $f$. Again, the solution with the LRN form of $\mu_t$ yields a larger error in $f$ than the ZPG profile, which is counterintuitive. However, there are still errors present in the boundary conditions. The most notable are the use of a one-dimensional equation to compute the IBCs and the use of Equation (7.12) to determine the $V$ boundary conditions. Hence the apparently-superior accuracy of the friction factor with the ZPG profile is caused by different errors nullifying each other.

The results of this section conclusively show that it is possible to obtain accurate friction factors with NDD using interface $A$. For this flow, an accurate profile of $R_U$ is more important than an accurate profile of $\mu_t$ in order to compute an accurate friction factor. The approach used in this section may be useful in studies where an approximate form of $R_U$ is known a priori. This could be obtained efficiently for example from a study of a reduced portion of a geometry. Even a coarse approximation of the source terms would yield reasonably accurate friction factors. This is demonstrated by simulation II in Table 7.3, where using only the pressure gradient in $R_U$ leads to just a 7% error in the friction factor.

### 7.3.3 NDD with non-local IBCs and interface $A$

It is possible to further improve the accuracy of the simulations above that of the simulations in Section 7.3.2 by using non-local NDD, which is described in Section 5.9. As the accuracy of the simulations increases, the friction factor should approach the LRN result.
In a one-dimensional case, the Robin boundary condition in Equation (5.10), repeated below,

\[ U^* = f_{1,U} \frac{\partial U}{\partial y} \bigg|_{y^*} + \tilde{f}_{2,U}, \quad (7.11) \]

is exact provided that the turbulent viscosity and source terms, \( R_U \), are correct. However, in a two-dimensional case the expressions for \( f_{1,U} \) and \( \tilde{f}_{2,U} \) in Equations (5.8) and (5.11) are no longer exact. Non-local IBCs capture the full two-dimensional nature of the solution in the inner region. In the one-dimensional case, the boundary conditions on \( V \) are calculated with Equation 5.16, which is repeated below,

\[ V(y^*) = K \int_{\xi = 0}^{\gamma^*} \frac{d\xi}{\Gamma_V(\xi)} - \frac{\dot{m}_S}{\rho S}, \quad (7.12) \]

In this section, the flow in the ribbed channel is studied again using the non-local formulation of NDD. As discussed in Section 5.9.2, the more auxiliary functions that are computed, the more accurate the domain decomposition method. However, in this section the approach of Utyuzhnikov (2009) is used, and only two auxiliary functions are computed. Equation (5.88), repeated below,

\[ \nabla \Phi \big|_{\Gamma_i} = \Phi \big|_{\Gamma_i} \nabla W_{i,0} \big|_{\Gamma_i} + \nabla W_{i,e} \big|_{\Gamma_i}, \quad (7.13) \]

is used to apply the NLIBC. An example of using this procedure is given in Appendix D.

NLIBCs are applied to \( U \) and the auxiliary functions are denoted \( W_0 \) and \( W_U^e \), where \( W_U^e \) contains the source term \( R_U \). A simulation is also performed in which NLIBCs are applied to \( V \), with the auxiliary functions \( W_0 \) and \( W_V^e \), where \( W_V^e \) contains the source term \( R_V \). The auxiliary functions are computed using the full form of \( \mu_t \) taken from the LRN solution. The forms of \( R_U \) and \( R_V \) include both the pressure gradient and convection terms from the LRN solution. There are now only two approximations that can affect the friction factor as calculated by Equation (7.10): the number of terms included in the expansion of \( U \) on the interface in Equation (5.69), and the procedure used to calculate the IBCs for \( V \).

Three simulations are performed in this section. In the first simulation \( V \) is computed with the usual NDD approach with a correction if the mass flux through the interface is non-zero. In the second simulation, the IBC on \( V \) is computed using the non-local boundary condition in Equation (7.13) with \( W_0 \), \( W_V^e \) and the continuity correction. This boundary condition should be more accurate than in the first simulation, since the exact form of \( R_V \) is used to compute the \( V \) boundary conditions. In the third simulation, the boundary conditions on \( V \) are of Dirichlet type, where the value of \( V \) is taken from the LRN solution on the interface boundary. This is the most accurate boundary condition in the three simulations. Thus, the theoretical accuracy of the boundary conditions on \( V \) increase with every simulation. The only factor that could affect the friction factor in the third simulation is the number of terms.
used in Equation (5.69) to compute the NLIBC\(\text{s}\) for \(U\).

The friction factors from the three simulations and the corresponding errors are shown in Table 7.4. The friction factor from simulation 1 is very close to that of simulation VI in Table 7.3, which is expected since the boundary conditions are theoretically similar. The only improvement that simulation 1 has over simulation VI is that it includes streamwise gradients in the computation of the interface boundary conditions. However, since the form of \(R_U\) comes from the LRN solution, the effects of streamwise gradients are already included implicitly in simulation VI. The small difference in \(f\) between simulations 1 and VI indicates that once \(R_U\) is known, a one-dimensional governing equation is sufficient to produce accurate enough boundary conditions.

<table>
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<th>Name</th>
<th>BC on (V)</th>
<th>(10^4 f)</th>
<th>(\varepsilon)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LRN</td>
<td></td>
<td>9.97</td>
<td>—</td>
</tr>
<tr>
<td>1</td>
<td>Equation (7.12) with continuity correction</td>
<td>10.6</td>
<td>7 %</td>
</tr>
<tr>
<td>2</td>
<td>Equation (7.13) with continuity correction</td>
<td>8.64</td>
<td>-13 %</td>
</tr>
<tr>
<td>3</td>
<td>from LRN solution</td>
<td>10.0</td>
<td>&lt; 0.5 %</td>
</tr>
</tbody>
</table>

Table 7.4: Friction factors for the simulations using non-local NDD.

When the non-local formulation of NDD is used to compute boundary conditions on \(V\) in simulation 2, the friction factor decreases, and the error in \(f\) becomes larger in magnitude by a factor of approximately two. This result is counterintuitive since using the correct form of \(R_V\) to compute the NLIBC\(\text{s}\) for \(V\) should lead to a more accurate solution. However, two other factors affect the boundary conditions on \(V\). The first approximation is that two terms are sufficient in Equation (5.69) to model \(V\) in the inner region. This is a good approximation, since the results in Table 7.4 demonstrate that it is a good approximation for \(U\). The second approximation that affects the boundary conditions on \(V\) is the continuity correction. When Equation (7.13) is used, the correction to \(V\) at each boundary face required to guarantee continuity is 21 times larger than it is when the one-dimensional form of NDD is used. This behaviour is caused by the larger magnitude of \(V\) near to the upstream corner of the rib, visible in Figure 7.4d, which leads to large source terms in \(R_V\) in this region. Thus, the boundary condition on \(V\) is distorted along the interface and the accuracy of the friction factor decreases.

Equation (7.13) is a Robin boundary condition and was found to be stable in Code_Saturne. This is in contrast to the Robin boundary condition in Equation (7.11), which was found to be unstable in Code_Saturne when applied to \(V\). This behaviour is expected since Equation (7.13) is more stable because \(W_2\) is computed using a fixed value of \(R_V\), whereas in Equation (7.11), the value of \(\tilde{f}_2\) changes at each iteration.
Because simulation 2 did not yield the predicted improvement in accuracy, simulation 3 was performed, in which the boundary condition on $V$ is “exact” because it is taken from the LRN solution. No continuity correction for the $V$ boundary conditions is required in this case, since continuity is already assured in the LRN simulation. Using the exact form of $V$ leads to an improvement in accuracy in the final term in Equation (7.10). This leads to an increase in the accuracy of the friction factor, as seen in Table 7.4. The error in the friction factor is reduced to less than 0.5\%. This result demonstrates that using only two terms in the functional expansion of $U$ at the interface boundary with Equation (7.13) is sufficiently accurate for $U$. It also demonstrates that the method has been correctly implemented into Code_Saturne.

Since $W_0$ and $W_U^{U, V}$ are computed a priori, fewer calculations are required at each iteration with the approach taken in this section than were required in Section 7.3.2. This makes it more straightforward to implement non-local NDD than to implement the usual NDD method. The drawback is that $R_U$ and $\mu_t$ must be known a priori, which can only be the case if a precursor solution is performed. However, this section has demonstrated that if $R_U$ and $\mu_t$ are known accurately enough then $f$ can be accurately predicted.

### 7.4 Results with interface $B$

In Section 7.3 it was shown that an accurate solution cannot be obtained with NDD with interface $A$ unless an accurate form of $R_U$ is known in advance of the simulation. In this section, simulations are performed with NDD using interface $B$. With interface $B$, only a thin layer around the ribbed wall is included in the inner region. With such an approach there can be no wall boundary faces in the outer region, which leads to a fast computation. In addition, the convection terms may be more accurately captured with the one-dimensional NDD algorithm since most of the region in between the ribs, shown in Figure 7.4, is included in the simulation. The thickness of the removed layer is a constant fraction of the rib height. Removing a thin region above each wall is similar to the situation encountered when using a wall function, whereby the near-wall cell centres lie in a thin layer surrounding the wall. In every case, the NDD mesh was created by removing cells from the LRN mesh.

However, there are drawbacks to using interface $B$. For example, the definition of $y^*$ around the top corners above the rib is not immediately obvious. IBCs are usually derived by integrating along a line normal to the interface, however on the vertical side of the interface at $y > h$, the normal to the interface never encounters a wall. In this region, $y^*$ is taken as the distance from the top corner of the rib to the interface, as indicated by the arrows in Figure 7.2.
Friction factors from simulations with interface $B$, with $y^* = 0.2h$ on the smooth wall and either $y^* = 0.1h$ or $0.2h$ on the ribbed wall, are shown in Table 7.5. The friction factors with NDD are significantly larger than they are in Table 7.1 and are closer to the corresponding LRN/HRN results. In particular, the simulation with the Spalart-Allmaras model with the ZPG viscosity profile and $y^* = 0.1h$ yields a friction factor in excellent agreement with the LRN result. However, the same configuration with the Duprat et al. (2011) profile yields an error of 45% in the friction factor. Since the Duprat et al. (2011) profile is sensitive to the pressure gradient at the interface boundary, which Figure 7.4b shows is large, the Duprat et al. (2011) profile will predict a larger turbulent viscosity than the ZPG profile over much of the inner region. This leads to a larger friction factor.

<table>
<thead>
<tr>
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<th>$10^3 f$</th>
<th>$\varepsilon$</th>
<th>$10^3 f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LRN</td>
<td>9.97</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>HRN</td>
<td>–</td>
<td>–</td>
<td>14.0</td>
</tr>
<tr>
<td>NDD $y^* = 0.1h$</td>
<td>14.4</td>
<td>45%</td>
<td>11.9</td>
</tr>
<tr>
<td>ZPG</td>
<td>9.97</td>
<td>&lt; 0.1%</td>
<td>–</td>
</tr>
<tr>
<td>NDD $y^* = 0.2h$</td>
<td>15.1</td>
<td>51%</td>
<td>12.6</td>
</tr>
<tr>
<td>ZPG</td>
<td>11.6</td>
<td>16%</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 7.5: Overall friction factors with interface $B$.

The NDD solution converges to the LRN solution as $y^* \to 0$, regardless of the turbulent viscosity profile. The excellent agreement of the NDD solution with the ZPG profile and $y^* = 0.1h$ suggests that this convergence has been achieved, but the same case with the Duprat et al. (2011) profile demonstrates otherwise.

Sensitivity to the turbulent viscosity profile at any $y^*$ is, in general, undesirable. The ZPG and Duprat et al. (2011) profiles were found in Chapter 6 to be reliable. However, for this flow, at $y^*/h = 0.1$ they yield friction factors that differ by 45% of the LRN result. Thus for $y^*/h = 0.1$, convergence to the LRN solution has not been achieved. However, $y^*/h = 0.1$ is already a relatively small value for $y^*$. Hence there is a source of considerable error in the NDD calculations, even for smaller $y^*$, with interface $B$, which makes this shape of interface undesirable. Figure 7.4 suggests that this error is caused by neglecting the effects of pressure and convection in the circled areas, around the top corners of the rib, in the NDD governing equations.

In addition, the friction factor is seen to change as $y^*$ is increased. With the $k – \varepsilon$ model, $f$ increases by around 5% when $y^*$ changes from $0.1h$ to $0.2h$ on the ribbed wall. The variation with the Spalart-Allmaras model depends on the turbulent viscosity profile.
7.5 Results with interface C

Interface C is similar to interface A but has $y^* \leq h$. Hence part of the rib wall is included in the outer region. These simulations are performed only with the Spalart-Allmaras turbulence model, since this is a LRN turbulence model that is capable of resolving the region of the ribbed wall included in the outer region. If the HRN $k-\varepsilon$ model in Code_Saturne were used then the SWF would be used around the parts of the rib included in the outer region. This would mix two near-wall approaches in the same simulation, and complicate the analysis of the results. Simulations are run with interface C for different $y^*$ on the ribbed wall, and constant $y^*/h = 0.2h$ on the smooth wall. As usual, in every case, the NDD mesh is created by removing cells from the LRN mesh.

The Duprat et al. (2011) and ZPG viscosity profiles are used for the simulations with NDD. The overall friction factors from these simulations are displayed in Figure 7.5 alongside the LRN result. Also shown in Figure 7.5 are the friction factors computed with interface A, where $y^*/h > 1$, using the Spalart-Allmaras and $k-\varepsilon$ models. These friction factors are also shown in Table 7.1.

Figure 7.5 shows that as $y^* \to 0$ the friction factor found with NDD converges to the LRN value with both the Duprat et al. (2011) and ZPG profiles. However, as $y^*$ increases the friction factor increases significantly with the Duprat et al. (2011) profile such that by $y^*/h = 0.9$, the friction factor is almost double the LRN value. In contrast, the ZPG profile yields an almost constant friction factor, which varies by less than 2.5% of the LRN value up to and including $y^*/h = 0.9$. This difference in behaviour indicates that the Duprat et al. (2011) profile is less accurate than the ZPG profile on this flow. This is caused by the sensitivity...
of the Duprat et al. (2011) profile to the pressure gradient, which is large between the ribs. Hence the Duprat et al. (2011) profile predicts a larger turbulent viscosity than the ZPG profile in between the ribs. However, in reality the turbulent viscosity is small over much of this region. Thus the ZPG profile performs better.

The friction factor decreases significantly for \( y^* \geq h \), where interface A is used, as discussed in Section 7.3. This result indicates that without any prior knowledge of \( R_U \) in the inner regions, it is essential to include the top corners of the ribs in the NDD simulations in order to accurately estimate the friction factor.

In Figure 7.6, \( C_f \), \( C_P \) and \( Nu \) are plotted in between the ribs, as well as \( U \) at \( y/h = 0.1 \) and \( V \) at \( y/h = 1 \). The NDD results were computed with the ZPG viscosity profile. The LRN simulation predicts \( C_P \), \( U \) and \( V \) with good enough accuracy compared to the data of Rau et al. (1998), however the Nusselt number is under-predicted by around half. More sophisticated \( \overline{u'^2} - f \) models make better predictions of the Nusselt number (Keshmiri and Gotts, 2011).

In every plot, the NDD solution converges to the LRN solution as \( y^* \to 0 \), which is the expected behaviour, with the notable exception of the Nusselt number in Figure 7.6d. For \( 2 \leq x/h \leq 7 \), the NDD solution converges to the LRN solution as \( y^* \to 0 \). However, near to the rib corners at \( x/h = 0.5 \) and \( x/h = 8.5 \), the NDD solution becomes increasingly
7.5. Results with interface C

Figure 7.6: Results for different $y^*$ with the Spalart-Allmaras model with the ZPG profile.
inaccurate as $y^* \to 0$. Despite this, in the limit $y^* = 0$, the NDD solution coincides exactly
with the LRN solution, since the governing equations are then identical.

The poor agreement at small $y^*$ is caused by the vertical wall of the rib. As the vertical wall
of the rib is approached ($x/h \to 0.5$ or $x/h \to 8.5$), there is a region in which both the bottom
wall of the channel and the vertical wall of the rib must be considered when computing the
IBCs. Hence in this region the NDD governing equations are not one-dimensional. However,
the one-dimensional boundary layer equation is used to compute IBCs by integrating along
a line from the interface to the bottom wall of the channel. Very near to the vertical wall of
the rib, the contribution to the temperature of the bottom wall of the channel is negligible
compared to the vertical wall of the rib. However, with NDD, the lower wall is the only wall
that is considered. Since the interface boundary is located relatively far from the bottom
wall of the channel and the contribution from the heated vertical wall of the rib is ignored,
the temperature at the interface is computed to be lower than it should be (since the walls
are heated). Likewise, the temperature at the wall, which is computed using Equation (5.26),
is also under-predicted since it depends on the temperature at the interface. However, the
bulk temperature is determined mainly by the flow in the outer region. Therefore, $T_w - T_b$
is under-predicted near to the vertical walls of the rib, which according to Equation (7.3),
leads to the increase in the Nusselt number, visible in Figure 7.6d.

The error in $Nu$ at the rib corners is most pronounced for the smallest $y^*$. This is because
for small $y^*$, the temperature at the wall computed by Equation (5.26) is most similar to
the temperature at the interface, since the magnitude of the integrals in Equation (5.26) is
smaller. Hence the outer region has less effect on $T_w$, and so cannot compensate for any
errors. Therefore $T_w - T_b$ is smallest for smaller $y^*$ near the rib corners, which leads to a
larger Nusselt number for smaller $y^*$.

As $y^*$ increases, the accuracy of all profiles in Figure 7.6 decreases. This trend continues up
to $y^*/h = 0.9$. These results are not displayed in Figure 7.6 because they skew the scales
of the graphs and because there is no reason they should be expected to be accurate with
such large $y^*$. A notable exception to this trend is $V$, shown in Figure 7.6f, which remains
accurate up to and including $y^*/h = 0.9$. This is because $V$ is plotted at $y/h = 1$, which is
in the outer region for $y^*/h < 1$. 
7.6 Example of a parametric design optimisation with interface C

Since the friction factor found with NDD with the ZPG profile is insensitive to \( y^* \), it is possible to study different rib heights with the same mesh. This allows a parametric design study to be performed straightforwardly, using only one mesh to study multiple rib heights. A new rib height is simulated by changing the definition of \( y^* \), which is a parameter in the NDD model. The results of Section 7.5 indicate that at least the top parts of the rib must be included in the mesh; therefore there is a minimum rib height that can be studied with a particular mesh, which is Reynolds number-dependent. The results in this section are for \( Re = 3 \times 10^4 \). In Chapter 8, similar ribbed flows are studied at larger Reynolds numbers up to \( 1.1 \times 10^6 \). In these cases the portion of the rib that must be included in the mesh is larger.

In this section, the mesh contains a rib of height \( h/H = 0.04 \), and corresponds to the mesh with \( y^*/h = 0.6 \) in Section 7.5. With this mesh it is possible to study any rib height \( h \geq 0.04H \) using NDD. In this section, \( y^* \) is defined such that the rib height in each simulation is \( h = 0.04H + y^* \). Simulations are performed in this section using the Spalart-Allmaras model with the ZPG viscosity profile. LRN computations are also performed for each rib height studied. For the LRN computations, a new mesh is generated for each rib height. Each NDD computation is initialised with the solution for the nearest rib height. The rib heights range from \( h/H = 0.05 \) to \( h/H = 0.1 \). The resulting friction factors are displayed in Figure 7.7.

The error in the NDD value of \( f \), expressed as a percentage of the LRN value, is always less than 2% for every rib height tested. The under-estimation of the friction factor is caused by effects occurring in the outer region, since the difference between the NDD and LRN value of \( f \) is constant for each rib height. If the mesh with \( y^*/h = 0.5 \) in Figure 7.5 had been used, the error in the corresponding version of Figure 7.7 would have been smaller. Regardless, the agreement between the LRN and NDD values of \( f \) in Figure 7.7 is excellent and would be of use in a parametric design optimisation study.

For example, a CFD model of a large fluid system can take a long time to converge. If part of the model contains a ribbed channel, and the objective is to optimise the rib height based on the friction factor, then the portion of ribbed channel in the system could be modelled with NDD. The value of \( y^* \) could be updated as the simulation converges, which allows the rib height to be optimised in a single computation, without having to perform separate computations with different meshes. This would lead to a significant saving of computation time.
Chapter 7. Ribbed channel flow

Figure 7.7: Friction factors for different rib heights computed with the Spalart-Allmaras model. The NDD simulations use the ZPG viscosity profile.

7.7 Conclusions

In this chapter it has been demonstrated that NDD can be used on the ribbed channel provided that:

- Either the form of $R_U$ is known in advance of the simulation, in which case interface $A$ can be used.
- Or the top corners of the rib are included in the outer region, in which case the Spalart-Allmaras model with the ZPG turbulent viscosity profile yields accurate friction factors.

The other conclusions that can be drawn from this chapter are that:

1. Applying NDD to the ribbed channel using the one-dimensional formulation of NDD tested in Chapter 6 and including the entire rib in the inner region leads to friction factors smaller than the LRN value by around 70%. Even in the case with small ribs, the friction factor predicted by NDD is closer to that of a smooth channel than a ribbed channel. The only way to obtain reliable and accurate friction factors, whilst still including the rib in the inner region, is to perform a precursor simulation in which the form of $R_U$ can be computed. If this form of $R_U$ is used to compute $\tilde{f}_{2U}$, then
the friction factors obtained with NDD are more accurate, with errors of less than 10% possible.

2. Using the non-local formulation of NDD, with the source terms computed from a precursor simulation, does not lead to significant improvements in the accuracy of the friction factor compared to the one-dimensional formulation of NDD. However, a significant improvement in the accuracy of the friction factor is seen if the exact boundary condition on $V$, taken from a LRN simulation, is imposed at the interface. Although this requires that a precursor simulation be performed, situations exist where such an approach is useful.

3. The one-dimensional formulation of NDD can yield accurate friction factors on the ribbed channel if the top corners of the rib are included in the mesh of the outer region. With the Spalart-Allmaras model with the ZPG viscosity profile, the error on the friction factor is less than 2.5% even when 90% of the height of the rib is included in the inner region.

4. When the top corners of the rib are included in the mesh of the outer region, simulations with a range of $y^*$ can be performed to study different rib heights with the same mesh. Hence NDD can be used for design optimisation problems without having to generate a new mesh in each case. This is useful for CFD models of large systems where the aim is to optimise a rib height. Only one mesh needs to be created, and the rib height can be changed by varying $y^*$ as the simulation converges. This leads to a significant saving of computation time.

5. Although the friction factor is accurately predicted with NDD for a large range of $y^* < h$, profiles of local properties such as the velocity or wall shear stress are only accurate for smaller $y^*$. 
Chapter 8

Industrial flows

This chapter contains results of flows in annular passages, where the inner surface of the annulus may contain a rib that protrudes into the passage. The inner surface is a model of a “fuel pin”, and is referred to as a pin. Flows over fuel pins were studied extensively by the Central Electricity Generating Board (CEGB) during the development of the AGR. In an AGR, the fuel pins house the fuel, which is where heat is generated. Carbon dioxide flows over the surface of the fuel pins to cool them.

The flows performed in two experimental studies are repeated in this chapter. The studies are those of Watson (1970) and Pirie (1974). The results of this chapter have been included in two reports, which were submitted to EDF Energy Generation during the EngD. These reports have been added to the document repository at EDF Energy Generation and have the reference numbers TSK9969/2015/1 and TSK9969/2015/2.

In normal circumstances, an AGR fuel assembly contains 36 fuel pins in the arrangement shown in Figure 8.1c. The fuel pins shown in Figure 8.1a are called “multistart” pins and the ribs are situated along the fuel pin in a helix. Figure 8.1b is a cross section of a rib along the axis of the pin. Both left- and right-handed pins are inserted into the fuel assembly in an arrangement that enhances flow mixing and heat transfer. Pins can also have “transverse” ribs, where the ribs form continuous rings around the pin.

The pin is characterised by parameters such as the rib angle, height and pitch. The optimal values of these were determined experimentally during the development of the AGR. One of the objectives of this chapter is to assess the accuracy of CFD on flows of this type, and to investigate the quality of the experimental data.

In normal operation, a deposit of carbon forms on the surface of the fuel pins in an AGR. The geometry of the deposit is complex, however its impact on the pin can be split into two main effects. The first effect is that the deposit fills in part of the region between the ribs,
8.1 Introduction

During the development of the AGR, many experiments were performed to study the pressure drop of different geometries of fuel pins. For simplicity, it was usual to study just one fuel pin placed concentrically in a smooth pipe. In particular, Watson (1970) studied the flow of either CO$_2$ or air over four fuel pins, one of which had no rib and the other three had transverse ribs. Pirie (1974) studied the flow of CO$_2$ over ten fuel pins, two of which had transverse ribs and the other eight had multistart ribs. The pins studied by Watson (1970) and Pirie (1974) differ in the number of rib starts, the rib angle of attack, the rib pitch and the rib height. The geometries of every pin and pipe combination studied in this chapter are given in Table 8.1. Each geometry is referred to as a “surface”. Surfaces 0 and 1 were studied by Watson (1970), and surfaces 1 to 10 were studied by Pirie (1974). Surface 1 was studied by both Watson (1970) and Pirie (1974). The names of the surfaces in Table 8.1 correspond to the names given to the surfaces by Pirie (1974) with the exception of surface 0, the name for which is introduced in this thesis.

A schematic of the geometry of a single pin in an annulus is shown in Figure 8.2. The pin root radius is the radius of the pin (ignoring the rib) and is denoted $R_1$. The radius of the
Chapter 8. Industrial flows

Table 8.1: Geometry of the 11 surfaces studied in this chapter. Surfaces 0 and 1 were studied by Watson (1970) and surfaces 1 to 10 were studied by Pirie (1974).

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<th>Surface</th>
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<th>Pipe radius $R_2$ /mm</th>
<th>Pitch $W$ /mm</th>
<th>Rib height $h$ /mm</th>
<th>Starts $N$</th>
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<td>9</td>
<td>24.15</td>
<td>52.05</td>
<td>8.46</td>
<td>1.14</td>
<td>32</td>
<td>60</td>
</tr>
<tr>
<td>10</td>
<td>24.15</td>
<td>52.05</td>
<td>8.46</td>
<td>1.14</td>
<td>32</td>
<td>60</td>
</tr>
</tbody>
</table>

smooth pipe into which the pin is placed is denoted $R_2$. In the experiments, the pipe was the same for every flow, however the value of $R_2$ for surface 0 is slightly different to the others because it has been converted into millimetres from the value in inches reported by Watson (1970). The length in the axial direction between identical points on a rib is the pitch and is denoted $W$. The axial rib pitch to rib height ratio is almost the same for every surface and ranges from 7.1 to 7.4.

Figure 8.2: Schematic of the end-on view of the geometry of a single multistart pin in an annulus.

All ribs have a square cross-section when measured in a $(r, z)$ plane, where $z$ is aligned with the axis of the pin and $r$ is the radial coordinate. The height of the rib measured in the radial direction is $h$. The width of the rib, measured in the axial direction is $w$ and for the
surfaces in Table 8.1, \( w = h \). The number of rib starts, \( N \), is defined as the number of ribs around the pin in an arbitrary slice in an \((r, \phi)\) plane at constant \( z \). For a transverse rib, \( N \) is defined as zero. The angle that the ribs make with an \((r, \phi)\) plane, \( \alpha \), is given explicitly in Pirie (1974), however it can also be calculated from \( R_1 \), \( N \) and \( W \) as

\[
\tan(\alpha) = \frac{NW}{2\pi R_1}.
\]  

(8.1)

The values of \( \alpha \) in Table 8.1 are those reported in Pirie (1974).

Of the 11 surfaces in Table 8.1, surfaces 0, 1 and 6 are studied the most extensively in this chapter. Surface 6 most closely resembles the multistart fuel pins in an AGR fuel assembly. It has a rib angle of 33°, a rib pitch to height ratio of 7.4 and 12 rib starts. AGR multistart fuel pins have a rib angle of 34°, an axial rib pitch to height ratio of 6.5 and 12 rib starts.

Figure 8.3 shows photographs of surfaces 1 and 6. These are the pins that were used in the experiments of Pirie (1974). The pipe wall is not shown.

![Photographs of surfaces 1 and 6 from Pirie (1974). The pipe wall is not shown.](image)

(a) Surface 1

(b) Surface 6

Figure 8.3: Photographs of surfaces 1 and 6 from Pirie (1974). The pipe wall is not shown.

### 8.1.1 Computations performed

For consistency with Watson (1970), the Reynolds number is defined as

\[
Re = \frac{\rho U_b d_e}{\mu},
\]

(8.2)

where the bulk velocity is \( U_b = \dot{m}/A \), where \( \dot{m} \) is the mass flow rate and \( A \) is the area between two cylinders of radii \( R_2 \) and \( R_1 \), ignoring the rib.

Table 8.2 shows the Reynolds number of each simulation for each surface. Each run is referred
to by a name. For example, S1R3 refers to run 3 of surface 1, which has a Reynolds number of $Re = 5.26 \times 10^5$. There appears to be an error in Pirie (1974) for S4R8 where the Reynolds number is listed as $123.35 \times 10^5$. It has been assumed that this should be $12.35 \times 10^5$. The Reynolds number increases as the run number increases. There are extra runs for surface 1 since it was studied by both Watson (1970) and Pirie (1974). The runs for surface 1 performed by Watson (1970) are denoted by letters instead of numbers. The runs for surface 0 have numerical names even though they were only performed by Watson (1970).

At the conditions in the experiments, the mach number of every flow in Table 8.2 is below 0.1, which indicates that compressibility effects are not important.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Run 1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.58</td>
<td>3.50</td>
<td>5.08</td>
<td>7.73</td>
<td>9.53</td>
<td>11.25</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2.72</td>
<td>3.61</td>
<td>5.26</td>
<td>6.76</td>
<td>8.72</td>
<td>10.44</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2.52</td>
<td>3.18</td>
<td>3.91</td>
<td>4.96</td>
<td>6.16</td>
<td>7.22</td>
<td>9.39</td>
<td>11.38</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2.64</td>
<td>3.29</td>
<td>4.10</td>
<td>5.04</td>
<td>6.52</td>
<td>7.75</td>
<td>9.97</td>
<td>12.22</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1.54</td>
<td>2.81</td>
<td>3.46</td>
<td>4.35</td>
<td>5.20</td>
<td>6.53</td>
<td>7.89</td>
<td>10.28</td>
<td>12.35</td>
</tr>
<tr>
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<td>2.58</td>
<td>3.53</td>
<td>4.52</td>
<td>4.57</td>
<td>6.54</td>
<td>7.78</td>
<td>9.86</td>
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<tr>
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<td>6.91</td>
<td>8.56</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>2.73</td>
<td>3.46</td>
<td>4.53</td>
<td>5.29</td>
<td>6.44</td>
<td>7.63</td>
<td>9.84</td>
<td>12.08</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>2.60</td>
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<td>3.78</td>
<td>5.72</td>
<td>6.74</td>
<td>8.72</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>2.82</td>
<td>3.52</td>
<td>4.43</td>
<td>5.26</td>
<td>6.79</td>
<td>8.00</td>
<td>10.41</td>
<td>11.62</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2.79</td>
<td>3.39</td>
<td>3.98</td>
<td>4.62</td>
<td>6.05</td>
<td>7.12</td>
<td>9.31</td>
<td>11.60</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Surface</th>
<th>Run A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.87</td>
<td>2.38</td>
<td>1.79</td>
<td>1.35</td>
<td>0.86</td>
<td>5.21</td>
</tr>
<tr>
<td>1</td>
<td>2.58</td>
<td>3.50</td>
<td>5.08</td>
<td>7.73</td>
<td>9.53</td>
<td>11.25</td>
</tr>
</tbody>
</table>

Table 8.2: Reynolds numbers of every run with each surface of Watson (1970) and Pirie (1974). Each run is referred to by a name. S1R3 refers to surface 1, run 3. There appears to be an error in Pirie (1974) for S4R8, where the Reynolds number is reported to be $123.35 \times 10^5$.

### 8.1.2 Computation outputs

Watson (1970) and Pirie (1974) report the friction factor, $f$, for each surface, which is calculated as

$$f = \frac{d_e A^2 \rho}{\dot{m}^2} = \frac{dP}{dz} \left( \frac{dT_g}{dz} \frac{\dot{m}^2}{\bar{T}_g \rho A^2} - \left| \frac{dP}{dz} \right| \frac{\dot{m}^2}{P \rho A^2} \right),$$

(8.3)

where $dP/dz$ is the average pressure gradient over the annulus and $\bar{P}$ is the mean pressure. The quantity $\bar{T}_g$ is the mean gas temperature, and $dT_g/dz$ is the change in gas bulk temperature per unit length.

Equation (8.3) can be expressed in terms of the bulk velocity as

$$f = \frac{d_e}{2W} \left( \frac{\left| \Delta P \right|}{\rho U_b^2} - \frac{\Delta T_g}{\bar{T}_g} - \frac{\left| \Delta P \right|}{\bar{P}} \right),$$

(8.4)

where $\Delta P$ is the pressure change per unit rib pitch and $\Delta T_g$ is the change in bulk gas
8.1. Introduction

temperature per unit rib pitch.

Although it is not completely clear how $T_g$ and $P$ were determined in the experiments, the contribution from these two terms to the friction factor is small. This is demonstrated now, using the results for S1RE, the data for which are given in Table 8.3, wherein $\dot{q}'$ is the heat input per unit length of pipe.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>$2.15 \times 10^{-5}$ kg m$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>3.33 kg m$^{-3}$</td>
</tr>
<tr>
<td>$U_b$</td>
<td>10.9 m s$^{-1}$</td>
</tr>
<tr>
<td>$T_g$</td>
<td>369 K</td>
</tr>
<tr>
<td>$\bar{P}$</td>
<td>353 kPa</td>
</tr>
<tr>
<td>$\dot{q}'$</td>
<td>2.3 kW m$^{-1}$</td>
</tr>
<tr>
<td>$A$</td>
<td>$6.28 \times 10^{-3}$ m$^2$</td>
</tr>
<tr>
<td>$dP/dz$</td>
<td>185 Pa m$^{-1}$</td>
</tr>
</tbody>
</table>

Table 8.3: Flow data and results for S1RE of Watson (1970).

Using the specific heat capacity of $c_p = 1.01$ kJ kg$^{-1}$ K$^{-1}$, the average bulk temperature change per unit length can be approximated as

$$\frac{\Delta T_g}{W} \approx \frac{\dot{q}'}{\rho U_b A c_p} \approx 10 \text{ K m}^{-1}. \quad (8.5)$$

With a pitch $W = 4.93$ mm, this gives

$$\frac{\Delta T_g}{T_g} \approx 1.3 \times 10^{-4}, \quad (8.6)$$

for one rib pitch. This can be compared to

$$\frac{|\Delta P|}{\bar{P}} \approx 2.6 \times 10^{-6}, \quad (8.7)$$

and

$$\frac{|\Delta P|}{\rho U_b^2} \approx 2.6 \times 10^{-3}. \quad (8.8)$$

This demonstrates that $|\Delta P|/\bar{P} \ll \Delta T_g/T_g$ and $\Delta T_g/T_g < |\Delta P|/(\rho U_b^2)$. Therefore to a good approximation the overall friction factor of the annulus can be expressed as

$$f = \frac{d_e |\Delta P|}{2W \rho U_b^2}. \quad (8.9)$$

Equation (8.9) is used to compute $f$ in the CFD calculations and means that the temperature equation does not need to be solved in order to compute the friction factor.

In practice, calculating $f$ in this way is likely to produce an over-estimate because the next largest term in Equation (8.3) is the term involving the temperature, which would decrease $f$. For example, the above calculations indicate that for S1RE, the effect of the temperature term in Equation (8.3) is to reduce the friction factor by approximately 5%.
Chapter 8. Industrial flows

The error in the friction factor is computed in terms of the experimental value, \( f_{\text{expt}} \) as

\[
\mathcal{E} = 100\% \times \left( f_{\text{CFD}} - f_{\text{expt}} \right) / f_{\text{expt}},
\]

where \( f_{\text{CFD}} \) is the friction factor from a CFD simulation. Values of \( \mathcal{E} \) are reported for some results in this chapter.

Stanton numbers are also reported in Pirie (1974). The experimental reports do not explain in detail how the Stanton number is calculated for the ribbed pins. However for the CFD results, the Stanton number is calculated for each boundary face as

\[
St = \frac{\dot{q}_w''}{\rho U_b c_p (T_w - T_b)}.
\]

The pin and rib surfaces are given a constant heat flux boundary condition, with the same heat flux everywhere on the surface. The pipe wall is insulated and is given a zero heat flux condition. The Prandtl number is quoted in Pirie (1974) as \( \sigma = 0.76 \), however it is not given in Watson (1970). In the CFD calculations, the Prandtl number is taken as \( \sigma = 0.71 \). The turbulent Prandtl number is \( \sigma_t = 1 \).

8.2 Smooth pins

Surface 0, which has a smooth pin, is similar to the annulus studied in Section 6.3. However the runs in this chapter have Reynolds numbers an order of magnitude larger. The smooth annulus is studied with the LRN \( k-\varepsilon \) (Chien, 1982) and Spalart-Allmaras turbulence models, the HRN \( k-\varepsilon \) model with the SWF, and with NDD using the Spalart-Allmaras and HRN \( k-\varepsilon \) models. The geometry of the mesh is shown in Figure 8.4, which is similar to that used in Section 6.3. In all cases the mesh contains one cell in the axial and azimuthal directions.

The LRN mesh has 522 cells in the radial direction. NDD meshes are created by removing cells from the LRN mesh that lie within the inner regions. The interfaces have the same radial extent at each wall, with \( y^*/d_e = 1 \times 10^{-3}, 5 \times 10^{-3}, 10 \times 10^{-3} \) or \( 20 \times 10^{-3} \). The mesh with \( y^*/d_e = 1.0 \times 10^{-3} \) is not studied with the HRN \( k-\varepsilon \) model because the maximum \( y^*_+ \) is too small for the model. The meshes used with the SWF have cell centres at the same location as the interface boundaries in the NDD meshes. The SWF meshes have 209, 104 and 13 cells, corresponding to \( y^*/d_e = 5 \times 10^{-3}, 10 \times 10^{-3} \) and \( 20 \times 10^{-3} \), respectively.

NDD results are computed using the piecewise linear viscosity profile for the \( k-\varepsilon \) model and the ZPG viscosity profile for the Spalart-Allmaras model.
8.2. Previous studies

There have been many studies of flows in smooth annuli over the last century. A review can be found in Childs and Long (1996). Experimental results have often been used to develop correlations for the friction factor and Nusselt number. These correlations are useful to compare simulation results against.

Jones Jr. and Leung (1981) found that if a new Reynolds number, $Re^* = Re \phi^*$ is introduced, then correlations for the friction factor in a pipe can also be used for flows in smooth annuli. The parameter $\phi^*$ depends on the radius ratio, $a = R_1/R_2$, as

$$\phi^* = \frac{1}{(1-a)^2} \left( 1 + a^2 + \frac{(1-a^2)}{\ln(a)} \right),$$

which for surface 0 is $\phi^* = 0.672$. The correlation for $f$, which is valid for $Re^* \gtrsim 7000$, is the Prandtl correlation for the friction factor in a smooth pipe (Jones Jr. and Leung, 1981)

$$\frac{1}{\sqrt{f}} = 4 \log_{10} \left( Re^* \sqrt{f} \right) - 0.4.$$  \hfill (8.13)

The Reynolds numbers for surface 0 in Table 8.2 correspond to $Re^*/10^5 = 1.73, 2.35, 3.41, 5.19, 6.40$ and 7.56. These are larger than those in Jones Jr. and Leung (1981), however the Prandtl correlation is valid up to $Re \approx 10^6$ (White, 2006) so it is likely to be valid for these flows.

Another correlation is that of Kaneda et al. (2003), who numerically integrated the momentum equations using a correlation for the turbulent shear stresses. The resulting correlation for the friction factor is complex, but can be simplified by assuming that the friction factor is independent of the ratio $R_1/R_2$. This is reported to be a good approximation (Kaneda et al., 2003). The simplified form of the correlation is (Kaneda et al., 2003)

$$\sqrt{2/f} = 1.610 + \frac{\ln(Re)}{0.436} - \frac{550 \sqrt{2/f}}{Re} - \frac{\ln(\sqrt{2/f})}{0.436},$$  \hfill (8.14)

for $Re \gtrsim 1 \times 10^4$. Equation (8.14) has been shown to produce agreement with experimental data up to $Re \approx 10^6$.  

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Heat transfer correlations often report the Nusselt number, which is related to the Stanton number as $Nu = St \sigma \Theta Re$. One of the earliest studies was performed by Kays and Leung (1963) and is still widely used. Kays and Leung (1963) used empirical eddy diffusivity profiles to produce tabulated values of $Nu$ for different wall boundary conditions, Reynolds numbers, Prandtl numbers and radius ratios. More recently, Yu et al. (2005) used empirical correlations for the turbulent fluctuations and the turbulent Prandtl number to compute various parameters which can be used to calculate the Nusselt number. The correlations of Kays and Leung (1963) and Yu et al. (2005) are reported as tabulated data. Consequently the correlations are, by definition, valid at the Reynolds numbers at which they are used.

### 8.2.2 Results and discussion

The range of $y^*/d_e$ used with NDD and the corresponding $y^*_{+\tau}$ on the outer wall is given in Table 8.4 for the results for S0R1 with the Spalart-Allmaras model. The inner wall has a larger $y^*_{+\tau}$, and other runs have larger Reynolds numbers, which leads to even larger values of $y^*_{+\tau}$. The largest $y^*_{+\tau}$ occurs on the inner wall for S0R6 with $y^*/d_e = 20 \times 10^{-3}$ and is equal to 971.

<table>
<thead>
<tr>
<th>$10^5 y^*/d_e$</th>
<th>1</th>
<th>5</th>
<th>10</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y^*_{+\tau}$</td>
<td>12</td>
<td>58</td>
<td>118</td>
<td>232</td>
</tr>
</tbody>
</table>

Table 8.4: The range of $y^*$ and the corresponding value of $y^*_{+\tau}$, which applies to the outer wall, for S0R1 with the Spalart-Allmaras model.

The friction factors from the LRN, HRN and NDD simulations are plotted against the experimental data and the correlations of Jones Jr. and Leung (1981) and Kaneda et al. (2003) in Figure 8.5. Figure 8.5a shows results for the $k-\varepsilon$ model and Figure 8.5b shows results for the Spalart-Allmaras model. The HRN $k-\varepsilon$ results with the SWF are in close agreement with the LRN results and the correlations of Kaneda et al. (2003), and agree well with the experimental result at the lowest Reynolds number. The NDD $k-\varepsilon$ friction factors are largest, and agree well with the experimental results at the highest Reynolds number. Except for the smallest Reynolds numbers, the NDD friction factors are always in closer agreement with the experimental results than the other $k-\varepsilon$ results. Since the LRN model is that of Chien (1982), whereas the NDD and SWF results are computed using the HRN $k-\varepsilon$ model, there is no particular reason why the NDD or SWF results should agree with the LRN results. Neither the SWF nor NDD friction factors vary significantly with $y^*$. The trend of $f$ with $Re$ is similar between all CFD results and the correlations.

LRN and NDD friction factors with the Spalart-Allmaras model are in good agreement with the experimental values, and are larger than the friction factor predicted by either correlation.
Figure 8.5: Friction factors for surface 0, showing LRN, HRN and NDD results against the experimental data of Watson (1970) and Pirie (1974) and the correlations of Kaneda et al. (2003) and Jones Jr. and Leung (1981).
When an allowance is made for experimental error, the trend in \( f \) with \( Re \) is similar between all results. The NDD results show little sensitivity to \( y^* \) and are in close agreement with the LRN results. There is clear convergence to the LRN result as \( y^* \to 0 \). As \( y^*/d_e \) increases, the friction factor tends to increase, but the deviation from the LRN result is never larger than 3\% in Figure 8.5b.

The friction factors with NDD vary less with \( y^* \) than they did in Section 6.3. This is because higher Reynolds numbers are studied in this chapter, and at higher Reynolds numbers the maximum \( y^*_+ \) in the annulus is larger and so the boundary layer near to the walls is better-defined.

The Stanton numbers are plotted in Figure 8.6, which also shows the tabulated data of Kays and Leung (1963) for \( \alpha = 0.5 \) and \( \sigma_\Theta = 0.7 \) and of Yu et al. (2005) for \( \alpha = 0.5 \) and \( \sigma_\Theta = 0.76 \). Figure 8.6a shows results for the \( k-\varepsilon \) model and Figure 8.6b shows results for the Spalart-Allmaras model.

All Stanton numbers computed with a \( k-\varepsilon \) model are smaller than the experimental results, however the values computed with NDD are the most similar. Stanton numbers computed with the SWF are the smallest. The LRN results are smaller than the experimental data, and the correlation of Kays and Leung (1963) but are in close agreement with the correlation of Yu et al. (2005). Neither the NDD nor SWF results show significant sensitivity to \( y^* \). The trend in \( St \) with \( Re \) is similar in all sets of results.

As with the friction factor, the LRN Spalart-Allmaras Stanton numbers are in agreement with the experimental data. The NDD results show little sensitivity to \( y^* \) and are in close agreement with the LRN results. The maximum discrepancy between the LRN and NDD Stanton numbers is less than 0.5\%. All Stanton numbers computed with the Spalart-Allmaras model are below the experimental values and above both the data of Kays and Leung (1963) and Yu et al. (2005), however the difference is smaller than for the \( k-\varepsilon \) model. The trend of \( St \) with \( Re \) is similar in all data plotted in Figure 8.6b.

The differences between the LRN \( k-\varepsilon \) and Spalart-Allmaras results for both \( f \) and \( St \) can be used to quantify the uncertainty associated with the computational model. Since at the lowest Reynolds number the LRN \( k-\varepsilon \) model is closer to the experimental result and at the largest Reynolds number the Spalart-Allmaras model is closer, it can be inferred that the modelling and experimental uncertainties in \( f \) are similar, although there could be undiagnosed systematic errors in the experimental data. When NDD is used, the \( k-\varepsilon \) and Spalart-Allmaras results agree more closely with the experimental results than when the LRN or HRN forms are used. This is despite the fact that different turbulent viscosity profiles are used for the two turbulence models with NDD.
8.2 Smooth pins

Figure 8.6: Stanton numbers for surface 0, showing LRN, HRN and NDD results against the experimental data of Watson (1970) and Pirie (1974) and the correlations of Yu et al. (2005) and Kays and Leung (1963).

(a) $k - \varepsilon$

(b) Spalart-Allmaras
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In Figure 8.6 both the $k-\varepsilon$ and Spalart-Allmaras models predict values of $St$ that are smaller than the experimental results. The spread in $St$ between the CFD models is larger than it is in the experimental results, however the trend in the $St$ with $Re$ is clearer in the CFD results. This implies that the random error in the experimental data is smaller than the uncertainty in the CFD results, although there may be unknown and unquantifiable systematic errors in the experimental results that affect the trend.

When discussing the results, Watson (1970) states that:

*Although the test surfaces may be aerodynamically smooth the slightest protuberance on a pressure tapping, or a centralising support can have a large effect on performance. It follows, therefore, that measured friction factors will always tend to be higher than the true values."

Hence there may be systematic errors in the experimental results, which cause both $f$ and $St$ to be over-predicted. Since the experimental procedure followed by Watson (1970) is similar to that followed by Pirie (1974), similar errors may be present in the results for the ribbed pins.

As discussed in Section 8.2.1, the correlations used in this section are within their ranges of applicability. The correlations of Jones Jr. and Leung (1981) and Kays and Leung (1963) are based on experimental data whereas the correlations of Kaneda et al. (2003) and Yu et al. (2005) are based on numerical calculations. Thus, while there may be systematic errors in the results used to build the experiment-based correlations, the numerical correlations are free from systematic experimental errors. In Figure 8.5, the correlation of Kaneda et al. (2003) yields friction factors lower than those of Jones Jr. and Leung (1981) by approximately 5%. Likewise, in Figure 8.6, the correlation of Yu et al. (2005) yields Stanton numbers lower than those of the data of Kays and Leung (1963) by approximately 5%. Thus, any systematic errors in the experimental correlations, for both the friction factor and the Stanton number are likely to be less than 5%. An estimate of the systematic errors in the experimental data for both $f$ and $St$ can be found by comparing the experimental data to the correlations in Figures 8.5 and 8.6. The correlations imply that the experimental results over-predict both $f$ and $St$, since all experimental data are above the correlations for both $f$ and $St$, with the exception of $f$ for S0R1. The over-prediction is no more than 10% in both $f$ and $St$, compared to the correlations in Figures 8.5 and 8.6.

When validating Equation (8.13), Jones Jr. and Leung (1981) found that much of the available experimental data was of poor quality and therefore unreliable. They emphasised the importance of validating the experimental procedure by computing friction factors in the laminar flow regime, where an analytical expression for $f$ exists. Thus it is not unusual for
experiments of annular flows to be affected by significant experimental errors, especially at
the time when the experiments of Watson (1970) and Pirie (1974) were performed (Jones Jr.

8.3 Ribbed pins

Surfaces 1 to 10 of Table 8.1 are studied in this section. The pins in these geometries all
have ribs on them. Surfaces 1 and 6 are the surfaces that are studied in most detail. There
is more experimental data available for surface 1, which has a transverse rib, than there is
for the other surfaces. In addition, as a transverse pin, there are experimental correlations
that can be used to compute results for this surface. Surface 6 has a multistart rib and is
the surface that most closely resembles the fuel pins found in AGRs and is therefore of more
interest to EDF Energy Generation.

8.3.1 Previous studies

Before discussing the computations performed, it is instructive to review flows over ribbed
pins similar to those studied in this chapter. There have been many experimental and com-
putational studies, however none are directly comparable to the study performed here.

Experimental studies

A large number of experimental studies were performed by the CEGB in addition to those
of Watson (1970) and Pirie (1974). Some of these concern just a single pin, such as the
studies of Lawn (1976) and Warburton et al. (1973), and some concern clusters of pins, such
as the studies of Lee (1971) and Bell (1987). The reports of Watson (1970) and Pirie (1974)
were chosen for this chapter because the reports contained clear, tabulated results and a
detailed description of the flow conditions, which many of the other reports do not. The
experimental procedures followed by other authors at the CEGB were similar and often the
same equipment was used. There is not much that can be gained by critically evaluating the
results of other studies by the CEGB since many features are also present in Watson (1970)
and Pirie (1974). Instead it is useful to compare data obtained independently.

Around the same time as the CEGB was studying flows over fuel pins, similar studies were
being performed in Germany. Feurstein and Rampf (1969) studied the pressure drop and heat
transfer of flows of air over 21 different smooth and transverse pins in annuli with Reynolds
numbers ranging from $2 \times 10^4$ to $2 \times 10^5$. There is a clear trend in the friction factor with

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Reynolds number, although the friction factors show noticeable scatter around the line of best fit. The results were used to build expressions for the friction factor of the form $f = C \text{Re}^q$, and for the Stanton number of the form $St = K \text{Re}^m$, where $C$, $q$, $K$ and $m$ are tabulated for different rib profiles. Images were taken of the instantaneous velocity field for the flow of water between the ribs at different Reynolds numbers. The results of Feurstein and Rampf (1969) were used by Maubach (1972) to develop an empirical correlation for the friction factor of a transverse pin in an annular channel. This correlation is used in Section 8.5.

Dalle Donne and Meyer (1977) also developed a correlation that can be used to predict the friction factor for transverse pins. While developing the correlation, Dalle Donne and Meyer (1977) performed a number of new experiments of transverse ribbed annular flows. Ten different pins were studied, each with four different smooth pipes. Two of the ribbed surfaces were studied with heat transfer. The data of 18 different authors, from a period of 31 years, including the data of Feurstein and Rampf (1969) and Watson (1970), were also used to develop the correlation. Dalle Donne and Meyer (1977) noted that their experimental results show less scatter than the data of the 18 other authors. The report of Dalle Donne and Meyer (1977) contains a thorough review of the studies performed up to the date of its publication. The correlation of Dalle Donne and Meyer (1977) is used in Section 8.5, and the full equations are given in Appendix E.

More recent studies exist of flows over helical structures. A review of heat transfer over these types of surfaces can be found in Webb (2005). However, the results are seldom relevant to flows over AGR fuel pins. Often the geometry is slightly different or the Reynolds numbers are smaller. For example, many studies have been performed over rods with helically-wrapped wires on them, since this type of pin is found in pressurised water reactors (Diller et al., 2009). Sometimes the helical rib is cut into the pin surface, so that it protrudes inwards rather than outwards, resulting in a “rifled” tube (Zhang et al., 2015). One study that is close to being appropriate for this chapter is that of Gee and Webb (1980), who studied multistart pins with different rib angles and built a correlation with the results. However the Reynolds number was never larger than $6.5 \times 10^4$ and therefore the results and correlation are not applicable to the flows in this chapter. Ravigururajan and Bergles (1996) built a correlation for the friction factor and Nusselt number of pipe flows where the pipe wall is ribbed with either a transverse or multistart rib. The maximum Reynolds number of any experimental data used to derive the correlation is $Re = 2.2 \times 10^5$. 

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Computational studies

Many similar flows have been studied computationally, however as is the case with experimental studies, it is difficult to find other work with a similar geometry at the Reynolds numbers studied in this chapter. For example, Rashkovan et al. (2010) studied transverse pins with variable rib width to pitch ratio in an annulus using a LRN $k - \varepsilon$ model. However the Reynolds number was never larger than $4 \times 10^4$. Takase (1996) studied transverse ribs using a HRN $k - \varepsilon$ model, up to a largest Reynolds number of $2 \times 10^4$, and compared the results to experimental correlations. The Reynolds numbers studied by these authors are significantly below the range in Table 8.2. However, two studies in particular stand out as relevant and are reviewed in detail below.

Study by Henry and Collins (1991)

Similar flows to those of Watson (1970) and Pirie (1974) have been studied by Henry and Collins (1991), who used a HRN $k - \varepsilon$ model with a wall function. Henry and Collins (1991) contains results for both transverse and multistart ribs. Although the flow conditions and geometry are similar, they do not correspond exactly to any flow in Pirie (1974), even though Pirie (1974) is given as a citation. Table 8.5 shows the geometry and flow conditions for one of the multistart cases studied by Henry and Collins (1991). The parameter $w_{HC}$ is the width of the rib in the axial direction, $h_{HC}$ is its height in the radial direction. The case in Table 8.5 is the only case that has a ribbed pin for which an experimental value of $f$ is reported in Henry and Collins (1991). The referenced value of the friction factor is cited by Henry and Collins (1991) as “personal communication”. As reported in Henry and Collins (1991), the friction factor in Table 8.5 has an error $\varepsilon = -32\%$. Experimental data of the fluid velocity is reported, but is also cited as “personal communication” and is therefore inaccessible.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_2$</td>
<td>49.045 mm</td>
</tr>
<tr>
<td>$R_1$</td>
<td>19.72 mm</td>
</tr>
<tr>
<td>$h_{HC}$</td>
<td>1.13 mm</td>
</tr>
<tr>
<td>$w_{HC}$</td>
<td>0.8609 mm</td>
</tr>
<tr>
<td>$W$</td>
<td>7.29 mm</td>
</tr>
<tr>
<td>$N$</td>
<td>12</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>34°</td>
</tr>
<tr>
<td>$Re$</td>
<td>$2.13 \times 10^5$</td>
</tr>
<tr>
<td>$f$ (experiment)</td>
<td>$5.06 \times 10^{-3}$</td>
</tr>
<tr>
<td>$f$ (CFD)</td>
<td>$3.43 \times 10^{-3}$</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>$-32%$</td>
</tr>
</tbody>
</table>

Table 8.5: Geometry and flow conditions of one of the multistart cases of Henry and Collins (1991). The parameter $w_{HC}$ is the width of the rib in the axial direction, $h_{HC}$ is its height in the radial direction.

The geometry used by Henry and Collins (1991) to create a mesh is shown in Figure 8.7.
The mesh has 1 active cell in the axial direction, 14 in the azimuthal direction and 22 in the radial direction, for a total of 308 cells. The height of the rib is covered by two cells. Such a mesh is not fine enough to adequately resolve the pressure field on a mesh with only two cells covering the height of the rib. Henry and Collins (1991) also states that the friction factors were mesh-dependent. Mesh independence could not have been achieved in any case because a wall function was used.

The simulations in this report are an improvement over the simulations of Henry and Collins (1991) because low Reynolds number turbulence models are used and the friction factors computed are mesh independent. This work considers a larger range of rib heights and Reynolds numbers than the work of Henry and Collins (1991) and uses the exact same flow conditions as those reported in Pirie (1974).

Study by Keshmiri (2011)

Keshmiri (2011) studied the flow over transverse pins. The pins were arranged in the form of a simplified AGR fuel element, which contains 36 pins in three rings. Transverse pins were chosen for computational efficiency because only a 30° sector of the fuel assembly had to be used to generate a mesh. Had multistart pins been used, it would have been necessary to study a 120° sector. The $\bar{v}^2 - f$ model in the commercial code STAR-CD was used for the simulations. The Reynolds number based on the entire fuel element was $Re = 3 \times 10^4$.

Keshmiri (2011) compared the region between the ribs in the fuel element simulation to the results of a ribbed channel flow (Keshmiri and Gotts, 2011), similar to that studied in Chapter 7. Three distinct types of sub-channel were identified in the fuel assembly. It was argued that a three-dimensional simulation of a fuel element is necessary to accurately compute the pressure, temperature and velocity fields because the two-dimensional simulations of a channel do not capture the span-wise flow present in the fuel assembly.

Keshmiri (2011) found that the friction factor computed from the simplified fuel element
agreed well with the empirical correlation of Ravigururajan and Bergles (1996) for a transverse ribbed pipe. However the Reynolds number is still an order of magnitude smaller than those considered in this chapter, and the use of transverse pins, while efficient, means that the swirl of the flow over a multistart pin is not captured.

The flows in this section differ from those of Keshmiri (2011) because they are of multistart pins and therefore contain swirling motion, because the Reynolds numbers studied are larger and because there are experimental data against which the results can be compared.

8.3.2 Computational set-up

All of the runs in Table 8.2 are performed with CFD. The section of the geometry used in the mesh for the simulations of ribbed pins is shown in Figure 8.8, and is similar to the geometry used for the ribbed channel in Chapter 7. The mesh contains a 1° sector of the geometry. Figure 8.9 shows how the 1° sector fits can be transformed to create the ribbed pin.

A mesh independence study was performed using one particular run, S6R4, with the Spalart-Allmaras model. This case was chosen because initially only surface 6 was to be studied, and run 4 has the highest Reynolds number. The Spalart-Allmaras model was chosen because the simulations converge quickly. A mesh with 27,880 cells and a fine mesh with 86,832 cells were created. The difference in the friction factor for S6R4 obtained with these two meshes, expressed as a percentage of the result obtained on the fine mesh was 0.9%. There was no noticeable difference in plots of the wall shear stress between the ribs. Therefore the mesh with 27,880 cells is assumed sufficiently fine to produce mesh independent results for all runs of surface 6.

With a mesh of a sector larger than 1°, it is possible that three-dimensional effects and unsteady phenomena may appear in the RANS solution. To investigate this, the mesh was copied, rotated and translated repeatedly, to create a mesh of a 30° sector with 30 × 27880 =
Figure 8.9: The $1^\circ$ (red) and $30^\circ$ (blue) mesh domains shown within a larger section of the flow geometry of surface 6.
8.3. Ribbed pins

836,400 cells, as shown in blue in Figure 8.9. When S6R4 was studied with this larger mesh, the difference in the friction factor, compared to the result found with the 1° mesh was 0.07%, and no unsteady flow effects were observed. Hence a mesh of a 1° sector is sufficient in order to calculate mesh-independent results that are representative of the underlying turbulence model. For clarity, some results in this chapter are plotted for the case with the 30° mesh.

The 1° mesh was then transformed appropriately into the geometry of all the other ribbed surfaces and used to study all runs for the other surfaces. Hence all results were obtained on a mesh with 27,880 cells, with no further mesh independence studies. The mesh with 27,880 cells is shown in Figure 8.10a, and a close up of the region near to the rib is shown in Figure 8.10b. The mesh is very refined near to the wall, with the smallest cell being approximately 0.02% of the rib height.

Figure 8.10: The mesh used in the computations, and a close-up around the rib.
To assess the extent to which mesh-dependence could affect the friction factor, a very coarse mesh with 3612 cells was made and used to study S6R4 again. The error on the friction factor, compared to the friction factor obtained on the mesh with 27,880 cells was 4%. Thus, even in the event that 27,880 cells is insufficiently fine for some runs on some surfaces, the error in the friction factor will be small.

### 8.3.3 Computation outputs

As well as the friction factor, profiles of the wall shear stress are plotted for some runs. The wall shear stress is plotted in terms of curvilinear coordinates, \( \eta \) and \( \xi \), where \( \eta \) points in the helical direction and \( \xi \) varies in the direction normal to \( \eta \) on the surface of the pin at constant radius. Unit vectors in the \( \eta \) and \( \xi \) directions are denoted \( \hat{e}_\eta \) and \( \hat{e}_\xi \), respectively. These vectors are shown in Figure 8.11, in which the pin is viewed from within the flow domain, looking at the pin. A component of \( \hat{e}_\xi \) points in the positive \( z \) direction, which is along the axis of the can, in the flow direction. A line moving in the \( \hat{e}_\xi \) moves perpendicular to the helix traced by the ribs.

![Figure 8.11: A view from within the flow domain, looking at the pin, which shows the definition of the coordinate vectors \( \hat{e}_\eta \) and \( \hat{e}_\xi \).](image)

The wall shear stress is resolved into the \( \eta \) and \( \xi \) directions to determine the skin friction coefficients

\[
C_{f,\eta} = \frac{\mu}{\frac{1}{2} \rho U_p^2} \left. \frac{\partial U}{\partial n} \right|_w \cdot \hat{e}_\eta, \tag{8.15}
\]

and

\[
C_{f,\xi} = \frac{\mu}{\frac{1}{2} \rho U_p^2} \left. \frac{\partial U}{\partial n} \right|_w \cdot \hat{e}_\xi. \tag{8.16}
\]

The derivatives are taken in the direction normal to the wall, pointing into the fluid, which defines the unit vector \( n \). Figure 8.11 shows that \( n = \hat{e}_\eta \times \hat{e}_\xi \).

The skin friction coefficients, the pressure coefficient,

\[
C_P = \frac{(P - P_{ref})}{\frac{1}{2} \rho U_p^2}, \tag{8.17}
\]

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and the local Stanton number are plotted along an axial line in the $z$ direction between two successive ribs for some runs. The reference pressure, $P_{\text{ref}}$, is arbitrarily defined such that $C_P = 0$ immediately downstream of the rib. The downstream corner of the rib is located at $z = 0$, and the upstream corner of the rib is always located at $z/W \approx 0.865$ by virtue of the choice of $W$ and $h$ by Pirie (1974). There is no experimental data against which $C_{f,\eta}$, $C_{f,\xi}$, $St$ or $C_P$ can be compared.

8.3.4 Friction factors for all surfaces

At first, only surface 6 was studied, since this pin is most similar to the pin in an AGR. However, there was a discrepancy between the computed friction factors and the experimental measurements. Therefore, friction factors for all ten surfaces of Pirie (1974) were computed, in order to investigate whether or not there is something specific to surface 6 that might cause this discrepancy. Surface 6 is unusual in that Pirie (1974) performed only four runs for it, compared to eight for most other surfaces. It is not clear why this is so. Therefore it was thought it would be worthwhile to study the other surfaces. The results for all 10 surfaces are reported in this section.

The friction factors in this section are all computed with the Spalart-Allmaras model and are displayed in Figure 8.12, alongside the experimental results of Pirie (1974). In general, the experimental data in Figure 8.12 show a decreasing trend in $f$ with increasing $Re$, which is consistent with the CFD results. However, the experimental results for surface 1 in Figure 8.12a show a different trend in $f$ with $Re$ to the CFD results. In contrast, for surface 10 in Figure 8.12j, the trends in the experimental and CFD results are similar. Although each surface has a different geometry, some features are similar in all plots. With the exception of S1RE, the CFD friction factor is always lower than the corresponding experimental value. For all surfaces, the CFD friction factor varies more smoothly with $Re$ than the experimental measurements. The experimental results clearly contain experimental uncertainty, which is visible as the scatter in the trend lines in the experimental data. In particular, in Figure 8.12e, the experimental friction factors for S5R3 and S5R4 differ by around 8%, whereas the Reynolds numbers differ by around only 1%. As well as the random error in each measurement, there are also likely to be systematic errors in the experimental results, as was suggested in Section 8.2 for surface 0.

The error in the friction factor is different for each surface. The arithmetic mean of the error,

$$
e = \frac{1}{N} \sum_{i=1}^{N} \epsilon_i,$$

where $\epsilon_i$ is the error in the friction factor for each run and the summation runs over all
Figure 8.12: Friction factors for all 10 surfaces of Pirie (1974) using the Spalart-Allmaras model.
8.3. Ribbed pins

runs that are performed with CFD for each surface, is shown in Table 8.6. Calculating $e$ with an arithmetic mean causes $e$ to be biased towards the Reynolds numbers at which more simulations were performed. This tends to be the lower end of the Reynolds number range, particularly for surface 1. According to Table 8.6, the CFD friction factors for surfaces 1 and 10 are the most accurate.

<table>
<thead>
<tr>
<th>Surface</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha/\degree$</td>
<td>0</td>
<td>0</td>
<td>3.5</td>
<td>18</td>
<td>33</td>
<td>33</td>
<td>33</td>
<td>33</td>
<td>45</td>
<td>60</td>
</tr>
<tr>
<td>$h/mm$</td>
<td>0.69</td>
<td>1.14</td>
<td>1.14</td>
<td>1.14</td>
<td>0.58</td>
<td>1.14</td>
<td>2.29</td>
<td>1.14</td>
<td>1.14</td>
<td>1.14</td>
</tr>
<tr>
<td>$e$</td>
<td>-11%</td>
<td>-16%</td>
<td>-17%</td>
<td>-25%</td>
<td>-19%</td>
<td>-28%</td>
<td>-41%</td>
<td>-32%</td>
<td>-29%</td>
<td>-11%</td>
</tr>
</tbody>
</table>

Table 8.6: $e$ for each surface, using the Spalart-Allmaras model.

Although it is not clear how accurate the RANS results are for the surfaces in Figure 8.12, experimental uncertainties are one possible cause of the discrepancy between the CFD and experimental friction factors. It is not unusual for the experimental uncertainties to be large for this type of flow. For example, there is noticeable scatter about the line of best fit in the data of Feurstein and Rampf (1969) such that if only the data for $Re > 1 \times 10^5$ were available, it would not be possible to identify the trend of $f$ with $Re$. This suggests that the data of Watson (1970) and Pirie (1974), which usually have $Re > 1 \times 10^5$, may be at such large Reynolds numbers that the experimental uncertainties are too large for the data to be reliably interpreted. This, coupled with the observation of Watson (1970) that the experimental friction factors are likely to be over-estimated, could explain the discrepancies between the CFD and experimental friction factors in Figure 8.12.

Figure 8.12 and Table 8.6 indicate that the error depends on the pin. Thus, whatever the sources of error are, they depend on the rib height and angle. The largest errors are found for surface 7, which has the largest rib height. Of surfaces 2, 3, 4, 6, 9 and 10, which differ only by the rib angle, the error is largest for surfaces with $\alpha = 33\degree$ or $45\degree$. Hence the swirl of the flow, determined by the angle, and the size of the swirling region, determined by the rib height, have a significant effect on the error.

The friction factors reported in Watson (1970) and Pirie (1974) are calculated with Equation (8.3) and are consistent with the values predicted by CFD and experimental correlations for surface 0 in Figure 8.5. Any terms in Equation (8.3) whose measurement could be affected by the presence of the rib would lead to experimental errors that depend on the rib profile. However there are no terms for which the measurement procedure would be significantly affected by the rib profile. The bulk gas temperature was computed from the power passed through the pin and assuming that $T_g$ varies linearly along the experimental apparatus. The validity of this assumption is unlikely to depend on the rib profile. The pressure was measured on the pipe wall and the same pipe was used for each surface. Pirie (1974) used only
four measurements of the pressure to compute the pressure gradient. The typical pressure
distribution along the experimental channel is plotted in Pirie (1974) in a figure which sug-
gests that there may be outliers in the pressure measurements. Therefore, four points may
be insufficient for an accurate measurement of the pressure gradient. However the accuracy
of this would not depend on the rib profile. Thus, there are no aspects of the experimental
procedure that would cause such large errors to appear for ribbed pins when the smooth pin
results are accurate.

8.3.5 Discussion of flow features

Figure 8.13 shows $C_{f,\eta}$ and $C_{f,\xi}$ between the ribs with the Spalart-Allmaras model for run 1
of all ten surfaces studied by Pirie (1974), except for surface 4, where run 2 is plotted because
the Reynolds number is more similar to the others. Each line style corresponds to a different
rib angle. There are several relationships between the rib profiles:

1. Surfaces 2, 3, 4, 6, 9 and 10 differ only by the rib angle.
2. Surfaces 5, 6, 7 and 8 all have $\alpha = 33^\circ$.
3. Surfaces 5, 6, and 7 have the same root diameter but different rib profiles.
4. Surfaces 6 and 8 differ only in the root diameter.
5. Surfaces 1 and 2 have $C_{f,\eta} = 0$ and so these lines are not visible in Figure 8.13a.

All multistart pins have $C_{f,\eta} > 0$ everywhere between successive ribs, which indicates that the
flow is attached in the helical direction. As the rib angle increases towards $45^\circ$ (comparing
surfaces 3, 4, 6 and 9), the magnitude of $C_{f,\eta}$ increases. The profile of $C_{f,\eta}$ also flattens as the
rib angle increases. Meanwhile, the magnitude of $C_{f,\xi}$ decreases as the rib angle increases.
This indicates that as the rib angle increases, the flow between the ribs tends to move along
the helical direction instead of normal to the ribs. This leads to a decrease in pressure on the
upstream face of the rib and hence to a lower total friction factor as the rib angle increases.

When the rib height increases but the rib pitch to height ratio remains constant (comparing
surfaces 5, 6 and 7), there is no obvious monotonic behaviour in either $C_{f,\eta}$ or $C_{f,\xi}$. This is
because the number of rib starts is different for these surfaces.

When the root diameter increases (surfaces 6 and 8), there is only a minor change in $C_{f,\xi}$,
whereas $C_{f,\eta}$ noticeably increases. Hence the flow is more strongly attached in the helical
direction for larger $R_1$. This is because the larger root diameter reduces the radius of curvature
of the helix, and therefore the centripetal force required to maintain a helical motion is
reduced.
Figure 8.13: $C_{f,\eta}$ and $C_{f,\xi}$ between successive ribs with the Spalart-Allmaras model for run 1 of every surface (except for surface 4, for which run 2 is shown). Each line style corresponds to a different rib angle. Surfaces 1 and 2 have $C_{f,\eta} = 0$. 

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Figure 8.14 shows $C_P$, which is directly related to the pressure, in the region around the rib for S1R1. It is seen that the pressure changes from its global maximum to its global minimum in a small region near to the upstream corner of the rib. The same behaviour is seen in the experimental results from the CEGB of Lawn (1976), for a similar pin geometry and Reynolds number. In order to resolve this pressure field, a very fine mesh is required around the rib corners. Any mesh fine enough to resolve the pressure field in this region will also be fine enough to use a LRN turbulence model in this region. The mesh used by Henry and Collins (1991) had only two cells covering the height of the rib and therefore could not have been fine enough to resolve the pressure fully.

![Figure 8.14: $C_P$ around the rib for S1R1 with the Spalart-Allmaras model.](image)

Figure 8.15 shows the streamlines between successive ribs for S1R1. Around two rib heights above the pin surface, the flow is approximately one-dimensional. There are three circulation regions visible between the ribs. Figure 8.19b, which is a plot of $C_{f,\xi}$ along the pin wall, indicates that $C_{f,\xi}$ is actually negative at the wall over much of the region between the ribs. This means that the two largest circulation regions in Figure 8.15 rotate in the same direction.

For the multistart surfaces, the streamlines do not form continuous cycles, since the flow moves helically around the rib. Streamlines for S6R4 are shown in Figure 8.16, and show the helical flow near the pin surface. Near to the pin wall, the flow moves around the rib in a helical path, with the helix angle equal to the angle of the rib. The azimuthal component of the velocity, $U_\phi$, shown in Figure 8.17, is large and negative near the pin wall. The region where the magnitude of $U_\phi$ is largest is between adjacent ribs. At larger radial distances, the magnitude of $U_\phi$ is smaller, but still non-zero, and negative, which indicates that the flow still moves in a helix and that the angle of the helix changes with the radius. This is also seen in the streamlines. The change in direction of the streamlines occurs in a thin radial region just beyond the top of the rib. The angle of the flow in the bulk is not equal to
the angle of the rib, and is thus flow-dependent. Thus, streamline curvature caused by the helical motion and the streamline rotation caused by changing the rib angle is an important flow feature. However LEVMs, such as the Spalart-Allmaras model, often fail to capture streamline curvature accurately (see Section 2.8.10). Thus it was decided to study surface 6 in more detail using curvature correction methods in the turbulence model equations, to quantify the effect of streamline curvature on the flows. Surface 6 is chosen because it is the most similar to the real pin in an AGR. In addition, surface 1 is studied more extensively, since the rib angle is zero in this case. It therefore provides a useful baseline case where streamline curvature is at a minimum. Furthermore, as a transverse pin, the CFD results for surface 1 can be compared to existing correlations to further assess the accuracy of both the CFD and experimental results.

8.3.6 Results and discussion for surfaces 1 and 6

In this section, simulations of all runs for surfaces 1 and 6 are performed with the Spalart-Allmaras, BL-\(\nu^2/k\), \(\varphi - f\) and EBRSM models, which are all LRN models. In addition, a run with \(Re = 1.85 \times 10^5\) is performed for surface 6. This is because an LES has been performed at this Reynolds number by Juan Uribe at the University of Manchester.

Two different types of curvature correction are used in this chapter: the correction of Shur et al. (2000), which modifies the turbulent production, and that of Cazalbou et al. (2005), which modifies the turbulent dissipation. Both types of correlation are implemented for the BL-\(\nu^2/k\) and \(\varphi - f\) models; whereas only the Shur et al. (2000) correction is implemented with the Spalart-Allmaras model because this model does not solve for the dissipation. The implementation of the curvature corrections is described in Appendix A.9. The curvature corrections are used to assess what effect streamline curvature has on the friction factor,
Figure 8.16: Streamlines for S6R4 with the 30° mesh.

Near the pin the streamlines follow the helix of the rib

Figure 8.17: Azimuthal velocity component, $U_\phi$ for S6R1 with the Spalart-Allmaras model.

compared to calculations where streamline curvature is not modelled.

The friction factors for surfaces 1 and 6 are shown in Figures 8.18a and 8.18b, respectively, alongside the experimental results and, for surface 6, the LES result of Juan Uribe at the University of Manchester.

For surface 1 the data of Watson (1970) and Pirie (1974) with CO$_2$ suggest that $f$ increases with $Re$ and the results of Watson (1970) with air show no clear trend. For S1RE, which has
8.3. Ribbed pins

Figure 8.18: Friction factors for surfaces 1 and 6 using many turbulence models.
the lowest Reynolds number, the Spalart-Allmaras friction factor is in close agreement with
the experimental result but by the largest Reynolds number, for S1R6, the Spalart-Allmaras
model under-predicts the friction factor, with $\epsilon = -20\%$. The friction factor in the CFD
results always decreases as $Re$ increases. The slope of the line is similar for the Spalart-
Allmaras and BL-$v^2/k$ models, but the $\varphi - f$ model has a flatter slope. The difference in
the value of $f$ predicted by the three turbulence models is largest for the smallest Reynolds
number. The $\varphi - f$ result for the lowest Reynolds number (S1RE) is unusually small, since
the trend in $f$ with $Re$ is noticeably different for this Reynolds number. This result was
investigated by performing S1RE with different meshes, convergence parameters and solver
options, however the result did not change. Hence this result is correct for the $\varphi - f$ model.

For surface 6 the data of Pirie (1974) suggest that $f$ decreases with $Re$, although there is
considerable uncertainty because there are only four data points. Although no CFD results
agree well with the experimental data, it could be argued that the slope of the CFD line
is similar to that implied by the experimental data. All turbulence models predict similar
slopes and the slope is unaffected by the curvature corrections.

Different behaviour is seen for the two curvature correction algorithms:

- With the correction of Shur et al. (2000), the friction factor always increases when
  either the Spalart-Allmaras or the $\varphi - f$ models are used, whereas it always decreases
  when the BL-$v^2/k$ model is used.

- With the correction of Cazalbou et al. (2005) the friction factor always decreases when
  the BL-$v^2/k$ and $\varphi - f$ models are used.

For the Spalart-Allmaras model with the Shur et al. (2000) correction, the average increase in
the friction factor is approximately 5%. Thus, streamline curvature is an important compo-
ment of the flow physics for surface 6. However the change in $f$ when the curvature correction
is activated depends not just on the correction algorithm used but also the turbulence model.
The same curvature correction can give either an increase or decrease in $f$, depending on the
turbulence model. Therefore it is unclear from the results in Figure 8.18b whether the effect
of streamline curvature is to increase or decrease the friction factor. Because of this mixed
behaviour, it was decided not to use the curvature corrections in future simulations but to
note that the friction factor could increase or decrease by around 5% for each simulation
because of the curvature.

As a Reynolds stress model, the EBRSM model naturally accommodates the effects of stream-
line curvature, whereas the other turbulence models do not. Thus the EBRSM results should
yield some insight into the effects of streamline curvature on the friction factor. The friction
factors computed with the EBRSM model are lower than those for the other models, which
suggests that the effect of streamline curvature is to reduce the friction factor. However, simulations were also run with the EBRSM model for surface 1 and the resulting friction factors were considerably smaller than those in Figure 8.18a. For S1RE the friction factor was \( f = 8.69 \times 10^{-3} \) and for S1R6 the friction factor was \( f = 6.56 \times 10^{-3} \). These results are not plotted in Figure 8.18a because they distort the scale on the friction factor axis. The poor agreement suggests that there is something wrong with either the model or the implementation of the model into Code_Saturne. In light of these spurious results on surface 1, the results with the EBRSM model on surface 6 should be treated with caution.

For surface 6, when no curvature correction is used, the largest friction factors are found with the \( \phi - f \) model, followed by the Spalart-Allmaras, BL-\( \nu^2/k \) and EBRSM models. The same pattern emerges in the results for surface 1 at the largest Reynolds numbers. This means that the \( \phi - f \) model agrees most closely with the experimental data. However, the Spalart-Allmaras model was chosen as the most suitable model to be used in future simulations because it converges an order of magnitude faster, since a larger pseudo time step can be used. The Spalart-Allmaras model also lends itself conveniently to domain decomposition.

The CFD results indicate that the experimental data of Pirie (1974) significantly overestimate the friction factor. It would not have been possible to reach this conclusion from RANS results alone but the LES result of Juan Uribe at the University of Manchester sits roughly in the middle of all the RANS predictions in Figure 8.18b at that Reynolds number. Moreover, the LES friction factor is lower than all of the experimental results for surface 6, despite having a smaller Reynolds number. If the LES were performed at a larger Reynolds number then the friction factor would be even smaller, which suggests that the experimental data over-estimate the friction factor.

Plots of \( C_{f,\eta} \), \( C_{f,\xi} \), \( C_P \) and \( St \) are shown for S6R1 for the four turbulence models (with no curvature correction) in Figure 8.19. Without any experimental data to compare to it is impossible to assess which model produces the most accurate profile of any of these parameters. It is seen that the \( \phi - f \) and BL-\( \nu^2/k \) models, which are both \( \nu^2 - f \) models, produce similar profiles for each parameter. Of the two models, the \( \phi - f \) model always produces the largest values of \( C_{f,\eta} \), \( C_P \) and \( St \). This is consistent with the \( \phi - f \) model predicting the largest overall friction factor for surface 6. The profiles obtained with the Spalart-Allmaras model are similar in shape to those found for \( C_f \), \( C_P \) and \( Nu \), respectively for the plane ribbed channel in Figure 7.6. This makes sense because in the direction normal to the ribs the two geometries are similar.

The profiles from the EBRSM model are different in shape to those found with the EVMs. For example, \( C_P \) is smaller and has a different curvature over much of the plotted region.
The peak in $C_{f,\eta}$ and the trough in $C_{f,\xi}$ for $z/W > 8$ are much sharper than they are for the EVMs and for $z/W < 8$, the magnitude of $C_f$ is smaller. However, the shape of the profile of $St$ is similar to the EVMs. The profile of $C_{f,\eta}$ is similar to the profile in Keshmiri et al. (2016) of $Nu$ on the wall of a heated ribbed channel flow similar to that studied in Chapter 7. In particular, Keshmiri et al. (2016) found a sharp peak in $Nu$ just upstream of the impingement face of the rib when using the EBRSM model or LES. The similarity to the profile of $C_{f,\eta}$ in Figure 8.19a is not surprising since in the $\eta$ direction the flow over surface 6 is similar to that over a ribbed channel.

Figure 8.19: $C_{f,\xi}$, $C_{f,\eta}$, $C_P$ and $St$ between two ribs for S6R1 with four different turbulence models.

Pirie (1974) reports that for S6R1, $St = 4.55 \times 10^{-3}$. Although it is not specified exactly how this value is calculated, it is known that $St$ is measured somewhere on the cylindrical surface of the pin, and not on the rib. Therefore the Stanton number as reported by Pirie (1974) can be computed from the data shown in Figure 8.19d. However none of the profiles in Figure 8.19d ever go above $3 \times 10^{-3}$. Therefore, no matter which turbulence model is used, the Stanton number found with CFD will be at least 33% lower that found in the experiment. The
8.3. Ribbed pins

Stanton number from the Spalart-Allmaras model peaks at around $2 \times 10^{-3}$ in Figure 8.19d, hence this model must under-predict the Stanton number by over 50%. Similar behaviour is seen for other runs and for other surfaces.

The agreement with the computed Stanton number and the experimental results is poor and means that CFD has not yet been validated for application to heat transfer problems on fuel pins. However the friction factors also contain significant errors. The solution to the enthalpy equation, from which the Stanton number is calculated, depends on the solution for the momentum equation. Thus, in order to improve the prediction of the Stanton number, attention must first be paid to reducing the error in the friction factor. The remainder of this chapter is devoted to investigating the reasons for the discrepancy between the computed and experimental friction factors.

8.3.7 Sources of discrepancy between the CFD model and the experiments

Since almost all CFD results in Figures 8.12 and 8.18 are lower than the corresponding experimental measurement it is natural to suspect that there may be features in the experiments that are not present in the CFD calculations. Any missing features could also explain why the errors in Table 8.6 depend on the rib profile.

In Section 8.2 it was suggested that the effect of systematic errors on the smooth pin is to increase both $f$ and $St$ by no more than 10%. However in Section 8.3.4 it was found that the systematic error depends on the rib height, angle and pitch, notwithstanding that the CFD results contain significant uncertainties themselves, due to the turbulence model.

A detailed list of the differences between the model and the experiments is given in this section, as well as an assessment of the effect that these differences have on the results of the CFD calculations.

1. There are uncertainties in the geometry quoted in the experiments.

   (a) Lengths in Watson (1970) are quoted in inches whereas in Pirie (1974) they are quoted in millimetres. When the lengths of Watson (1970) for surface 1 are converted into millimetres using the standard conversion, the resulting values are sometimes different to the values quoted in Pirie (1974). For example, the value of $R_2$ quoted in Watson (1970) is equivalent to 52.07 mm, but according to Pirie (1974), $R_2 = 52.05$ mm, even though the two values are supposed to be the same.

   (b) In Watson (1970) the rib height is quoted to the nearest 0.001 inch, which is 25 µm. In Pirie (1974), the rib height is quoted to the nearest 10 µm, which is more accurate. Thus in the experiments, the rib height may vary over the length
of the pin, although it is difficult to quantify by how much. In contrast, in the CFD model, the rib height is constant and has no uncertainty.

(c) There are minor inconsistencies in the redundant information given in Pirie (1974) about the rib angle. For example, the rib angle of attack for surface 6 is reported as $33^\circ$. However the angle can be calculated from the number of rib starts, the rib pitch and the pipe diameter to be

$$\alpha = \tan^{-1} \left( \frac{NH}{\pi D} \right) = 33.7^\circ,$$

which is slightly different to the quoted value.

Since the geometrical errors are small, the effect on the friction factor will also be small. Therefore geometrical uncertainties do not explain the discrepancy between the CFD and experimental results.

2. Traces of the ribs in Pirie (1974) and Watson (1970) indicate that the ribs are not exactly square. Figure 8.20, which is taken from Pirie (1974), shows the profile of the rib for surface 6 used in the experiments. Watson (1970) reports that the radius of curvature at the rib corners is approximately 10% of the rib height. Increasing the curvature of the rib corners will decrease the friction factor. Curvature of the rib could lead to a decrease in the friction factor of around 10% (Watson, 1972). Hence the experimental friction factors are smaller than they would be if the rib were perfectly square. In the CFD model, however, the ribs are perfectly square. Curving the ribs in the CFD model would increase the discrepancy in the results. However the maximum change in the friction factor would be no more than 10% (Watson, 1972).

![Figure 8.20: Cross sections of ribs for surface 6 along the axis of the pin, from Pirie (1974).](image)

3. It is possible that the experimental surfaces were not completely smooth, and that there was a surface roughness on the experimental surfaces in addition to the rib. The roughness average on the outer pipe wall in the experiments of Watson (1970) was 0.127 $\mu$m, which is small compared to the rib height. The effect of surface roughness is studied in Section 8.6.

4. There are restrictions on the CFD model imposed by the use of periodic boundary conditions.
8.3. Ribbed pins

(a) Periodicity requires the experimental flow to be fully-developed. If the experiments were not fully developed in the region where measurements were taken, then significant errors would be introduced. However both Watson (1970) and Pirie (1974) are careful to demonstrate that the experimental flows are fully developed in the measurement region. Therefore this is not a significant source of error.

(b) In the experiments there were grids and braces used to hold the pins in a concentric position. This would lead to an increase in the friction factor over the whole length of the experiment. However the experimenters only took measurements between the braces. Therefore this omission does not cause significant errors.

Including the effects of grids and braces would yield a roughly-constant increase in \( f \) for each surface at a fixed Reynolds number. Therefore even if the grids and braces did affect the experimental friction factors, including the effect in the CFD model would not lead to agreement in \( f \) for all surfaces since Figure 8.12 shows that different increases in \( f \) are required for each surface in order to achieve consistency.

5. The computations ignore the change in fluid properties with temperature over the length of the pipe. However this is a good approximation, as will be demonstrated in Section 8.5 using an empirical correlation built using experimental results.

6. The omission of the last two terms on the right hand side of Equation (8.4) also affects the computed friction factor. The CFD predictions are likely to over-estimate the friction factor by around 5%, as discussed in Section 8.1.2.

7. In reality the heat flux on the pin wall in the experiments would not have been uniform. The pin was heated by passing an electric current through it. The rib tips are likely to have received a slightly different current to the cylindrical surface of the pin and would also have been cooled more by the fluid flow. Hence the boundary conditions on the temperature in the CFD calculations are incorrect.

A more accurate way to model the thermal boundary condition is to solve the heat conduction equation in the rib itself, as is done in Mantle et al. (1971) and Iacovides et al. (2003). The effect of changing the thermal boundary condition would only affect the friction factor via the second term in Equation (8.3), which is small. Therefore this discrepancy is does not have a significant effect on the friction factor. The Stanton numbers in Figure 8.19d have such large errors that a modest change to the boundary conditions would not lead to agreement between the CFD and experimental results. In any case, the Stanton numbers will always be incorrect if the velocity field is incorrect. Therefore it is essential to compute an accurate friction factor before considering the
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Stanton number.

8. The CFD results could be affected by the mesh resolution. However the test with a very coarse mesh, discussed in Section 8.3.2, indicates that the friction factor is unlikely ever to vary by more than 5% if the mesh is not sufficiently fine for some reason. In addition, the case with a 30° mesh produced a friction factor in excellent agreement with the 1° mesh. Therefore the angular extent of the mesh is not a source of error.

The results reported in this section are all obtained on meshes with hexahedral cells. Further tests were performed on three-dimensional meshes with tetrahedral and polyhedral cells. The friction factor was unaffected by the choice of cell topology.

9. The meshes themselves contain small geometrical errors. For instance, the faces of the mesh are always straight, even on the pin and pipe walls, which are supposed to be curved. However because the mesh is rotated through only 1°, there is only a small error. The effect on the friction factor of these errors is negligible. This is confirmed by the accurate results for surface 0 in Figure 8.5, since the same errors are present for every surface.

10. The turbulence model equations may not be sufficiently accurate for these flows. One feature that EVMs often fail to capture is the effects of streamline curvature, which affects all multistart surfaces. The effects of streamline curvature were studied for surface 6 in Section 8.3.6 using two curvature correction algorithms and it was inconclusive whether streamline curvature causes an increase or decrease in the friction factor. Regardless of the sign of the change, the magnitude of the change in $f$ was around 5%. Modelling turbulence is known to be difficult and one way to estimate the error on a result is to study the same problem with multiple models, which was done in Section 8.3.6. The EBRSM model, which as a Reynolds stress model can account for the effects of curvature naturally, did not yield a significantly different friction factor to the eddy-viscosity models. Furthermore, the LES result for surface 6 by Juan Uribe at the University of Manchester is free from much of the modelling restrictions of RANS, and the friction factor is in reasonable agreement with the RANS models.

11. There could also be unknown bugs in the computational code used for the simulations. As a consistency check, one run was also performed on the commercial code Star-CCM+ with the Spalart-Allmaras model using the same numerical options, but this time with a polyhedral mesh of a 30° sector of the flow geometry, shown in Figure 8.21. After a separate mesh independence study, the friction factor computed by Star-CCM+ for S6R4 with the Spalart-Allmaras model was within 2% of the value predicted by Code_Saturne with the mesh in Figure 8.8. This is consistent with the findings of
Keshmiri et al. (2015), who showed that these two codes produce similar results in benchmarking tests of forced convection flows. This validates Code_Saturne on the flows in this chapter.

![Figure 8.21: The mesh of a 30° sector of the flow domain used in the Star-CCM+ study.](image)

Although the differences between the CFD model and the experiments are many, there is no obvious omission from the CFD model that could reasonably be expected cause the CFD friction factors to increase enough to be consistent with the experimental values. It seems that errors in the experiments must be at least partially responsible for the discrepancy. In addition, it is difficult to conceive of any source of error that would affect the friction factor more for multistart pins with rib angles near to 45° more than any other angle and simultaneously lead to a small error in a case with no rib. Such behaviour would be required to mollify the errors in Table 8.6.

### 8.4 Friction factors for surfaces 1 and 6 using NDD

Although the agreement between the CFD and experimental friction factors in Section 8.3 is poor, the CFD simulations can still be repeated with NDD. The benchmark solution for the NDD method is the LRN solution with the corresponding turbulence model. In this section, NDD simulations are only performed with the Spalart-Allmaras model with the ZPG profile. Interface boundaries are placed above both the pin and pipe walls, with the same offset from each wall. On the pin wall, the interface boundary is always located between two successive ribs and never goes beyond the top of a rib. This is analogous to interface C in Figure 7.2, and $y^*$ is defined in the same manner. Different $y^*$ are studied for both surfaces 1 and 6.
The friction factors are shown for surface 1 in Figure 8.22a and for surface 6 in Figure 8.22b. For small $y^*$ the friction factors are very close to the LRN values for every Reynolds number for both surfaces. The trend in $f$ with $Re$ with NDD is independent of $y^*/h$ and is the same as the trend in the LRN results. As $y^*$ increases the friction factor increases. The same result was found for surface 0 in Section 8.2.

The friction factor varies by less than 5% of the LRN result for all cases with $y^*/h \leq 0.76$ for surface 1 and for all cases with $y^*/h \leq 0.39$ for surface 6. For $y^*/h > 0.5$, the solutions for surface 6 did not converge. This gives an indication of the range of rib heights that could be studied using a mesh with a fixed height of rib included in it. More of the rib can be excluded from the mesh for the transverse case than for the multistart case. This result could have been anticipated by considering the azimuthal velocity component shown in Figure 8.17. Near to both the pin and pipe walls, the direction of the velocity vectors changes as the azimuthal component of the velocity changes. A one-dimensional governing equation is assumed to govern the wall-parallel velocity when computing IBCs for NDD. Thus with NDD there is no rotation of the velocity vector in the inner regions, which reduces the accuracy of the IBCs especially for larger $y^*$. It is possible that the results for multistart ribs with NDD could be improved by modelling more terms in the NDD governing equation or by using the non-local formulation. However this is not explored in this thesis because it was deemed more useful to investigate the reason for the discrepancy between the LRN and experimental results in Figure 8.12. In addition, EDF Energy Generation already have data to determine how the friction factor is affected by the rib height and do not require a further study.
8.4. Friction factors for surfaces 1 and 6 using NDD

Figure 8.22: Friction factors with NDD for surfaces 1 and 6 using the Spalart-Allmaras model with the ZPG turbulent viscosity profile.
8.5 Modelling the rib as a roughness element

Most of the friction factors found with CFD in Figures 8.12 and 8.18 do not agree with the experimental values. To assess which results are more accurate, it is useful to have a third, independent method of computing the friction factor. Although no such methods exist for multistart pins, numerous studies have been performed on transverse pins by many different authors in the 1970s. These studies were used to generate correlations that can be used to compute the friction factor for different transverse pin geometries for different Reynolds numbers. The correlations were designed to be used in transformation methods, wherein the effects on the flow of the fuel pin and the pipe can be separated from one another. With such an approach, the friction factor for a fuel assembly can be calculated using the result for a single pin in an annulus.

Many correlations were derived during the development of the AGR in the UK, and the helium cooled fast reactor in Germany, for flows over fuel pins in similar conditions to those in this chapter. The oldest correlation is that of Hall (1958) but subsequent correlations have made numerous improvements. For example, while the Hall (1958) transformation requires measurements of the velocity profile in the annulus, the Wilkie (1966) transformation requires only the position of maximum velocity. Eventually the position of maximum velocity was replaced with the surface of zero shear stress, which is used in the transformations of Maubach (1972) and Warburton and Pirie (1973). Dalle Donne and Meyer (1977) reviewed the development of early transformation methods, before introducing an even more sophisticated method.

Two correlations are used in this section: that of Maubach (1972) and that of Dalle Donne and Meyer (1977). Both correlations assume that the rib can be treated as a roughness element, and so the flow in a transverse pin is treated as the flow in an annulus with a rough pin wall and a smooth pipe wall. Since the flow is treated as a one-dimensional annular flow, there is a surface where the wall shear stress is zero, which has a circular cross-section with a well-defined radius, $R_0$. Hence the annulus is split into two distinct regions, which touch at the surface of zero shear, as shown in Figure 8.23. Region 1 is between the pin and the surface of zero shear. In region 1 the fluid velocity is described by the rough wall function, expressed in terms of the rib height as

$$U_{1+}^+ = \frac{1}{\kappa} \ln(y/h) + R(h_+^+),$$

(8.20)

where the subscript refers to region 1. Region 2 is between the surface of zero shear and the pipe wall. In region 2 the fluid velocity is assumed to be governed by the smooth wall function (Equation (3.17)).
8.5. Modelling the rib as a roughness element

Figure 8.23: The geometry assumed by the transformation methods of Maubach (1972) and Dalle Donne and Meyer (1977).

8.5.1 The correlation of Maubach (1972)

The data of Feurstein and Rampf (1969) were used by Maubach (1972) to investigate the link between $f$ and $R(h_+)$ in Equation (8.20). The link is given as a set of simultaneous equations that link $R(h_+)$ with $\beta = R_0/R_1$. If, by some method, $R(h_+)$ is known then $f$ can be computed, or vice versa. The full set of equations is given in Maubach (1972) and is not repeated here. The equations can be considered as simplifications of the correlations of Dalle Donne and Meyer (1977), the equations for which are given in Appendix E.

Maubach (1972) assumed that $R(h_+)$ reaches an asymptote for $Re > 10^5$. This allowed a plot of $R(h_+)$ against $W/h$ to be made. Using this plot, $R(h_+)$ can be estimated. According to Figure 4 in Maubach (1972), for surface 1, $R(h_+) \approx 3.1$. This gives an independent method of computing $f$ for surface 1, assuming $Re > 10^5$. The data of Feurstein and Rampf (1969) have a maximum Reynolds number of $2 \times 10^5$, which only overlaps 3 of the flows of Watson (1970) for surface 1. However, the results for surfaces 1 and 2 in Figure 8.12 show no major qualitative differences for Reynolds numbers larger than this. In addition, the Maubach (1972) has been applied for Reynolds numbers up to $1.3 \times 10^6$ in Warburton and Pirie (1974). Therefore the correlation of Maubach (1972) can be used for flows at the higher Reynolds numbers studied by Pirie (1974).

The transformation can also be used in reverse to compute values of $R(h_+)$ using the friction factors of Watson (1970) and Pirie (1974). The experimental data yield values of $R(h_+)$ between 2.03 and 3.40, which is consistent with the value from Figure 4 in Maubach (1972).
The LRN Spalart-Allmaras results yield values of $R(h_+)$ between 3.38 and 3.55. The Spalart-Allmaras results yield larger values of $R(h_+)$ than the experimental data, but the spread of these values is smaller.

The relationships between $f$ and $Re$ for three different values of $R(h_+)$ are shown in Figure 8.24. The three values correspond to the maximum and minimum values yielded by the experimental data and the value predicted by Figure 4 in Maubach (1972) ($R(h_+) = 3.1$). By construction, the line for $R(h_+) = 2.03$ yields the largest friction factors and $R(h_+) = 3.40$ yields the smallest, with both lines passing through only one experimental data point. The size of the space between the lines for these two values of $R(h_+)$ is a measure of the uncertainty in the experimental data. For all values of $R(h_+)$, the trend is for $f$ to decrease with $Re$. This trend is similar to that found by the Spalart-Allmaras results. The friction factors computed with $R(h_+) = 3.40$ show reasonable agreement with the Spalart-Allmaras results across all Reynolds numbers.

![Figure 8.24: Friction factors for surface 1 from the equations of Maubach (1972) with different $R(h_+)$.](image)

Only two of the friction factors predicted by Watson (1970) and Pirie (1974) are below the trend line for $R(h_+) = 3.1$, which is the value of $R(h_+)$ implied by the data of Feurstein and Rampf (1969) used by Maubach (1972). In contrast, all of the Spalart-Allmaras friction factors are below this trend line. Across the range of Reynolds numbers, the Spalart-Allmaras
8.5. Modelling the rib as a roughness element

results are closer to the trend line than the experimental data. Assuming that the trend line for $R(h_\tau^+) = 3.1$ is correct, the correlation indicates that:

1. The friction factors of Watson (1970) and Pirie (1974) are mostly over-estimates and the friction factors from the Spalart-Allmaras model are always under-estimates.

2. The over-estimation by the experimental data is larger than the under-estimation by the Spalart-Allmaras model.

3. The trend in $f$ with $Re$ in the experimental results is incorrect, whereas the trend in the Spalart-Allmaras results is accurate.

4. With the exception of the $\varphi - f$ model, the other turbulence models in Figure 8.18a predict smaller friction factors than the Spalart-Allmaras model. Hence RANS turbulence models tend to under-estimate the friction factor.

However, drawing any conclusions from Figure 8.24 affords much significance to the experimental results of Feurstein and Rampf (1969), since these were the only data used to develop the correlation. These data were obtained around the same time as the experiments of Watson (1970) and Pirie (1974), and therefore may be subject to similar experimental errors.

8.5.2 The correlation of Dalle Donne and Meyer (1977)

Following on from the work of Maubach (1972) and other authors, Dalle Donne and Meyer (1977) developed an improved, more accurate correlation. The correlation of Dalle Donne and Meyer (1977) assumes that the rough wall function has the same form as the correlation of Maubach (1972) (Equation (8.20)), but that the slope of the velocity profile in region 2 of the annulus is variable, and is a function of the flow near the ribbed wall. This is necessary because the turbulence generated by the ribs is seen in experiments to flatten the velocity profile near the pipe wall. The correlation can also account for variations in fluid properties with temperature if the ratio of wall to bulk temperature is known. This is an improvement on the isothermal correlation of Maubach (1972).

In Dalle Donne and Meyer (1977) a new parameter, $R(h_\tau^+)_1\%$, is introduced, which is related to $R(h_\tau^+)$ as

$$R(h_\tau^+)_1\% = R(h_\tau^+) - 0.4 \ln \left( \frac{h/\hat{y}}{0.01} \right) - \frac{5}{\sqrt{h_\tau^+}} \left( \frac{T_W}{T_B} - 1 \right)^2,$$  \hspace{1cm} (8.21)

where $T_W$ is the wall temperature, $T_B$ is the bulk temperature, $\hat{y} = R_0 - R_1$ and $h_\tau^+_{r,W}$ is $h_\tau^+$ computed in terms of the fluid properties at the wall temperature. If $h/\hat{y} < 0.235$ then the ribs can be adequately modelled as roughness elements, otherwise, the flow is better considered as an orifice plate (Dalle Donne and Meyer, 1977).
Dalle Donne and Meyer (1977) used the data of 18 authors (including that of Watson (1970) and Feurstein and Rampf (1969)) and results of their own experiments to develop a correlation for $R(h^+)_{1\%}$. For $h^+ > 70$ (which is always the case with the Watson (1970) and Pirie (1974) experiments), $R(h^+)_{1\%}$ reaches an asymptote and is approximately independent of $h^+$ (Dalle Donne and Meyer, 1977). In this flow regime, $R(h^+)_{1\%}$ is renamed $R(\infty)_{01}$. For square ribs with $(W - h)/h < 6.3$, which is the case for surface 1, the correlation is

$$R(\infty)_{01} = 9.3 \left(\frac{W - h}{h}\right)^{-0.73} \pm 1.$$  \hspace{1cm} (8.22)

According to Dalle Donne and Meyer (1977), the term $\pm 1$ in Equation (8.22) leads to a variation of around $\pm 15\%$ in the computed friction factor.

In Equation (8.21), $R(h^+)_{1\%}$ depends on $h/\hat{y}$, which depends on the Reynolds number. This means that $R(h^+)_{1\%}$ is not constant for a particular geometry but must be calculated for each Reynolds number. The Reynolds number range of the data used to derive the correlation of Dalle Donne and Meyer (1977) spans at least the range in Watson (1970), in which the largest Reynolds number of any study is $1.125 \times 10^6$. Many of the supporting results used to build the correlation are valid up to $1.3 \times 10^6$ (Dalle Donne and Meyer, 1977). Therefore the correlation is applicable for the flows in this chapter. The full equations of the correlation and a brief outline of the methodology are given in Appendix E.

Values of $R(\infty)_{01}$ are computed for all runs of Watson (1970) and Pirie (1974) for surface 1 where carbon dioxide was used as a coolant. The correlations of Merriman (1980) are used to account for the variation of the properties of carbon dioxide with temperature, in order to include thermal effects in the correlation. The average pressure is required in order to compute the properties of carbon dioxide but is not given in Pirie (1974). It is estimated to be equal to the mean of the average pressures from each run performed by Watson (1970) with carbon dioxide. The sensitivity of $R(\infty)_{01}$ to the mean pressure is small over the range of pressures in the experiments of Watson (1970), so the estimation of the mean pressure does not significantly affect the results in this section. Values of $R(\infty)_{01}$ are also computed from the Spalart-Allmaras friction factors using the isothermal form of the correlation. For the experimental results, $R(\infty)_{01}$ is computed using both the isothermal and non-isothermal forms of the correlation, to quantify the effects of the variation of fluid properties with temperature. The computed values of $R(\infty)_{01}$ are displayed in Table 8.7.

The isothermal and non-isothermal transformations yield similar values of $R(\infty)_{01}$, which indicates that the variation of fluid properties with temperature has only a small effect on the results. This confirms that the analysis in Section 8.1.2 is correct and that Equation (8.9) is accurate enough. The values of $R(\infty)_{01}$ computed from the Spalart-Allmaras friction factors
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Table 8.7: \( R(\infty)_{01} \) computed for surface 1 from the friction factors of Watson (1970) and Pirie (1974), the LRN Spalart-Allmaras results and Equation (8.22). Only the results of experiments that used carbon dioxide are considered.

are larger than the most-likely value predicted by Equation (8.22) and larger than the value implied by any of the experimental results. When computed from the experimental data, \( R(\infty)_{01} \) is often lower than the most-likely value implied by Equation (8.22), which could have been seen already for the data of Watson (1970) in Figure 36 of Dalle Donne and Meyer (1977). The spread in \( R(\infty)_{01} \) from the Spalart-Allmaras results is smaller than it is from the experimental results, which reveals that the trend in \( f \) with \( Re \) is captured more accurately by the Spalart-Allmaras model than the experiments. The largest spread in \( R(\infty)_{01} \) is given by Equation (8.22), which also yields both the largest and smallest values of \( R(\infty)_{01} \). Values of \( h/\hat{\gamma} \) computed from the experimental data ranged from \( 3.39 \times 10^{-2} \) to \( 3.67 \times 10^{-2} \), which are less than 0.235. Therefore it is a good approximation to treat the rib as a roughness element.

Given a Reynolds number and a value of \( R(\infty)_{01} \), the correlation of Dalle Donne and Meyer (1977) can be used to compute the friction factor. The correlation in Equation (8.22) provides a means to do this. This is done for an isothermal case with \( T_W/T_B = 1 \) and a case with \( T_W/T_B = 1.17 \), which is the average value from all experimental runs with carbon dioxide, in order to elucidate the effect on the friction factor of heating the experiment. The resulting friction factors are shown in Figure 8.25.

The trend of \( f \) with \( Re \) in Figure 8.25 is similar to that in Figure 8.24 found with the correlation of Maubach (1972). All of the experimental and Spalart-Allmaras friction factors lie within the lines for \( R(h_{\pm})_{01} = 1.47 \) and 3.47, which was already implied by Table 8.7. This is unsurprising because the range \( \pm 1 \) in Equation (8.22) was introduced by Dalle Donne and Meyer (1977) to enable the correlation to reproduce the results of many different authors. Friction factors obtained with the Spalart-Allmaras model are always lower than the trend lines for \( R(\infty)_{01} = 2.47 \) whereas most experimental results are above the line. Heating the annulus is seen to lead to a decrease in the friction factor, which is consistent with the thermal term in Equation (8.4). The average decrease in \( f \) caused by heating the annulus is approximately 0.9% of the value of the isothermal friction factor across the range of Reynolds numbers in Figure 8.25. The trend in \( f \) with \( Re \) is almost independent of the effects of heating the annulus, however the difference between the heated and unheated friction factors does
Figure 8.25: Friction factors for surface 1 computed using the correlation of Dalle Donne and Meyer (1977) with $R(\infty)_{01}$ calculated using Equation (8.22). The properties of carbon dioxide are determined using the correlations of Merriman (1980).

Assuming the results of the correlation of Dalle Donne and Meyer (1977) with $R(\infty)_{01} = 2.47$ are correct, the following conclusions can be drawn from Figure 8.25:

1. The friction factors of Watson (1970) and Pirie (1974) using both carbon dioxide and air are accurate for $Re \lesssim 4 \times 10^5$. However as the Reynolds number increases above this, the friction factors become increasingly inaccurate such that most of the friction factors found using carbon dioxide are over-estimates.

2. The friction factors from the Spalart-Allmaras model are under-estimates.

3. The trend in $f$ with $Re$ is captured accurately by the Spalart-Allmaras model, but not captured by the experimental data.

4. Heating the annulus produces a decrease in the friction factor of approximately 0.9% of the isothermal result.

5. The trend in $f$ with $Re$ is similar between the isothermal and non-isothermal results, although the difference between the trends grows slightly as the Reynolds number in-
creases.

The conclusions are similar to those found with the correlation of Maubach (1972). Since the correlation of Dalle Donne and Meyer (1977) is based on the data of 19 authors, these conclusions are reliable. The data used to derive the correlation are all experimental results and so they contain experimental uncertainties. The results for $R(\infty)_{01} = 1.47$ and $R(\infty)_{01} = 3.47$ are useful for bounding the uncertainty in the data used to derive the correlation. However, Watson (1970) stated that in their experiments the errors in the experimental procedures would lead to increases in $f$, rather than decreases. Therefore there may be a tendency for correlations based on experimental data to over-estimate $f$.

The difference between the friction factor predicted by the correlation of Dalle Donne and Meyer (1977) and the data of Watson (1970) and Pirie (1974) grows as the Reynolds number increases. For S1R6, the difference is over 12%, when expressed as a percentage of the value of $f$ computed with the correlation. The smallest Reynolds number studied with surface 6 is $4.76 \times 10^5$, which is in the range where the data of Pirie (1974) over-predicts the friction factor for surface 1. This implies that the friction factors for surface 6 in Pirie (1974) are indeed over-estimates.

### 8.5.3 Modelling the rib as a roughness element using CFD

The results of Sections 8.5.1 and 8.5.2 suggest that, at least for a transverse pin, it is a good approximation to model the rib as a roughness element. In such cases, the effect of the rib is included in the constant term in the rough wall function, as written in Equation (8.20). Therefore it should be possible to run CFD calculations of an annular flow with a rough inner wall and obtain reasonable predictions of the friction factor. This is done in this section with the rough wall function in *Code_Saturne*, which is discussed in Section 4.7.

For sufficiently large $y_+^z$ the rough wall function can be written as Equation (3.96), which is repeated below,

$$ U^+ = \frac{1}{\kappa} \ln y_+^z. \tag{8.23} $$

Therefore the only requirement to model the rib as a roughness element is an estimate of the roughness length, $z_0$, which can be found by equating Equations (8.23) and (8.20) to yield

$$ z_0 = h \exp \left( -\kappa R(h_+^z) \right), \tag{8.24} $$

where $\kappa = 0.40$ should be used for consistency with Maubach (1972) and Dalle Donne and Meyer (1977).

For surface 1, according to Figure 4 in Maubach (1972), $R(h_+^z) \approx 3.1$, and so $z_0 = 200 \mu m$. 238
Equation (8.22) from the correlation of Dalle Donne and Meyer (1977) gives $R(\infty)_{01} = 2.47$, which can be turned into $R(h_+^\tau)$ at a particular Reynolds number. For $T_W/T_B = 1.17$, the average roughness length over the Reynolds number range studied by Watson (1970) and Pirie (1974) is computed to be $z_0 = 209 \, \mu m$. These roughness lengths are used in this section to model surface 1.

For surface 6, which has a multistart pin, the computation of the roughness length is complicated because the rib angle of attack should be included in the calculation and there are no existing means to do this. Hence a range of roughness lengths is tested, with $z_0 \in \{100, 200, 300, 400\} \, \mu m$. If a suitable roughness length can be found such that a multistart rib can be incorporated into the rough wall function, then it may be possible to significantly simplify the modelling of a cluster of fuel pins with CFD.

A simulation is set up on a $1^\circ$ sector of an annulus, as shown in Figure 8.4, and a mesh of only 7 equidistant cells. The intention of these simulations is to obtain an accurate-enough friction factor in the fastest possible time. The rough wall function is used on the pin wall and the smooth wall function is used on the pipe wall. The simulations in this section are performed using the HRN $k - \varepsilon$ turbulence model, since it is the only turbulence model implemented in Code_Saturne for which the rough wall function is properly implemented. The roughness lengths used for surfaces 1 and 6 are those discussed above.

The computed friction factors are shown in Figure 8.26 for surfaces 1 and 6. The value of $y_+^\tau$ on both walls for both surfaces is typically around 1000, which indicates that the mesh is suited to the use of a wall function.

For surface 1, the trend in $f$ with $Re$ in Figure 8.26a is similar to the LRN Spalart-Allmaras result, although the values of $f$ are smaller by around 5%. The friction factors are also smaller than the correlations of Maubach (1972) and Dalle Donne and Meyer (1977) by approximately 10%. Thus, the rough wall function in Code_Saturne tends to yield smaller friction factors than the experimental data. Figure 8.26a shows that a larger value of $z_0$ would be needed in order to find agreement with the HRN $k - \varepsilon$ and LRN Spalart-Allmaras friction factors. However, since the LRN simulations are performed with a different turbulence model, there is no particular reason why the LRN and HRN results should match. No choice of $z_0$ would ever yield good enough agreement with the experimental data since the trend in $f$ and $Re$ is different.

For surface 6, Figure 8.26b shows that $z_0 = 100 \, \mu m$ gives good enough agreement with the LRN Spalart-Allmaras results across all Reynolds numbers, and that $z_0 = 300 \, \mu m$ gives reasonable agreement with the experimental data of Pirie (1974). Since there are fewer experimental data for surface 6, the trend in $f$ with $Re$ is less clear but it is reasonably
Figure 8.26: Friction factors for surfaces 1 and 6 when the rib is modelled as a roughness element with the rough wall function using the HRN $k - \varepsilon$ model in *Code_Saturne*.
approximated by the $k - \varepsilon$ simulations.

The results of this section indicate that it is possible to model both a transverse and multistart pin with a rough wall function. It may therefore be possible to perform a simplified calculation of a fuel assembly by modelling the ribs with the rough wall function instead of including them in the mesh. However Figure 8.26b cannot accurately determine which value of $z_0$ should be used, since it is not clear what the true friction factor is, and whether the experimental or CFD data are closer to the true value. In addition, in a fuel assembly the enhanced mixing caused by the right- and left-handed multistart pins will also tend to increase the friction factor. Modelling this would require a larger value of $z_0$. However given that it is possible to use a transformation method to compute the friction factor of a fuel assembly from that of a single pin, it should be possible to compute an appropriate roughness length for use in a fuel assembly once an accurate value of $z_0$ is known for a single pin using a similar procedure.

8.6 Modelling roughness on the pin surface

In Section 8.3, the experimental friction factors are almost always larger than the CFD friction factors and the profile of $f$ against $Re$ is flatter. Surface roughness can cause both of these effects. Therefore it was postulated that, although the pin surface contains a rib, the actual surfaces of the pin (including the rib) and pipe might have had a non-smooth surface finish left over by the manufacturing process. Hence there could have been an additional source of surface roughness in the experiments. If this additional surface roughness is included in the CFD model, the results might agree more closely with the experimental data. In this section the rough wall function in *Code_Saturne* is used to study different surface finishes on surfaces 1 and 6.

In addition, one of the objectives of this project is to quantify the change in the friction factor when a rough deposit of carbon forms on the surface of the pin. This can also be studied using the rough wall function on the pin wall. Thus, this section addresses two questions:

1. Could the discrepancy between the CFD and experimental results of Watson (1970) and Pirie (1974) be caused by surface roughness on the experimental surfaces?

2. What happens to the friction factor when a carbon deposit roughens the pin surface?

In order to address these two questions, reasonable estimates for the roughness length on the pin wall are required. As discussed in Section 3.6, Equation (3.99) shows that in a fully rough flow, the roughness length is less than the equivalent sand grain roughness. The methodology of Adams et al. (2012), expressed as Equation (3.95), indicates that the roughness average is also less than the equivalent sand grain roughness. The roughness average of any non-smooth
8.6. Modelling roughness on the pin surface

Surface finish must be significantly smaller than the rib height, otherwise it would surely have been mentioned in the experimental reports. Since measurements of the rib height in Pirie (1974) are given to the nearest 10 µm it is anticipated that the actual surface finish is less than 10 µm, although the rib heights in Watson (1970) were given to the nearest 25 µm and so the uncertainty could be larger.

The roughness lengths tested are shown in Table 8.8. In addition, a case with no surface roughness, which uses the smooth wall function was studied. Also shown in Table 8.8 are the equivalent sand grain roughnesses for the roughness lengths, which are calculated assuming the flow is fully rough, and the roughness average, which has been calculated using the methodology of Adams et al. (2012).

<table>
<thead>
<tr>
<th>$z_0$</th>
<th>1</th>
<th>3</th>
<th>5</th>
<th>10</th>
<th>15</th>
<th>20</th>
</tr>
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<tbody>
<tr>
<td>$s$</td>
<td>30</td>
<td>90</td>
<td>150</td>
<td>300</td>
<td>450</td>
<td>600</td>
</tr>
<tr>
<td>$R_a$</td>
<td>5</td>
<td>15</td>
<td>25</td>
<td>50</td>
<td>75</td>
<td>100</td>
</tr>
</tbody>
</table>

Table 8.8: The roughness lengths and corresponding equivalent sand grain roughnesses and roughness averages used to model surface roughness.

The pipe wall is quoted in Watson (1970) to have a surface finish of 5 microinches, which is 0.127 µm, which is much smaller than any $R_a$ tested in this section. It seems reasonable that the surface roughness on the pipe wall should be similar to the roughness on the pin wall, and certainly not different by several orders of magnitude. Thus it seems that $R_a = 5$ µm is likely to be an over-estimate of the surface finish on the pin wall in the experiments. Therefore any increase in $f$ that occurs for $R_a = 5$ µm is an upper bound for the increase caused by surface roughness that could have been present in the experiments.

Values of $R_a > 5$ µm are used to model the effects of carbon deposition on the pin surface. Images of deposits from post irradiation examination of real fuel assemblies indicate that the carbon deposit varies significantly along a pin. Therefore it is useful to test a range of surface roughness values to begin to quantify how the friction factor is affected by the deposit.

The simulations in this section are performed using the HRN $k - \varepsilon$ turbulence model, since it is the only turbulence model implemented in Code_Saturne for which the rough wall function is properly implemented. The geometry of the mesh is the same as that in Figure 8.8. The mesh has 4840 cells, with six cells covering the height of a rib in the radial direction and six cells covering the length of the rib in the axial direction. This particular distribution of cells gives a reasonable near-wall cell size that can be used to study different roughness lengths and is still fine enough to resolve some flow features. As in Section 8.3.2, the mesh of surface 1 is created by transforming the mesh of surface 6. Since HRN solutions inevitably depend on the mesh, the same mesh is used for every computation of each surface in this section.
Chapter 8. Industrial flows

Hence differences between simulations in this section are caused only by the choices of flow parameters. For surface 1, runs 1, 5, 6, E and F are performed. These runs span a range of Reynolds numbers that is representative of the full range in Table 8.2.

Since the surface finish of the pipe wall is known to be 0.127 µm, a set of simulations was run with \( z_0 = 0.127 \mu m \); on the pipe wall. In reality, \( z_0 = 0.127 \mu m \) corresponds to a roughness average larger than 0.127 µm. A larger roughness average yields a larger friction factor. Therefore any increase in \( f \) with \( z_0 = 0.127 \mu m \) is an over-estimate the increase that would occur with \( R_a = 0.127 \mu m \). When the simulation is run with the smooth wall function on the pin wall and \( z_0 = 0.127 \mu m \) on the pipe wall, the computed friction factor is lower than it is when the smooth wall function is used on both the pin and pipe walls. This behaviour is incorrect because the smooth wall case should produce the smallest friction factor. With \( z_0 = 0.127 \mu m \), the value of \( z_0^+ \) on the pipe wall is 0.05. If the flow were in the fully rough regime, this would correspond to \( s_0^+ = 1.5 \), which would put the flow in the fully smooth regime. Hence the pipe wall, with a roughness average of \( R_a = 0.127 \mu m \), is hydrodynamically smooth. Therefore in this section, the pipe wall is always treated as hydrodynamically smooth with the smooth wall function.

Using the value of \( \nu/u_\tau \) from the smooth wall case, a roughness length of \( z_0 = 6 \mu m \) would be required in order to have a fully rough flow with \( s_0^+ > 70 \). This would correspond to \( s \approx 180 \mu m \) or \( R_a \approx 30 \mu m \). The value of \( \nu/u_\tau \) on the pin wall varies depending on position, however its average value is similar to that on the pipe wall. Thus, to have a fully rough flow, \( z_0 \gtrsim 6 \mu m \) is required on the pin wall. Therefore the smallest three roughness lengths in Table 8.8 are not fully rough but transitionally rough. In this regime, the relationship between \( z_0 \) and \( s \) is not straightforward. However, the relationship between the two can be computed given \( \nu/u_\tau \) and an expression for the roughness function (see Section 3.6). The relationship between \( s \) and \( z_0 \) for the roughness function of Durbin et al. (2001) and \( \nu/u_\tau = 2.5 \mu m \), which is the average value of \( \nu/u_\tau \) on the pipe wall, is shown in Figure 8.27. Figure 8.27 can be used to compute the roughness length given an equivalent sand grain roughness, or vice versa.

Roughness lengths below approximately 0.3 µm do not have a corresponding equivalent sand grain roughness. In such cases the wall is hydrodynamically smooth.

Figure 8.28 shows the friction factors computed with the roughness lengths in Table 8.8 on the pin and rib surface and a smooth pipe wall for surfaces 1 and 6, as well as the case with the smooth surface finish on the pin, including the rib, with the HRN \( k - \varepsilon \) model.

The results with the SWF for the smooth pin wall agree well with the LRN Spalart-Allmaras results for both surfaces 1 and 6, with the agreement for surface 6 especially close. This indicates that a wall function method is appropriate for this flow, and that the mesh is.
8.6. Modelling roughness on the pin surface

suitable. When the pin wall is roughened the friction factor always increases. The increase in the friction factor grows as \( z_0 \) increases, however there are diminishing returns in the sense that the increase in \( f \) per unit \( z_0 \) decreases as \( z_0 \) increases. The effect of the roughness is to shift the plot of \( f \) upwards; the trend in \( f \) with \( Re \) is unaffected. Hence the increase in \( f \) is approximately independent of Reynolds number at the range of Reynolds numbers studied in Figure 8.28. For surface 1, this means that no amount of surface roughness on the pin wall could ever make the CFD results agree with the experimental results, since the trends in the two data sets different. For surface 6, a large roughness length could cause the CFD and experimental results to agree with each other. However the roughness length required to achieve agreement would be larger than \( z_0 = 20 \) µm, which corresponds approximately to \( R_a = 100 \) µm, which is well above the measurement uncertainty on the rib height in Pirie (1974). Therefore, surface roughness is not the cause of the discrepancy between the CFD and experimental results.

Surface 6 is geometrically similar to a fuel pin in an AGR. Therefore Figures 8.27 and 8.28b can be used to estimate the increase in \( f \) that occurs when a deposit of a given equivalent sand grain roughness forms on a real fuel pin. For example, with \( s = 100 \) µm, which corresponds to \( z_0 = 3 \) µm according to Figure 8.27, the friction factor increases by roughly 10% for surface 6, compared to the smooth case, as shown in Figure 8.28b. The rib height and pitch of surface 6 of Pirie (1974) are approximately twice those of a real AGR fuel pin. Therefore, for any

Figure 8.27: The relationship between \( z_0 \) and \( s \) for \( \nu/u_r = 2.5 \) µm, computed in the transitional region using the roughness function of Durbin et al. (2001).
Figure 8.28: Friction factors for surfaces 1 and 6 with the rough wall function on the pin wall and the smooth wall function on the pipe wall.
8.7 Conclusions

Although the flows in this chapter are conceptually straightforward and can be modelled with only a two-dimensional mesh, it has proved difficult to obtain any agreement between the experimental data and a CFD model. Even among experimental results of different authors, there is considerable variation in the measured friction factors for similar geometries and flow conditions (Dalle Donne and Meyer, 1977).

The results of this chapter are useful from a commercial perspective since the experiments of Watson (1970) and Pirie (1974) have never been studied before with CFD in such detail. In a situation such as this, CFD provides a useful estimate of the error in the experimental data. It is likely that the experimental results have over-estimated the friction factor. This over-estimation may also affect other experimental results from the same time period. Therefore it may be necessary to re-assess any predictions that have been made with this old experimental data.

The following useful conclusions can be drawn from this chapter:

1. The smooth pin results of Watson (1970), with no rib, are consistent with the CFD results and the correlations used in this chapter.

2. For the ribbed pins, the CFD results and the correlations of Maubach (1972) and Dalle Donne and Meyer (1977) imply that the friction factors in Watson (1970) and Pirie (1974) are over-estimates of the true friction factor. The degree of over-estimation is unknown but differs for each surface.

3. The Stanton number is also over-estimated in the experiments on surface 0. On the other surfaces, the CFD predictions of $St$ are also likely to be inaccurate since the flow velocity field is inaccurate.

4. NDD can be used on all pins. Especially good results are found for smooth pins with no ribs. The maximum size of the inner region that can be used for multistart pins is...
smaller than it is for transverse pins, in order to have an acceptable error on the friction factor.

5. The discrepancy between CFD and experimental results cannot be explained by surface roughness on the experimental surfaces.

6. It is possible to replace the rib by a representative roughness length for both surfaces 1 and 6. Therefore it should be possible to find a roughness length that can be used to perform efficient computations of an entire fuel assembly.

7. Carbon deposition on a fuel pin leads to an increase in the friction factor which can be estimated using Figure 8.28b.
Chapter 9

Conclusions and recommendations

This thesis contains two main threads of work. Firstly, the near-wall domain decomposition method of Utyuzhnikov (2006) has been implemented into an industrial code for the first time and applied to a range of test cases with complex flow phenomena and multiple turbulence models. Secondly, a detailed CFD study of the experiments performed by Watson (1970) and Pirie (1974) has been performed and the effects of surface roughness investigated. This chapter contains a summary of the previous chapters of this thesis and the overall conclusions from the work. More detailed conclusions can be found at the end of each chapter. Recommendations for future work that could follow this thesis are also given.

9.1 Summary of the work

Chapter 5 gave an introduction to the near-wall domain decomposition method and interface boundary conditions. The implementation of NDD for a $k-\varepsilon$ model by Utyuzhnikov (2006) was described and adapted to implement NDD for the $k-\varepsilon$ and Spalart-Allmaras models in Code_Saturne for the first time. Details of the implementations for the $k-\varepsilon$ and Spalart-Allmaras models are given in this chapter and the implementations for the $k-\omega$ SST and BL-$\overline{u^2}/k$ model are given in Appendix C. The results in this thesis are the first results from using NDD in an unstructured code and also the first results of using NDD in complex geometries. It was found that the treatment used by Utyuzhnikov (2008) for the interface-normal velocity component, $V$, is unstable in Code_Saturne and a new implementation was suggested. A list of other options explored is given in Appendix B. Chapter 5 also contains a comparison of NDD to conventional wall functions and the non-local formulation of NDD, first introduced by Utyuzhnikov (2009), is described and discussed. Many previous authors have identified wall functions as examples of overlapping domain decomposition methods (Knopp et al., 2006; Durbin, 2009; Lampropoulos et al., 2013). However the NDD method introduced
Chapter 9. Conclusions and recommendations

by Utyuzhnikov (2006), and developed further in this thesis, is unique in that it is a non-overlapping domain decomposition method, which requires a different implementation.

Chapter 6 presented results from five distinct test cases using the NDD method with the $k - \varepsilon$ and Spalart-Allmaras turbulence models. The test cases were two channel flows (at $Re_\tau = 590$ and $Re = 1.1 \times 10^4$), an annular flow, an impinging jet flow and an asymmetric diffuser flow. Different turbulent viscosity profiles were tested for each turbulence model and it was ultimately decided that the piecewise linear profile is most appropriate for the $k - \varepsilon$ model and the ZPG solution is most appropriate for the Spalart-Allmaras model. Different locations of the interface boundary, expressed in terms of $y^*$, were tested, to assess the performance of NDD as a HRN and LRN model. For all test cases, the results showed little sensitivity to $y^*$, and it was repeatedly demonstrated that the NDD solution approaches the LRN solution as $y^* \to 0$ for the Spalart-Allmaras model. The SWF implemented in Code_Saturne for the HRN $k - \varepsilon$ model tended to perform well on the simpler test cases. However on the diffuser flow, the SWF never predicts a recirculation region whereas one can be predicted with NDD because of the more accurate near-wall modelling that is possible. A comparison of computation times demonstrated that computation times with NDD tend to be greater than those with the SWF, but smaller than a fully-resolved LRN computation. Hence with NDD it is possible for a user to choose how much of a trade-off to make between the computation time and accuracy.

In Chapter 7 the NDD method was applied to the case of a ribbed channel flow. This study was intended as a precursor to the industrial computations in this thesis because there is reliable experimental data for this test case. The most ambitious aim of this chapter was to use NDD to exclude the entire rib and the region between the ribs from the main computational mesh, and hence to greatly simplify the problem. Many attempts were made to do this using interface A in Section 7.3 and it was found that unless the source terms in the momentum equations are known in advance of the simulation and used to compute the IBCs, the friction factor obtained with NDD is under-estimated by up to 70%. However, it was found that it is possible to remove from the computational mesh a large portion of the rib and the region between the ribs and still compute an accurate friction factor with NDD if the top surface of the rib remains within the mesh. Specifically, when 90% of the height of the rib is excluded from the main computational mesh, the error on the friction factor is 2%. This approach makes it straightforward to study different rib heights with only one mesh. An example of such a study is given, which fulfils one of the initial ambitions of this project.

Chapter 8 presented results of CFD calculations that model the experiments of Watson (1970) and Pirie (1974). A review of previous computational studies showed that these flows had never before been studied with LRN turbulence models at Reynolds numbers as high as the
9.2 Future work

Initial results for a smooth annulus matched the experimental data, and NDD simulations were found to produce accurate friction factors and Stanton numbers. For all except one run with the ribbed pins, with all turbulence models the friction factor from the LRN calculations was lower than the experimental value. It was briefly demonstrated that NDD could be used on fuel pin flows using the approach developed in Chapter 7. It was also demonstrated that the rib can be removed from the simulations and replaced by a roughness length in the rough wall function in Code_Saturne. With such an approach the friction factors can be calculated quickly and accurately. Figure 8.26 could be used to determine the appropriate roughness length to greatly simplify the study of a fuel assembly, if the true friction factor were known. However since the various methods of calculation produce such a large range of values of $f$, the true value is not known. More information is needed before any such computation could be performed. Assessment of RANS results and the LES result computed by Juan Uribe at the University of Manchester, and comparison of the trend in the experimental data to the correlations of Maubach (1972) and Dalle Donne and Meyer (1977) imply that the experimental results contain significant errors. The differences between the CFD simulations and the experiments were assessed and it was postulated that surface roughness in the experiments might be the cause of the discrepancy in the results. The effects of additional surface roughness on the fuel pin were studied and the results were sufficient to demonstrate that a non-smooth surface finish in the experiments is not the cause of the discrepancy between the experimental and the CFD results. It was also indicated how the results can be used to quantify the effects of carbon deposition on the friction factor. These results can be used to estimate how the friction factor in an AGR fuel assembly is affected by carbon deposition.

9.2 Future work

During this work, every effort was made to stay on time and on track to produce a useful set of results to satisfy both the academic requirements of the EngD degree and the commercial requirements of EDF Energy R&D UK Centre Limited.

On the commercial side, the most important output of this project is to have identified the discrepancy between the CFD simulations, the correlation of Dalle Donne and Meyer (1977) and the data of Watson (1970) and Pirie (1974). Investigating the sources of this discrepancy, and assessing whether it originates in the experimental data or in the CFD model took a great deal of time. The next objective should be to reduce the discrepancy between the experimental and CFD results in Chapter 8. In order to help do this, EDF Energy R&D UK Centre Limited have commissioned a new experiment, in which a real AGR fuel pin will
be studied in an annular flow, similar to those in Chapter 8. It is hoped that more modern experimental techniques will be able to reduce the experimental uncertainty in the results. The results in Chapter 8 were used to help decide the geometry and flow parameters of the experiment. In addition, EDF Energy R&D UK Centre Limited are hiring an intern to work with the results of the new experiment, and the results of this thesis, to continue the study.

Possible avenues for future work, which may use the results of the new experiments are given below.

1. It is important to ensure that a good enough agreement is found between the results of the new experiment and a CFD model of it. Therefore a CFD model of the real pin geometry in an annulus should be performed at the same Reynolds numbers as the experiment.

2. If a reasonable agreement is found then it will be possible to study a periodic flow in a fuel assembly and obtain reliable results. Once the friction factor of the fuel assembly is known, it should be possible to find a roughness length to represent the ribs on the fuel pins, similar to what was done in Section 8.5.3. In this way, the ribs could be excluded from a simulation of the fuel assembly, which would greatly simplify the mesh and reduce the computation time. An elongated mesh of an entire reactor core may then be created and used to study a number of scenarios. These include the effects of sleeve leakage, bowing of fuel pins and of blockages in a channel.

3. Carbon deposition on a real AGR fuel pin can also be studied with a method similar to that in Section 8.6.

On the academic side of this project, the most important output of this project has been the development of the NDD method, its implementation into Code_Saturne and its application to a range of flows. Many avenues for further work with the NDD method were identified in this course of this work. The most interesting possibilities are outlined below.

1. By including non-local effects, NDD should be applicable to an even greater range of flows, including those where the near-wall regions contain two-dimensional or non-linear effects. This was explored in Chapter 7, where it was demonstrated that accurate results can be obtained on the ribbed channel if the source terms are known accurately. It may be possible to perform a simulation of a smaller section of a geometry in order to obtain an approximation of the source terms. These source terms could be used to compute NLIBC's in a study of a larger section of the geometry. This would be helpful in a simulation of a large geometry, to remove the computational requirement of resolving the flow near walls far from the principal regions of interest.
2. NDD was only used with steady flows in this thesis, however it is possible to extend the method to unsteady flows, as explained in Utyuzhnikov (2014). Such an approach promises to simplify the study of flows with, for example, moving or oscillating boundaries, and can be implemented with the same procedures outlined in this thesis.

3. It is common for LES simulations to use near-wall models (Piomelli, 2008). Although in this thesis NDD has only been used with RANS, the methodology is also applicable to LES. Applying NDD to LES would require time-dependent effects to be included in the calculations of the IBCs. However one advantage of applying NDD to LES instead of RANS is that there would be no turbulence model functions that require IBCs.

4. While the implementation of NDD is conceptually straightforward since it only requires the computation of some boundary conditions, in practice a number of issues are encountered when applying NDD to an engineering problem. For example, in industry it is usual to take a CAD geometry of a particular component and create a mesh from it. With NDD it would be necessary to modify the CAD geometry to remove the near-wall regions (or create a mesh and remove some cells from it). Whilst this is conceptually simple, in practice, especially with unstructured meshes, generating a smooth mesh would be a complex procedure if the geometry is complex. Thus, while NDD is a useful tool for design optimisation problems on relatively simple geometries, difficulties with implementation are likely to be a barrier to its application to more complex geometries.

The similarities between the AWF and NDD are detailed in Chapter 5. A research project could apply the Robin boundary condition derived in NDD at the centre of the near-wall cell in a coarse mesh to calculate the required boundary conditions at the wall; exactly how the log law is used in the SWF. In this way, the underlying theory of the NDD method in this thesis would replicate the AWF without using long analytical expressions and would enable code developers to implement the AWF more straightforwardly. Thus a conventional wall function with many of the advantages of NDD would be obtained. This would allow the improved accuracy of NDD to be used on complex geometries without added complications.
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Appendix A

Turbulence models

This appendix gives the equations of the turbulence models that have been used in this thesis.

The mean strain and vorticity tensors appear frequently in turbulence model equations. They are defined respectively as

\[ S_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right), \] (A.1)

and

\[ \Omega_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right), \] (A.2)

and are used to define the scalars

\[ S = \sqrt{2S_{ij}S_{ij}}, \] (A.3)

and

\[ \Omega = \sqrt{2\Omega_{ij}\Omega_{ij}}. \] (A.4)

Note that in incompressible flow, \( \nabla \cdot \mathbf{U} = 0 \). Every simulation in this thesis is performed for incompressible flow. Additional terms may be required in some of the equations in this Appendix for compressible flows. Quantities evaluated at the wall are denoted with a subscript \( w \).

A.1 Wall-distance calculation

LRN models frequently use the distance from the wall as a parameter to damp the turbulence in a flow. In \textit{Code_Saturne} there are two options for calculating the distance to the wall. Either the distance is calculated directly from the mesh, or a Poisson equation is solved (Tucker, 1998). The preferred method is the Poisson equation method, since the geometrical method is incompatible with the parallelisation procedure of \textit{Code_Saturne}. The equation solves for a variable, \( \Psi \), which obeys the following equation

\[ \nabla^2 \Psi = -1, \] (A.5)
with $\Psi = 0$ at the wall and $\partial_n \Psi = 0$ at every other boundary, where $n$ is the normal to the boundary. The distance to the wall, $d$, is then computed as

$$d = -|\nabla \Psi| + (\nabla \Psi \cdot \nabla \Psi + 2\Psi)^{1/2}.$$  \hspace{1cm} (A.6)

\section*{A.2 The standard HRN $k-\varepsilon$ model}

The $k-\varepsilon$ model implemented in \textit{Code_Saturne} is the HRN model of Launder and Spalding (1974). This model uses the scalable wall function and cannot resolve the flow in regions closer to the wall than the logarithmic region of the turbulent boundary layer. The model solves for the turbulent kinetic energy, $k$, and the turbulent dissipation, $\varepsilon$. Since it is one of the oldest turbulence models, it is one of the most widely-used. However it has some well-known deficiencies, for example in flow regions with adverse pressure gradients or streamline curvature, rotating flows and flows with heat transfer (Nallasamy, 1987; Rodi and Scheuerer, 1986).

- The $k$ equation is

$$\rho \frac{Dk}{Dt} = \rho P - \rho \varepsilon + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right),$$  \hspace{1cm} (A.7)

where

$$\rho P = \mu_t S^2.$$  \hspace{1cm} (A.8)

- The dissipation equation is

$$\rho \frac{D\varepsilon}{Dt} = c_{\varepsilon 1} \frac{\rho P \varepsilon}{k} - c_{\varepsilon 2} \frac{\varepsilon^2}{k} + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right).$$  \hspace{1cm} (A.9)

- The turbulent viscosity is calculated as

$$\mu_t = c_\mu \rho k^2 \frac{\varepsilon}{\varepsilon}.$$  \hspace{1cm} (A.10)

- The model constants are $c_\mu = 0.09$, $c_{\varepsilon 1} = 1.44$, $c_{\varepsilon 2} = 1.92$, $\sigma_k = 1$ and $\sigma_\varepsilon = 1.3$.

- The implementation of the boundary conditions for this turbulence model is given in detail in Section 4.6.

\section*{A.3 The LRN $k-\varepsilon$ model of Chien (1982)}

The LRN $k-\varepsilon$ model of Chien (1982) solves for a modified dissipation, $\tilde{\varepsilon}$, where

$$\tilde{\varepsilon} = \varepsilon - 2\nu \frac{k}{dT}.$$  \hspace{1cm} (A.11)

Damping functions are used to produce the required near-wall behaviour. The model is not implemented by default in \textit{Code_Saturne}, but was implemented during this project and verified against published results for the same model. Only one-dimensional problems have
Appendix A. Turbulence models

been solved with this turbulence model, since there were issues with convergence on two-
dimensional flows due to the association of every control volume with the wall shear stress
at the nearest wall boundary face.

• The $k$ equation is

$$
\rho \frac{Dk}{Dt} = \rho P - \rho \bar{\varepsilon} - 2\mu \frac{k}{d^2} + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right),
$$  \hspace{1cm} (A.12)

with

$$
\rho P = \mu_t S^2.
$$  \hspace{1cm} (A.13)

• The equation for $\bar{\varepsilon}$ is

$$
\rho \frac{D\bar{\varepsilon}}{Dt} = c_{\varepsilon 1} \frac{\rho P \bar{\varepsilon}}{k} - f_2 c_{\varepsilon 2} \rho \frac{\bar{\varepsilon}^2}{k} - 2\mu \frac{\bar{\varepsilon}}{d^2} e^{-y^+/2} + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_{\bar{\varepsilon}}} \right) \nabla \bar{\varepsilon} \right),
$$  \hspace{1cm} (A.14)

where $y^+ = \rho d \sqrt{\tau_w/\rho/\mu}$, $\tau_w$ is the wall shear stress at the nearest wall,

$$
f_2 = 1 - \frac{5}{9} e^{-R_{\text{et}}/36},
$$  \hspace{1cm} (A.15)

and $R_{\text{et}} = \rho k^2/(\bar{\varepsilon} \mu)$.

• The turbulent viscosity is calculated as

$$
\mu_t = f_{\mu}^2 \frac{c_{\mu} \rho}{\varepsilon} k^2,
$$  \hspace{1cm} (A.16)

where $f_{\mu} = 1 - e^{-0.015 y^+}$.

• The model constants are $c_{\mu} = 0.09$, $c_{\varepsilon 1} = 1.35$, $c_{\varepsilon 2} = 1.8$, $\sigma_k = 1$ and $\sigma_{\bar{\varepsilon}} = 1.3$.

• The boundary conditions at the wall are $k = 0$ and $\bar{\varepsilon} = 0$.

A.4 The $k - \omega$ SST model

The $k - \omega$ model (Wilcox, 2006) solves for a transported variable $\omega \equiv \varepsilon/k$. Like the $\varepsilon$ equation, the $\omega$ equation is modelled empirically with the form

$$
\rho \frac{D\omega}{Dt} = \gamma \frac{\rho P \omega}{k} - \beta \rho \omega^2 + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_{\omega}} \right) \nabla \omega \right) + \frac{\sigma_d \rho}{\omega} \nabla k \cdot \nabla \omega,
$$  \hspace{1cm} (A.17)

for constants $\beta$, $\gamma$, $\sigma_{\omega}$ and $\sigma_d$. In the $k$ equation, $\varepsilon$ is replaced by $\beta^* \omega k$.

The essential difference between $k - \varepsilon$ and $k - \omega$ models is the last term in Equation (A.17). If it is included in the equation, the model behaves like the $k - \varepsilon$ model. The $k - \omega$ SST turbulence model\(^1\) (Menter, 1994; Menter et al., 2003) is effectively a blending between the two types of model. It was initially formulated to improve the calculations of flows with separation or adverse pressure gradients, where the original $k - \omega$ model tends to over-predict the shear stress. A limiter is placed on $\mu_t$ which forces $|\nabla \omega|/k$ to be smaller than it would be for the $k - \omega$ model in boundary layers. Near to the wall, the $k - \omega$ SST model is similar to the

\(^1\)SST stands for “shear stress transport.”
k – ω model since in this region the model damping functions are \( F_1 \approx 1 \) and \( SF_2 \ll a_1 \omega \). This is beneficial because the \( k – \omega \) model is generally more accurate than the \( k – \varepsilon \) model in the near-wall region (Menter et al., 2003), especially with the limiter on \( \mu_t \). Far from the wall, in free-stream regions, the \( k – \omega \) SST model behaves like the \( k – \varepsilon \) model, which is less sensitive to the levels of free-stream turbulence than the \( k – \omega \) model (Menter et al., 2003).

The model is written here in the form implemented in Code_Saturne. For completeness, the equations contain the effects of the acceleration due to gravity, \( g \), which was never included in this work. For incompressible flows considerable simplifications are possible.

- The \( k \) equation is
  \[
  \frac{\rho Dk}{Dt} = \rho P_k - \beta^* \rho k \omega + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right),
  \]  
  where
  \[
  P_k = \min \left( -\bar{u}_i \bar{u}_j \frac{\partial U_i}{\partial x_j}, c_1 \beta^* \omega \right) - \frac{\mu_t}{\rho} \nabla \rho, \quad (A.19)
  \]
  and
  \[
  -\rho \bar{u}_i \bar{u}_j = \mu_t \left( 2S_{ij} - \frac{2}{3} \nabla \cdot \nabla \delta_{ij} \right) - \frac{2}{3} \rho k \delta_{ij}. \quad (A.20)
  \]

  The limitation of \( P_k \) prevents the production term from growing too large near stagnation points (ANSYS Inc., 2009).

- The \( \omega \) equation is
  \[
  \frac{\rho D\omega}{Dt} = \gamma \mu_t \rho P_\omega \rho \omega^2 + \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_\omega} \right) \nabla \omega \right) + \frac{2\rho}{\sigma_{\omega^2}} (1 - F_1) \frac{1}{\omega} \nabla k \cdot \nabla \omega, \quad (A.21)
  \]
  where
  \[
  P_\omega = -\bar{u}_i \bar{u}_j \frac{\partial U_i}{\partial x_j} + \max \left( -\frac{\mu_t}{\rho} \nabla \rho , 0 \right), \quad (A.22)
  \]
  \[
  F_1 = \tanh(\varphi_1^4), \quad (A.23)
  \]
  \[
  \varphi_1 = \min \left( \max \left( \frac{k^{1/2}}{\beta^* \omega y}, \frac{500 \mu}{y^2 \rho \omega} \right), \frac{4 \rho k}{\sigma_{\omega^2} CD_{k\omega} y^2} \right), \quad (A.24)
  \]
  and
  \[
  CD_{k\omega} = \max \left( \frac{2 \rho}{\sigma_{\omega^2} \omega} \nabla k \cdot \nabla \omega , 10^{-20} \right). \quad (A.25)
  \]

- The turbulent viscosity is given by
  \[
  \mu_t = \frac{a_1 \rho k}{\max (a_1 \omega, SF_2)}, \quad (A.26)
  \]
  where
  \[
  F_2 = \tanh(\varphi_2^2), \quad (A.27)
  \]
  and
  \[
  \varphi_2 = \max \left( \frac{2k^{1/2}}{\beta^* \omega y}, \frac{500 \mu}{\rho \omega y^2} \right). \quad (A.28)
  \]

- The model constants are found by blending the constants of the \( k – \varepsilon \) and \( k – \omega \) models
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with the expression

\[ \alpha = \alpha_1 F_1 + \alpha_2 (1 - F_1), \]  

(A.29)

where \( \alpha \) is any model constant and the subscripts 1 and 2 refer to the subscripts in Table A.1, which contains the model constants. The values of \( \gamma \) are calculated in terms of other model constants as

\[ \gamma_i = \frac{\beta_i}{\beta^*} - \frac{\kappa^2}{\sqrt{\beta^*} \sigma_{\omega i}}, \quad \text{for } i = 1, 2. \]  

(A.30)

- The boundary condition on \( k \) at the wall is a homogeneous Dirichlet one:

\[ k_w = 0. \]  

(A.31)

- The correct boundary condition on \( \omega \) at the wall should strictly be infinity. This cannot be imposed computationally, so another approach is taken. Many different treatments can be found in the literature. A common boundary condition is \( \omega_w = 6 C_w \mu / (\rho \beta_1 y^2) \), which is based on the asymptotic solution to the \( \omega \) equation at the wall. Typically \( y \) is taken to be the distance of the first near-wall cell centre from the wall. Menter (1993) uses \( C_w = 10 \) whereas Wilcox (2006) uses \( C_w = 1 \). Code_Saturne uses the Neumann condition

\[ \frac{\partial \omega}{\partial y}_{|w} = \frac{960 \mu}{\rho \beta_1 d^2}. \]  

(A.32)

- A wall function exists in Code_Saturne for the \( k - \omega \) SST model, however it has not been used in this work and therefore is not explained here.

<table>
<thead>
<tr>
<th>( \sigma_{k1} )</th>
<th>( \sigma_{k2} )</th>
<th>( \sigma_{\omega1} )</th>
<th>( \sigma_{\omega2} )</th>
<th>( \beta_1 )</th>
<th>( \beta_2 )</th>
<th>( \alpha_1 )</th>
<th>( c_1 )</th>
<th>( \kappa )</th>
<th>( \beta^* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.85</td>
<td>1</td>
<td>2</td>
<td>0.85</td>
<td>0.075</td>
<td>0.0828</td>
<td>0.31</td>
<td>10</td>
<td>0.42</td>
<td>0.09</td>
</tr>
</tbody>
</table>

Table A.1: The constants for the \( k - \omega \) SST model.

A.5 The Spalart-Allmaras model

The Spalart-Allmaras model (Spalart and Allmaras, 1994) is a one equation turbulence model. It is a low Reynolds number model, designed to solve down to the wall without using wall functions. The model solves for a variable \( \tilde{\nu} \), which when combined with a damping function \( f_{\nu 1} \), gives the turbulent viscosity directly. The model was intentionally developed to admit the solution \( \tilde{\nu} = \nu \kappa y^+ \) near to the wall, with \( f_{\nu 1} \) responsible for damping \( \mu_t \) to give the correct near-wall behaviour (Allmaras et al., 2012). Because it uses only one equation, the model can fail to capture complex flow phenomena such as separation and transition to turbulence accurately. However, an advantage of the model is its simplicity; as a one-equation model with simple wall boundary conditions, it tends to be relatively simple to make computations with it converge.

The model implemented in Code_Saturne differs from that in the original reference of Spalart and Allmaras (1994). The original model has a “trip” term, involving a damping function \( f_{t1} \), which is useful only at low Reynolds numbers and when interested in the transition to
A.5. The Spalart-Allmaras model
turbulence. This term is not included in Code_Saturne. Also missing are any terms involving
the damping function, \( f_{t2} \). As with the “trip” term, this term was included to enhance the
model’s ability to capture the transition to turbulence. Since the flows in this work are at
high Reynolds numbers, the absence of these terms does not make any measurable difference
to any results.

- The model equation, as implemented in Code_Saturne is
\[
\rho \frac{D\tilde{\nu}}{Dt} = c_{b1} \rho \tilde{S} \tilde{\nu} - c_{w1} \rho f_w \left( \frac{\tilde{\nu}}{d} \right)^2 + \frac{c_{b2} \rho}{\sigma} \nabla \tilde{\nu} \cdot \nabla \tilde{\nu} + \frac{1}{\sigma} \nabla \cdot ((\mu + \rho \tilde{\nu}) \nabla \tilde{\nu}).
\] (A.33)

- The turbulent viscosity is calculated as
\[
\mu_t = \rho \tilde{\nu} f_{\nu1},
\] (A.34)
where the damping function \( f_{\nu1} \) is given by
\[
f_{\nu1} = \frac{\chi^3}{\chi^3 + c_{\nu1}^3},
\] (A.35)
and
\[
\chi = \frac{\rho \tilde{\nu}}{\mu}.
\] (A.36)

- The calculation of \( \tilde{S} \) requires an additional function \( \overline{S} \), defined as
\[
\overline{S} = \frac{\tilde{\nu}}{\kappa S^2 f_{\nu2}},
\] (A.37)
then \( \tilde{S} \) is calculated as
\[
\tilde{S} = \begin{cases}
\Omega + \overline{S} & \text{if } \overline{S} \geq -c_2 \Omega, \\
\Omega + \frac{\Omega(\nu_3 \Omega + c_6 S)}{(c_3 - 2c_2) \Omega - S} & \text{if } \overline{S} < -c_2 \Omega.
\end{cases}
\] (A.38)
This definition of \( \tilde{S} \) ensures that it is always positive (Oliver, 2008).

- The damping function \( f_{\nu2} \) is computed as
\[
f_{\nu2} = 1 - \frac{\chi}{1 + \chi f_{\nu1}}, \] (A.39)
and the damping function \( f_w \) is calculated as
\[
f_w = g \left( \frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right)^{1/6},
\] (A.40)
where \( g = r + c_{w2} (r^6 - r) \) and
\[
r = \min \left( \frac{\tilde{\nu}}{\kappa S^2 f_{\nu2}}, 10 \right). \] (A.41)

- The boundary condition on \( \tilde{\nu} \) at the wall is the homogeneous Dirichlet condition
\[
\tilde{\nu}_w = 0.
\] (A.42)
Appendix A. Turbulence models

- The model constants are given in Table A.2.

<table>
<thead>
<tr>
<th>( \sigma )</th>
<th>( \kappa )</th>
<th>( c_{b1} )</th>
<th>( c_{b2} )</th>
<th>( c_{w1} )</th>
<th>( c_{w2} )</th>
<th>( c_{w3} )</th>
<th>( c_{v1} )</th>
<th>( c_{2} )</th>
<th>( c_{3} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{2}{3} )</td>
<td>0.42</td>
<td>0.1355</td>
<td>0.622</td>
<td>( \frac{c_{b1}}{\sigma} + \frac{1+c_{b2}}{\sigma} )</td>
<td>0.3</td>
<td>2</td>
<td>7.1</td>
<td>0.7</td>
<td>0.9</td>
</tr>
</tbody>
</table>

Table A.2: The constants for the Spalart-Allmaras model.

A.6 The \( \varphi - f \) model

The original \( \overline{v^2} - f \) model of (Durbin, 1991) introduces two new functions into a \( k - \varepsilon \) model. These are \( \overline{v^2} \), which models the turbulence fluctuations normal to the mean streamlines, and \( f \), which is an elliptic relaxation function. The direction normal to the mean streamlines is treated with special interest because it is in this direction that the flow is most damped near to a wall. The equation for \( \overline{v^2} \) is based on the equation for the Reynolds stress itself. It contains a source term on the right hand side, of the form \( kf \), which models the redistribution term \( \phi_{22} \), the pressure diffusion and the dissipation tensor (Billard, 2011). The elliptic relaxation function obeys the following equation:

\[
L^2 \nabla^2 f - f = \frac{1}{T} (c_1 - 1) \left( \frac{\overline{v^2}}{k} - \frac{2}{3} \right) - c_2 \frac{\rho}{\varepsilon}.
\]  
(A.43)

This equation means roughly that \( f \) contains information about the non-local effects on \( \overline{v^2} \) within a sphere whose radius is the turbulent length scale. A significant issue for this model is the limiting behaviour of \( f \) at the wall, where the limit is (Laurence et al., 2004)

\[
f \to \left( \frac{-20\rho^2 \overline{v^2}}{\varepsilon y^4} \right) \text{ as } y \to 0.
\]  
(A.44)

Since \( \overline{v^2} \) is of order \( y^4 \) at the wall, the ratio in Equation (A.44) is very sensitive to changes in \( \overline{v^2} \) between iterations, which necessitates the use of a small time step. Laurence et al. (2004) introduced a new variable, \( \varphi = \overline{v^2}/k \) and used a change of variable \( \overline{f} = f + 2\nu \nabla k \nabla \varphi /k - \nu \nabla^2 \varphi \), which, after neglecting two terms in the \( \overline{f} \) equation, resulted in an equation set where \( \overline{f} \) receives a homogeneous Dirichlet boundary condition at the wall.

The \( \varphi - f \) turbulence model implemented in Code_Saturne is that of Laurence et al. (2004) with some minor modifications. For example, in the original reference, only the turbulent viscosity contributes to the diffusive term for \( \varphi \). However, since at the wall \( \mu_t \) goes to zero, the diffusion term can become numerically unstable. Therefore the molecular viscosity is included as well in Code_Saturne. At the wall, \( k \to 0 \) and so the production term dominates over diffusion even when molecular diffusion is included. Therefore this modification has only a small impact on the results.

- The \( k \) equation is

\[
\frac{\rho Dk}{Dt} = \rho P - \rho \varepsilon + \nabla \cdot \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k,
\]  
(A.45)
A.6. The $\varphi - f$ model

where $\mathcal{P}$ is the production of turbulent kinetic energy,

$$\mathcal{P} = \frac{\mu_S^2}{\rho}. \quad (A.46)$$

- The $\varepsilon$ equation is

$$\rho \frac{D\varepsilon}{Dt} = \frac{c_{e1}\rho\mathcal{P} - c_{e2}\rho\varepsilon}{T} + \nabla \cdot \left( \left( \mu + \frac{\mu}{\sigma_\varepsilon} \right) \nabla \varepsilon \right), \quad (A.47)$$

with the turbulent time scale

$$T = \max \left( \frac{k}{\varepsilon}, c_{dt} \sqrt{\frac{\mu}{\rho\varepsilon}} \right), \quad (A.48)$$

and

$$c_{e1} = 1.4 \left( 1 + \frac{c_{e1}}{\sqrt{\varphi}} \right). \quad (A.49)$$

- The $\varphi$ equation is

$$\rho \frac{D\varphi}{Dt} = \rho \mathcal{F} - \rho \mathcal{P} \frac{\varphi}{k} + 2\mu \frac{\varepsilon}{\sigma_k \varepsilon} \nabla \varphi \cdot \nabla k + \nabla \cdot \left( \left( \mu + \frac{\mu}{\sigma_\varphi} \right) \nabla \varphi \right). \quad (A.50)$$

- The equation for $\mathcal{F}$ is

$$L^2 \nabla^2 \mathcal{F} - \mathcal{F} = \frac{c_1 - 1}{T} \left( \varphi - \frac{2}{3} \right) - c_2 \frac{\mathcal{P}}{k} - \frac{2\mu}{\rho T} \nabla \varphi \cdot \nabla k - \frac{\mu}{\rho} \nabla^2 \varphi, \quad (A.51)$$

where the turbulent length scale is

$$L = c_L \max \left( \frac{k^{3/2}}{\varepsilon}, c_\eta \left( \frac{\mu^3}{\rho^2 \varepsilon} \right)^{1/4} \right). \quad (A.52)$$

- The turbulent viscosity is

$$\mu_t = c_\mu \rho T \varphi k. \quad (A.53)$$

- The boundary conditions at the wall are

$$k_w = 0, \quad (A.54)$$

$$\varepsilon_w = \frac{2\mu k_{fl}}{\rho d_{fl}}, \quad (A.55)$$

$$\varphi_w = 0, \quad (A.56)$$

$$\mathcal{F} = 0, \quad (A.57)$$

where $k_{fl}$ and $d_{fl}$ are respectively the turbulent kinetic energy and the distance from the wall at the near-wall cell centre.

- The model constants are given in Table A.3.
Appendix A. Turbulence models

<table>
<thead>
<tr>
<th>$c_{e1}$</th>
<th>$c_{e2}$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
<th>$\sigma_\varphi$</th>
<th>$c_\mu$</th>
<th>$c_{st}$</th>
<th>$c_L$</th>
<th>$c_\eta$</th>
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<th>$c_2$</th>
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<td>0.22</td>
<td>6</td>
<td>0.25</td>
<td>110</td>
<td>1.4</td>
<td>0.3</td>
<td></td>
</tr>
</tbody>
</table>

Table A.3: The constants for the $\varphi - f$ model.

A.7 The BL-$\overline{u'^2}/k$ model

Billard and Laurence (2012) took the $\varphi - f$ model and introduced a new dimensionless function $\alpha$ to describe the non-local effects. The dissipation was also modified by the change of variables

$$\epsilon = \epsilon_h + \frac{k}{\epsilon} E + \frac{1}{2} \nu \nabla^2 k,$$

where the so-called $E$ term is active predominantly in the buffer layer of wall-bounded flows. For consistency, the change of variables to $\epsilon_h$ necessitates halving the viscous diffusion of the three transported variables, $k$, $\epsilon_h$ and $\varphi$.

- The $k$ equation is

$$\rho \frac{Dk}{Dt} = \rho P - \rho \epsilon_h - \rho E + \nabla \cdot \left( \left( \frac{\mu}{2} + \frac{\mu_1}{\sigma_k} \right) \nabla k \right),$$

where the production term $P$ is

$$P = \frac{\mu_t S^2}{\rho},$$

and the $E$ term is

$$E = 2c_k (1 - \alpha)^{\frac{3}{2}} k \frac{\mu_t}{\epsilon_h} \rho^2 \left( \frac{\partial^2 U_i}{\partial x_k \partial x_j} \right) \left( \frac{\partial^2 U_i}{\partial x_k \partial x_j} \right).$$

- The $\epsilon_h$ equation is

$$\rho \frac{D\epsilon_h}{Dt} = \frac{c_{e1} \rho P - c_{e2} \rho \epsilon_h}{T} + \nabla \cdot \left( \left( \frac{\mu}{2} + \frac{\mu_1}{\sigma_{\epsilon_h}} \right) \nabla \epsilon_h \right).$$

This equation uses a constant $c_{e2}^*$, which is calculated as

$$c_{e2}^* = c_{e2} + \alpha^3 (c_{\varphi} - c_{e2}) \tanh \left( \frac{1}{\epsilon_h} \nabla \cdot \left( \frac{\mu}{\rho \sigma_k} \nabla k \right)^{3/2} \right).$$

- The $\varphi$ equation is

$$\rho \frac{D\varphi}{Dt} = \rho \left( 1 - \alpha^3 \right) f_w + \rho \alpha^3 f_h - \frac{\rho P \varphi}{k} + \frac{2\mu_t}{\mu_{st}} \nabla \cdot \nabla k + \nabla \cdot \left( \left( \frac{\mu}{2} + \frac{\mu_1}{\sigma_\varphi} \right) \nabla \varphi \right),$$

where

$$f_w = -\frac{\epsilon_h \varphi}{2k},$$

and

$$f_h = -\frac{1}{T} \left( c_1 - 1 + c_2 \frac{P}{\epsilon_h} \right) \left( \varphi - \frac{2}{3} \right).$$
A.8. The EBRSM model

• The function $\alpha$ obeys the equation

$$\alpha - L^2 \nabla^2 \alpha = 1.$$  \hfill (A.67)

• The turbulent length scale, $L$, is

$$L = \sqrt{c_L^2 \left( \frac{k^3}{\varepsilon_h^2} + c_\eta^2 \frac{\mu^3/2}{\rho^{3/2} \varepsilon_h^{1/2}} \right)},$$  \hfill (A.68)

and the turbulent time scale is

$$T = \sqrt{\frac{k^2}{\varepsilon_h^2} + c_T^2 \frac{\mu}{\rho \varepsilon_h}},$$  \hfill (A.69)

however $T$ is limited to

$$T_{lim} = \frac{0.6}{\sqrt{3 \varepsilon_\mu \varphi S}},$$  \hfill (A.70)

such that the turbulent viscosity is

$$\mu_t = \rho c_\mu \varphi k \min(T, T_{lim}).$$  \hfill (A.71)

• The boundary conditions at the wall are

$$k_w = 0,$$  \hfill (A.72)

$$\varepsilon_h|_w = \frac{\mu k_{I'}}{\rho d_{I'}},$$  \hfill (A.73)

$$\varphi_w = 0,$$  \hfill (A.74)

$$\alpha_w = 0,$$  \hfill (A.75)

where $k_{I'}$ is the turbulent kinetic energy at the near-wall cell centre.

The model constants are given in Table A.4.

<table>
<thead>
<tr>
<th>$\sigma_k$</th>
<th>$\sigma_{\varepsilon_h}$</th>
<th>$\sigma_\varphi$</th>
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<th>$c_\kappa$</th>
<th>$c_\eta$</th>
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<th>$c_2$</th>
<th>$c_T$</th>
<th>$c_L$</th>
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<td>0.164</td>
<td>1.44</td>
<td>1.83</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Table A.4: The constants for the BL-$\overline{v^2}/k$ model.

A.8 The EBRSM model

The EBRSM model is a Reynolds stress model with eight model equations. Six of these are for Reynolds stress components, $\overline{u_i u_j}$, one is for the turbulent dissipation, $\varepsilon$, and the other is for an elliptic blending function, $\alpha$. It is a low Reynolds number turbulence model. The full set of equations is documented clearly in Manceau and Hanjalić (2002) and for brevity
Appendix A. Turbulence models

is not repeated here. The required boundary conditions are

\[ u_i u_j w = 0, \quad (A.76) \]
\[ \varepsilon_w = \frac{2\mu k'_I}{\rho d'_I}, \quad (A.77) \]
\[ \alpha_w = 0. \quad (A.78) \]

A.9 Rotation and curvature corrections

Rotating reference frames are defined by the rotation vector, \( \Omega' \). This rotation must be included in the definition of the vorticity, which for clarity is denoted \( \omega_{ij} \) here. The vorticity is now defined as

\[ \omega_{ij} = \frac{1}{2} \left( \left( \frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right) + 2\varepsilon_{mji} \Omega'_m \right), \quad (A.79) \]

with \( \omega^2 = 2\omega_{ij}\omega_{ij} \).

Two different rotation correction methods are implemented in \textit{Code_Saturne}. These are discussed in Section 2.8.10. The first of the two corrections modifies the dissipation of turbulence, the second modifies the production of turbulence.

A.9.1 Correction by modification of dissipation

This rotation/curvature correction method is that of Cazalbou et al. (2005) and is used with the BL-\( \nu^2/k \) and \( \varphi - f \) turbulence models. The method modifies the constant \( c_\varepsilon^2 \) in the dissipation equation. Consequently, this method cannot be used with the Spalart-Allmaras model, since it does not solve for the dissipation.

- The new value of \( c_\varepsilon^2 \) is

\[ c_{\varepsilon^2}^{\text{new}} = c_\varepsilon^2 + \frac{c_\varepsilon^2 - 1}{1 + a R_0^{3/2}} + c_\varepsilon^2 c_{sc} \frac{S_k}{\varepsilon} (\tanh (b B_R + c) - d), \quad (A.80) \]

where the Rossby number is

\[ R_0 = \frac{\varepsilon}{\omega k}, \quad (A.81) \]

and the Bradshaw Richardson number is

\[ B_R = -\frac{2k}{S^3 \varepsilon} \omega_{ik} S_{jk} \left( \frac{D S_{ij}}{Dt} + (\varepsilon_{imn} S_{jn} + \varepsilon_{jmn} S_{in}) \Omega'_m \right), \quad (A.82) \]

where \( DS_{ij}/Dt \) is the total derivative of the strain rate tensor.

- The constants are \( a = 4.3, c_{sc} = 0.119, d = 5.13, c = 0.453 \) and \( d = 0.682 \). The value of \( c_{\varepsilon^2}^{\text{new}} \) is limited to a minimum value of zero.

- With the BL-\( \nu^2/k \) model, both \( c_{\varepsilon^2}^* \) and the \( E \) term are multiplied by \( c_{\varepsilon^2}^{\text{new}} / c_\varepsilon^2 \).
A.9.2 Correction by modification of production

This rotation/curvature correction method is that of Shur et al. (2000) and is used with the Spalart-Allmaras, BL-$v^2/k$ and $\varphi - f$ turbulence models. The method multiplies the production term by a function $F_{r1}$. For the Spalart-Allmaras model, the production term in Equation (A.33) is $c_{b1}\rho\tilde{S}\tilde{v}$. During the course of the project, this rotation correction was implemented for the BL-$v^2/k$ and $\varphi - f$ models, and results are given in Section 8.3.6.

- The multiplicative correction factor is defined as
  \[
  F_{r1} = (1 + c_{r1}) \frac{2r^*}{1 + r^*} (1 - c_{r3} \arctan(c_{r2}\tilde{r})) - c_{r1},
  \]  
  \[
  (A.83)
  \]
  where
  \[
  r^* = \frac{S}{\omega},
  \]  
  \[
  (A.84)
  \]
  and
  \[
  \tilde{r} = \frac{2\omega_{ik}S_{jk}}{D^4} \left( \frac{DS_{ij}}{Dt} + (\varepsilon_{imn}S_{jn} + \varepsilon_{jmn}S_{in}) \Omega'_{m} \right),
  \]  
  \[
  (A.85)
  \]
  which is similar to Equation (A.82), and
  \[
  D^2 = \frac{1}{2} (S^2 + \Omega^2).
  \]  
  \[
  (A.86)
  \]

- The constants are $c_{r1} = 1.0$, $c_{r2} = 12.0$ and $c_{r3} = 1.0$. The correction $F_{r1}$ is limited to a minimum value of zero, which is most likely to occur in flows over convex surfaces (Dufour et al., 2008).

The effect of the curvature correction is negligible in the flow boundary layer where the magnitude of the strain approximately balances the magnitude of the vorticity. The term is most important at the centre of a vortex, where the strain is zero but the vorticity is large. In such regions $0 \leq F_{r1} < 1$. This reduces the production of turbulence and hence reduces the turbulent viscosity. In turn this means that the vortex is less damped than it would be without the correction.

This rotation correction model has been shown to yield more accurate results than the standard Spalart-Allmaras model in rotating and curved channel flows in both two and three dimensions (Shur et al., 2000).
Appendix B

Treatment of the interface-normal velocity with NDD

As discussed in Section 5.3, the original Robin boundary condition in Equation (5.10), which was used by Utyuzhnikov (2006) with success, was found to be numerically unstable in Code_Saturne. Therefore another method of computing the IBCs for $V$ was required. This appendix describes the methods that were considered. The notation is the same as in Chapter 5.

For any method to work, the velocity and pressure gradient at $y^*$ must be able to determine $V$ down to the wall quickly and to good-enough accuracy.

In this appendix, a list of methods for enforcing continuity are outlined. The methods were tested on the diffuser flow from Section 6.5. The local coordinates in the inner region are $x$, which is parallel to the interface and $y$, which is perpendicular to it. Similarly, $U$ is parallel to the interface and $V$ is perpendicular to it.

The features required of the successful method are that:

1. It should give the correct wall-limiting behaviour of $V$ and $\partial_y V$.
2. The boundary condition on $V$ should be consistent with the pressure profile assumed in the sublayer.
3. The procedure should be able to handle flows where $V = 0$ everywhere, as well as flows where $V$ is non-zero.
4. The method should conserve mass.

Many conventional wall functions apply the boundary conditions $V = 0$ and $\partial_y V = 0$ at a wall using a first order finite difference-type approximation. However with the NWF (Gant, 2002), $V$ is given a special set of boundary conditions. The treatment of $V$ with the NWF is reviewed in Section B.1 and provides a starting point for some of the methods outlined in this appendix. The various methods considered for computing the IBCs for $V$ are described in Section B.2. The most robust and successful method is described in Section B.3 as well as in Section 5.3.
B.1 Treatment of $V$ with the NWF

In the NWF (Gant, 2002), which is described in Section 3.5.2, $V$ is obtained from the continuity equation over the sub-grid. Convective fluxes are calculated using an upwind difference scheme. At the face marked $N$ in Figure 3.5, which is at the equivalent to $y^*$ for IBCs, the value of $V$ in the sub-grid is scaled to match the value in the primary grid. Such an approach could be taken with NDD, however there are two issues which make it impractical.

1. The method cannot be easily extended to unstructured meshes of irregular geometries where there is no general way to calculate interface-parallel gradients accurately.

2. The storage requirements of the method would be greatly increased because $U$ would have to be stored across the numerical sub-grid at each boundary cell in order to calculate the convective fluxes.

B.1.1 Other approaches considered for the NWF

Explicitly specifying a profile of $V$ was another approach considered for the NWF. Motivated by LRN results of an impinging jet flow, which showed $V$ to be almost linear, Gant (2002) tried imposing a profile

$$V(y) = \frac{V_N}{y_N^{1.1}},$$

(B.1)

where the exponent, 1.1, is chosen to be greater than unity so that $\partial_y V_w = 0$, but $V(y)$ is approximately linear. This gave superior Nusselt number predictions on the impinging jet flow, however the approach based on the continuity equation was more faithful to the LRN model. The results were also found to be sensitive to the value of the exponent in Equation (B.1).

Gant (2002) also tried to solve the momentum equation for $V$, however the results were sensitive to the assumed profile of $V$. It is not possible to know the pressure explicitly because to do so would require a pressure-correction algorithm and would eliminate any speed advantage of the wall function over a LRN computation.

B.2 Treatments of $V$ considered for NDD

The following methods were considered but not adopted for use in NDD.

1. The simplest approach is to use a homogeneous Dirichlet boundary condition at the interface, $V^* = 0$. This approach is fast, stable, obeys continuity over periodic domains and is exact in one-dimensional flows. However it is clearly wrong near to recirculation regions and can be improved upon. It is also always wrong in cases where flow should leave through the interface, such as the impinging jet flow in Section 6.4.

2. A mass flux correction for continuity can be directly added to the Robin boundary condition in Equation (5.10) for $V$. This is done by modifying the value of $\tilde{f}_{2,V}$ as

$$\tilde{f}_{2,V}^{\text{new}} = \tilde{f}_{2,V}^{\text{old}} - \frac{1}{S} \int_{\Gamma} (f_1 \partial_y V + \tilde{f}_{2,V}^{\text{old}}) d\gamma,$$

(B.2)
where the integration is over the interface boundary with surface area $S$. The second term on the right hand side of Equation (B.2) is the mass flux leaving through the interface before any correction is applied. On the diffuser flow the correction term was unstable. Its value became large before the simulation diverged.

3. It is possible to modify case 2 to scale the corrections for each face. In one approach that was tested, the flux leaving through the interface was related to the near-interface cell-centre values of $V$ by

$$\int_{\Gamma} (f_1 \partial_y V + \tilde{f}_{2, V}) \, d\gamma = k \int_{\Gamma} V_I' \, d\gamma, \quad (B.3)$$

It was thought that this might make the method more stable, since $V_I'$ is known at the previous iteration and is therefore more stable than the integral in Equation (B.2). The correction is then $\tilde{f}_{2, V}^{\text{new}} = \tilde{f}_{2, V}^{\text{old}} - k S V_I'$. While this sometimes produced reasonable results, the simulations often diverged, especially for poorly-initialised problems.

4. Another approach that was tested used the continuity equation, since in two-dimensional flows the gradient $\partial_y V$ is known because

$$\partial_x U + \partial_y V = 0. \quad (B.4)$$

The $U$ boundary conditions can be used to calculate $\partial_x U$ on each face. A first-order finite-difference scheme gives $\partial_x U = (U^{i+1} - U^i) / \Delta x$, where adjacent faces on the interface are denoted by the counters $i$ and $i + 1$.

Although theoretically correct, in practice this approach did not lead to zero flux through the interfaces. This is because there is no way to modify the pressure at the interface at each iteration.

Other issues with this method include the calculation of $\partial_x U$ being unstable and inaccurate. Even when a minmod procedure was used, this procedure did not always converge. Because $\Delta x$ is small, any errors in $U$ are increased by a factor of $1/\Delta x$, which leads to large errors in $V$.

This approach does not extend well to unstructured, three-dimensional meshes, where the gradient calculation is non-trivial due to the arbitrary number of neighbouring boundary faces.

5. In two-dimensions, the continuity equation can be integrated with respect to $y$ over the inner region to

$$V^* = -\partial_x \int_0^{y^*} U \, dy. \quad (B.5)$$

The integral follows immediately from governing equation for $U$. This method produced reasonable results, however it was not always stable and does not generalise easily to complex geometries.

6. The continuity equation can be used to improve the value of the term on the right-hand side of the governing equation using the result that $\partial_y U = -\partial_x V$, and hence

\footnote{For the minmod procedure, $\partial_x U$ is calculated two ways: as $A = (U^{i+1} - U^i) / \Delta x$ and as $B = (U^i - U^{i-1}) / \Delta x$, then $\text{minmod}(A, B) = \min(|A|, |B|)$ if $AB > 0$, otherwise $\text{minmod}(A, B) = 0$.}
B.3 The treatment of $V$ used for NDD

The following method was chosen as the method to be implemented into \textit{CodeSaturne} and is also outlined in Section 5.3.

The approach is to integrate Equation (5.3) twice from 0 to $y^*$, and use $V = \partial_y V = 0$ at the wall to obtain

$$V(y) = \int_0^y \frac{d\xi}{\Gamma_V(\xi)} \int_0^\xi R_V(\eta) d\eta.$$  \hfill (B.7)

It is assumed that $R_V(y) = \partial_y P(y)$, where the pressure gradient is unknown. Using the constant value of $\partial_y P^*$ across the entire inner region was unstable and theoretically inaccurate.

The pressure can be considered to arise due to a dynamic pressure $\rho V^2$ in the sublayer. This is proportional to $y^4$ because $V \propto y^2$, hence $\partial_y P \propto y^3$. To a good approximation, at large Reynolds numbers the gradient of the pressure at the wall is zero.

The boundary condition on the pressure in the NWF is (Gant, 2002)

$$\partial_n P + \partial_j \overline{u_j} n_i = 0,$$  \hfill (B.8)

where $n$ is the interface-normal vector. Writing this in the local coordinates used in NDD transforms it into

$$\frac{\partial P}{\partial y} + \frac{\partial \overline{u^2}}{\partial x_j} = 0.$$  \hfill (B.9)

Neglecting interface-parallel gradients reduces this further to

$$\frac{\partial P}{\partial y} + \frac{\partial \overline{v^2}}{\partial y} = 0,$$  \hfill (B.10)

and because $\overline{v^2} \propto y^4$, this approach yields $\partial_y P \propto y^3$.

Taking $\partial_y P = \partial_y P^* y^3/y^3$ was numerically unstable and led to the simulations diverging. This is due to the pressure boundary conditions in the outer region, where $\partial_y P^* = 0$ is imposed at the interface. At the cell centre the pressure gradient is an average for the cell that enforces continuity throughout the outer domain. However, because of the boundary condition on the pressure at $y^*$, the pressure correction at the interface must be zero. Therefore the pressure at the cell centre does not correctly consider the region between the cell centre and the wall.
and the interface boundary. Hence it is wrong to use $\partial_y P^*$.
Instead, another profile of the pressure must be used. The cubic form of $\partial_y P$ is a good enough approximation.

The pressure gradient term in Equation (B.7) integrates to a term proportional to $y^4$, hence $V$ is imposed as

$$V(y) = K \int_0^y \frac{\xi^4 d\xi}{\mu + \mu_t(\xi)}, \quad (B.11)$$

with $K$ defined by

$$V_I' = K \int_0^{y^*} \frac{\xi^4 d\xi}{\mu + \mu_t(\xi)}, \quad (B.12)$$

such that the assumed profile returns the same value of $V$ as is stored in the main grid in the outer region. This profile is stable and can be made consistent with all of the requirements above. It allows for fluid to enter and leave the domain and it is impossible for more fluid to leave the domain through an interface boundary than enters the main computational domain through any inlets.

Mass conservation can be guaranteed by adding a second term to the right hand side of Equation (B.11) so that it becomes

$$V(y^*) = K \int_0^{y^*} \frac{\xi^4 d\xi}{\Gamma v(\xi)} - \frac{\dot{m}_S}{\rho S}, \quad (B.13)$$

where $S$ is the surface area of the interface boundary and $\dot{m}_S$ is the mass flux leaving through the interface boundary before any correction for continuity is applied. The correction term is computed using the first term on the right hand side of Equation (B.13). As mentioned in Section 5.3, the mass flux correction is always small compared to the flux entering through an inlet on the flows in this thesis.

This mass flux correction is only necessary if the mass flux through an interface must be zero. In some flows, such as the impinging jet flow in Section 6.4, the mass flux through the interface boundary is non-zero. On such cases, the mass flux correction algorithm should not be used.
Appendix C

IBCs for other turbulence models

This appendix outlines the implementation of NDD for the \( k - \omega \) SST and BL-\( v^2/k \) models. Results of NDD simulations with these two models on some of the flows studied in this thesis are also given. The test cases are the channel flow at \( Re = 590 \) of Section 6.1, the channel flow at \( Re = 1.1 \times 10^4 \) of Section 6.2, the annulus studied in Section 6.3, the annular flows over surface 0 of Section 8.2 and the asymmetric diffuser of Section 6.5. All NDD simulations for the test cases are performed using the turbulent viscosity profile of Duprat et al. (2011). The results form part of Jones and Utyuzhnikov (2015), which was published during this project.

The methodology used to derive IBCs for the BL-\( v^2/k \) model in Section C.2 could be adopted for use with any turbulence model. Therefore it is possible to use NDD with any turbulence model.

C.1 IBCs for the \( k - \omega \) SST model

The full governing equations for the \( k - \omega \) SST model are given in Appendix A.4. The coupled term \( \beta^* \rho k \omega \) in the \( k \) equation makes it complicated to calculate a Robin boundary condition for \( k \). Since \( k \) is a physically meaningful quantity, it is assumed that the turbulent kinetic energy in the \( k - \omega \) SST model corresponds to that in the \( k - \varepsilon \) model. Hence the procedure outlined in Section 5.6.1 is used to calculate the IBC for \( k \).

The \( \omega \) equation contains many non-linear terms. Therefore it is difficult to compute a Robin boundary condition for \( \omega \). Instead, \( \omega \) is determined using the blending approach of Knopp et al. (2006). This approach blends the solutions for \( \omega \) in the viscous sub layer \( (\omega_v) \) and the logarithmic sub layer \( (\omega_l) \) to specify \( \omega \) across the entire inner region. The blending uses the
Appendix C. IBCs for other turbulence models

definitions

\[
\omega_v = \frac{6\mu}{\rho\beta_1 y^2}, \quad (C.1)
\]

\[
\omega_l = \frac{u_\tau}{\sqrt{\beta_2} y}, \quad (C.2)
\]

\[
\phi = \tanh\left(\zeta^4\right), \quad (C.3)
\]

\[
\zeta = y^+ / 10, \quad (C.4)
\]

\[
\omega_{b1} = \omega_v + \omega_l, \quad (C.5)
\]

and

\[
\omega_{b2} = \left(\omega_v^{1.2} + \omega_l^{1.2}\right)^{1/1.2}, \quad (C.6)
\]

which allow \(\omega\) to be given the Dirichlet boundary condition

\[
\omega^* = \phi\omega_{b1}^* + (1 - \phi)\omega_{b2}^*. \quad (C.7)
\]

C.1.1 Results on test cases

The results of simulations using NDD with the \(k - \omega\) SST model are shown in Figure C.1.

Figure C.1a shows \(Re\) calculated from the channel flows at \(Re_\tau = 590\). It varies by no more than 10% over the range of \(y^*\) studied.

Figure C.1b shows \(f\) from the channel flow at \(Re = 1.1 \times 10^4\). It varies by around 15% over the range of \(y^*\) studied.

Figure C.1c shows \(C_f\) and \(Nu\) on both walls of the annular flow at \(Re = 8.9 \times 10^3\). The trends in \(Nu\) with \(y^*\) are similar to those in \(C_f\).

Figure C.1d shows \(C_f\) on the inclined wall of the diffuser flow. The recirculation region is accurately captured for every \(y^*\). The NDD solutions compare well to the LRN solution.

Figure C.1e shows the Stanton number for surface 0 of Chapter 8. Both the LRN and NDD solutions lie within the range defined by the results of Yu et al. (2005) and Watson (1970). NDD results for different \(y^*\) vary by no more than 8% of the LRN value.

In all Figures in Figure C.1 there is a clear convergence of the NDD solution to the LRN solution as \(y^* \rightarrow 0\). The trend is less obvious for Figure C.1e because the minimum \(y^+_\tau\) is 12, and therefore convergence could only reasonably be expected for \(y^*\) an order of magnitude smaller than the smallest \(y^*\) plotted in Figure C.1e.
C.1. IBCs for the $k - \omega$ SST model

(a) $Re$ of channel flow at $Re_\tau = 590$.

(b) $f$ of channel flow at $Re = 1.1 \times 10^4$.

(c) $C_f$ and $Nu$ on both walls of the annulus at $Re = 8.9 \times 10^3$ for different $y^*/d_e$.

(d) $C_f$ on the inclined wall of the diffuser.

(e) $St$ for flows over surface 0.

Figure C.1: Results of the test cases using NDD with the $k - \omega$ SST model.
C.2 IBCs for the BL-\(\overline{v^2}/k\) model

The governing equations of the BL-\(\overline{v^2}/k\) models contain main non-linear terms which make it difficult to compute Robin boundary conditions for them. To make progress, the implementation of NDD borrows heavily from the look-up table approach of Billard et al. (2015), who developed an adaptive wall function for the BL-\(\overline{v^2}/k\) model.

In the look-up table approach of Billard et al. (2015), the turbulence model equations are made non-dimensional by writing

\[
\varepsilon^+_h B = \frac{\mu \varepsilon}{\rho u^+_k},
\]  

(C.8)

Distances are made non-dimensional by introducing a dimensionless distance \(y^+_B\), which is calculated with a cubic spline interpolation (Billard et al., 2015)

\[
y^+_B = (2t^3 - 3t^2 + 1)f_i + (t^3 - 2t^2 + t)m_i \Delta x_i + (3t^2 - 2t^3)f_{i+1} + (t^3 - t^2)m_{i+1} \Delta x_i,
\]  

(C.9)

where the arguments are \(x = ky^2 \rho^2 / \mu^2\), \(t = (x - x_i) / \Delta x\), \(\Delta x = x_{i+1} - x_i\) and \(x_i < x < x_{i+1}\). The interpolation data \(x_i, m_i\) and \(f_i\) are given in Table C.1, which is taken from Billard et al. (2015).

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<td>1.53</td>
<td>2.846</td>
<td>5.058</td>
<td>9.926</td>
<td>16.21</td>
<td>53.64</td>
<td>217.451</td>
</tr>
<tr>
<td>(m_i)</td>
<td>10</td>
<td>0.77</td>
<td>0.143</td>
<td>0.0386</td>
<td>0.0123</td>
<td>0.007295</td>
<td>0.003025</td>
<td>0.00159</td>
</tr>
</tbody>
</table>

Table C.1: The data used to interpolate \(y^+_B\) for the BL-\(\overline{v^2}/k\) model (Billard et al., 2015).

Billard et al. (2015) sought analytical solutions for \(\varepsilon^+_h B\) and \(\varphi\) in the viscous and logarithmic sub layers of the boundary layer. The analytical solutions contain constants that are tuned to the solution of a plane channel flow at \(Re_\tau = 1020\), which is obtained from a LRN computation. The channel flow solution is also used to build cubic spline interpolations for \(\varepsilon^+_h B\) and \(\varphi\) for the buffer region between the viscous and logarithmic sub layers.

For \(\alpha\), an analytical solution is found near to the wall by assuming that the turbulent length scale is constant for \(y^+_B < 17\). The channel flow solution is used to build an empirical expression for \(\alpha\) above this limit. The solutions for \(\varepsilon^+_h B\), \(\varphi\) and \(\alpha\) are (Billard et al., 2015):

\[
\varepsilon^+_h B = \begin{cases} 
\frac{500C_T^2}{C_{\kappa}(y^+_B + 12.43)^4} & \text{if } y^+_B < 1, \\
3 \varepsilon_h(y^+_B) & \text{if } 1 \leq y^+_B < 30, \\
\frac{1}{\alpha y^+_B} & \text{if } 30 \leq y^+_B, 
\end{cases}
\]  

(C.10)

\[
\varphi = \begin{cases} 
0.0015 y^+_B^2 & \text{if } y^+_B < 1, \\
3 \varphi(y^+_B) & \text{if } 1 \leq y^+_B < 30, \\
0.1336 \log(y^+_B) - 0.2775 & \text{if } 30 \leq y^+_B, 
\end{cases}
\]  

(C.11)

\[
\alpha = \begin{cases} 
1 - \exp\left(\frac{-y^+_B}{24.52}\right) & \text{if } y^+_B \leq 17, \\
1 + \left(\frac{17}{y^+_B}\right)^{4/3} & \text{if } 17 < y^+_B. 
\end{cases}
\]  

(C.12)
The functions $\mathcal{F}_{\varepsilon h}$ and $\mathcal{F}_\varphi$ are spline interpolation functions. The interpolation formula, written in terms of $s = \{\varepsilon^{+}_{hB}, \varphi\}$, is (Billard et al., 2015)

$$
\mathcal{F}_s(y^+) = (2t^3 - 3t^2 + 1) f_i^s + (t^3 - 2t^2 + t) m_i^s \Delta y_i^+ + (3t^2 - 2t^3) f_{i+1}^s + (t^3 - t^2) m_{i+1}^s \Delta y_i^+, 
$$

(C.13)

where

$$
t = \frac{1}{\Delta y^+} \log \left( \frac{y^+}{y_i^+} \right),
$$

(C.14)

$$
\Delta y^+ = \log \left( \frac{y_{i+1}^+}{y_i^+} \right),
$$

(C.15)

and $y_i^+ < y_B^+ < y_{i+1}^+$. Equation (C.13) uses the data in Table C.2, which is taken from Billard et al. (2015).

<table>
<thead>
<tr>
<th>$i$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
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<tr>
<td>$y_i^+$</td>
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<td>5</td>
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<table>
<thead>
<tr>
<th>$f_i^k$</th>
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<th>0.063</th>
<th>0.091</th>
<th>0.149</th>
<th>0.0793</th>
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<tr>
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<td>-0.021</td>
<td>0.025</td>
<td>0.082</td>
<td>0</td>
<td>-0.074</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$f_i^\varphi$</th>
<th>0.00147</th>
<th>0.008</th>
<th>0.0165</th>
<th>0.0596</th>
<th>0.177</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_i^\varphi$</td>
<td>0.00299</td>
<td>0.0123</td>
<td>0.0264</td>
<td>0.088</td>
<td>0.138</td>
</tr>
</tbody>
</table>

Table C.2: Data used to interpolate $\varepsilon^{+}_{hB}$ and $\varphi$ between $1 \leq y^+ < 30$ (Billard et al., 2015).

When using the spline interpolations, it is important to use the definition of $y_B^+$ in Equation (C.9), and not any other definition, otherwise the interpolations will be incorrect.

Equation (C.10), (C.11) and (C.12) are used to impose Dirichlet boundary conditions at $y^*$.

The $k$ boundary conditions for the BL-$\nu^2/k$ model are calculated with the same procedure as they are for the $k - \varepsilon$ model. However in this case Equation (C.10) is used for $\varepsilon_h$ and the additional $E$ term in the $k$ equation (see Appendix A.7) is computed using the wall function of Billard et al. (2015). To compute the $E$ term, a non-dimensional quantity $E_B^+$ is calculated as

$$
E_B^+(y) = 0.0875 \exp \left[-(\log_{10}(y_B^+) - 1.01)^2/0.0484\right],
$$

(C.16)

which is converted into its dimensional form as $E(y) = E_B^+ u_k^4 \rho / \mu$ (Billard et al., 2015).

### C.2.1 Results on test cases

The results of simulations using NDD with the BL-$\nu^2/k$ model are shown in Figure C.2.

Figure C.2a shows $Re$ calculated from the channel flows at $Re_\tau = 590$. The trend with $y^*$ is not monotonic. The maximum error, expressed as a percentage of the LRN value is never larger than 8%.

Figure C.2b shows $f$ from the channel flow at $Re = 1.1 \times 10^4$. The trend with $y^*$ is not monotonic. The maximum error, expressed as a percentage of the LRN value is never larger than 15%.

Figure C.2c shows $C_f$ and $Nu$ on both walls of the annular flow at $Re = 8.9 \times 10^3$. Again
Appendix C. IBCs for other turbulence models

(a) $Re$ of channel flow at $Re_τ = 590$.

(b) $f$ of channel flow at $Re = 1.1 \times 10^4$.

(c) $C_f$ and $Nu$ on both walls of the annulus at $Re = 8.9 \times 10^3$ for different $y^*/d_e$.

(d) $C_f$ on the inclined wall of the diffuser.

(e) $St$ for flows over surface 0.

Figure C.2: Results of the test cases using NDD with the BL-$\overline{u^2}/k$ model.

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the trend in $y^*$ in both $C_f$ and $Nu$ on both walls is not monotonic. The trends in $Nu$ with $y^*$ are similar to those in $C_f$.

Figure C.2d shows $C_f$ on the inclined wall of the diffuser flow. The recirculation region is captured for every $y^*$ and the NDD solutions compare well to the LRN solution.

Figure C.2e shows the Stanton number for surface 0 of Chapter 8. The LRN and NDD solutions lie below the experimental results of Watson (1970). NDD results for different $y^*$ vary by no more than 7.5% of the LRN value.

In all Figures in Figure C.2 there is a clear convergence of the NDD solution to the LRN solution as $y^* \to 0$. As with the $k-\omega$ SST model, the trend is less obvious for Figure C.2e because the minimum $y^*_+ \tau$ is 12. Therefore convergence could only be reasonably expected for $y^*$ an order of magnitude smaller than the smallest $y^*$ plotted in Figure C.2e.

Although the magnitude of the error is still small, it seems that there is more variation with $y^*$ in the results with the BL-$\overline{v^2}/k$ model than there is with either the $k-\varepsilon$, Spalart-Allmaras or $k-\omega$ SST model. The behaviour of NDD for different $y^*$ is less steady than for the other turbulence models. This is caused by the mixing of two methodologies – the look-up table approach of Billard et al. (2015) and the NDD approach of Utyuzhnikov (2006). Mixing the two approaches leads to minor inconsistencies in the assumed values of functions in the inner region. A more accurate implementation might use a custom-built look-up table for the required functions that is built using the turbulent viscosity profile employed in the NDD approach. With this method there would be no inconsistency.
Appendix D

A one-dimensional example of non-local NDD

This appendix contains an example of the application of non-local NDD to a plane channel flow wherein the auxiliary functions are computed concurrently with the solution in the outer region. Information is exchanged between the inner and outer regions to enable the turbulent viscosity and source terms to be approximated in the inner regions. Since the channel flow is one-dimensional, and the mesh is merely a one-dimensional strip of cells, there are no non-local effects to be included in the auxiliary functions. However the same procedure could be followed on more complicated flows. As mentioned in Section 5.9.2, coupling information between the inner and outer regions is inefficient, since the value of all functions on the interface boundary could be exchanged instead, which would be more efficient.

The height of the channel is \( H \) in the \( y \) direction and the flow moves in the \( x \) direction with a Reynolds number \( Re = 1.8 \times 10^4 \). In this case, only one basis function for the sets \( \{ u_\alpha \} \) and \( \{ v_\alpha \} \) is required. The auxiliary functions are denoted \( W_0 \), which has \( u_0 = 1 \), and \( W^e \), which has \( v_0 = 1 \). There are two inner regions, \( \Omega_1 \) and \( \Omega_2 \) near to the bottom and top walls of the channel, respectively. For both \( \Omega_1 \) and \( \Omega_2 \), \( y^* = H/20 \). The auxiliary functions are one-dimensional and obey

\[
\frac{\partial}{\partial y} \left( (\mu + \mu_t) \frac{\partial W_0}{\partial y} \right) = 0, \quad (D.1) \\
W_0|_w = 0, \quad (D.2) \\
W_0^* = 1, \quad (D.3)
\]

in each inner region. Since Code_Saturne is a three-dimensional code, boundary conditions are required in the \( x \) and \( z \) directions. Periodic boundary conditions are applied in the \( x \) direction and symmetry boundary conditions are applied in the \( z \) direction.

In a one-dimensional channel flow, Equation (5.71) becomes

\[
U^* = U^* W_0^* + \partial_y P W_0^*, \quad (D.7)
\]

where \( R_U = \partial_z P \) is a constant. The Robin boundary condition in Equation (5.73) becomes

\[
\partial_y U^* = U^* \partial_y W_0^* + \partial_z P \partial_y W_0^*, \quad (D.8)
\]
and the wall shear stress can be calculated as

$$\tau_w = \mu \partial_y U \big|_w = \mu U^* \partial_y W_0 \big|_w + \mu \partial_x P \partial_y W_e \big|_w.$$  \hfill (D.9)

The \( k - \varepsilon \) turbulence model was used in the simulation with the exponential viscosity profile. The values of \( \mu^* \), \( k^* \) and \( \partial_x P^* \) are sent from \( \Omega_e \) to \( \Omega_1 \) and \( \Omega_2 \) at each iteration. The standard formulation of NDD was used to compute the IBCs for \( k \) and \( \varepsilon \), as described in Section 5.6.

The auxiliary functions \( W_0 \) and \( W^e \) in \( \Omega_1 \) are shown in Figure D.1a. The auxiliary functions in \( \Omega_2 \) were calculated independently but since the geometry of the two inner regions is the same, they could have been computed from the auxiliary functions in \( \Omega_1 \) by transforming \( y \rightarrow H - y \). The resulting velocity field across the whole channel is shown in Figure D.1b. The NDD result is compared to the LRN solution computed with the BL-\( \nu^2/k \) model.

Figure D.1: Functions computed during application of non-local NDD to a channel flow.

Figure D.1a shows the effect of the boundary conditions at \( y^* \) on \( W_0 \) and \( W^e \). Without the source term, \( \tau_{1,0} = 1 \), \( W^e \) would be zero everywhere. The effect of \( W_{1,0}^e \) in this example is small, and similar results are found if it is excluded. This demonstrates why most wall functions are accurate on simple flows, even though they ignore momentum source terms. The NDD solution in \( \Omega_1 \) and \( \Omega_2 \) is built as a linear combination of \( W_0 \) and \( W^e \). Since the profile of \( U \) obtained with NDD in Figure D.1b is accurate in the inner regions, the approach is verified to be accurate and correctly implemented.

In a one-dimensional case such as this example, there are no non-local effects. This means that the IBCs computed with Equation (5.11) are identical to those computed with Equation (D.8). This explains why, despite the different derivations, the non-local formulation of NDD is an extension of the one-dimensional formulation of NDD. In a two or three-dimensional case, the non-local formulation is more accurate, as is demonstrated in Chapter 7.
Appendix E

The correlation of Dalle Donne and Meyer (1977)

The full equations used in the correlation of Dalle Donne and Meyer (1977) are provided in this appendix to facilitate future use of the correlation. The equations are never fully written down in Dalle Donne and Meyer (1977). Instead, they are split over at least two papers (Dalle Donne and Meyer, 1977; Dalle Donne and Meerwald, 1970). A similar correlation can be found in Maubach (1972). However, the Maubach (1972) correlation applies only to isothermal flows.

The most important equations of the correlation are written in boxes, for emphasis.

The inner radius of the annulus is \( R_1 \); the outer radius is \( R_2 \) and the radius of zero shear is \( R_0 \). Thus, the annulus is split into two regions as shown in Figure 8.23. Region 1 of the annulus is bounded by \( R_1 \) and \( R_0 \); region 2 is bounded by \( R_0 \) and \( R_2 \). These radii are used to define

\[
\alpha = \frac{R_1}{R_2},
\]
\[
\beta = \frac{R_0}{R_2},
\]
\[
\gamma = \frac{R_0}{R_1} = \frac{\beta}{\alpha}.
\]

The equivalent diameters for the three regions are defined in the usual way as

\[
d_e = 2(R_2 - R_1),
\]
\[
d_1 = \frac{2(R_0^2 - R_1^2)}{R_1},
\]
\[
d_2 = \frac{2(R_2^2 - R_0^2)}{R_2}.
\]

The overall friction factor is defined as

\[
f = \frac{dP}{dz} \frac{d_e}{2\rho\bar{U}^2},
\]

where \( \bar{U} \) is the bulk velocity. There are equivalent expressions for the friction factor in regions
1 and 2, which are denoted with subscripts as
\[ f_1 = \frac{dP}{dz} \frac{d_1}{2\rho U_1^2}, \quad \text{(E.8)} \]
and
\[ f_2 = \frac{dP}{dz} \frac{d_2}{2\rho U_2^2}, \quad \text{(E.9)} \]
respectively.

The pressure in regions 1 and 2 is equal to the bulk pressure. It is this pressure that is used to compute the thermodynamic properties of the fluid. Fluid properties are computed at one of four temperatures. The appropriate temperature is indicated by a subscript. The meanings of the subscripts are given in Table E.1. To compute \( T_1' \) and \( T_2' \), the parameter \( T_2' \) is first evaluated, followed by \( T_1' \). Then, \( T_1 \) and \( T_2 \) can be found using the correlations of Wilkie (1966):

\[
T_2' = \begin{cases} 
\frac{T_B}{0.902 + 0.09(T_w/T_B)} & \text{for } T_w/T_B < 1.25, \\
\frac{T_B}{0.883 + 0.0911(T_w/T_B)} & \text{otherwise}, 
\end{cases} \quad \text{(E.10)}
\]
\[
T_1' = \begin{cases} 
T_2' \left(1.06 - 0.235(T_w/T_B) + 0.175(T_w/T_B)^2\right) & \text{for } T_w/T_B < 1.4, \\
T_2' \left(0.731 + 0.245(T_w/T_B)\right) & \text{otherwise}, 
\end{cases} \quad \text{(E.11)}
\]
\[
T_2 = \frac{T_2'}{1.0484 - 0.009133 \log_{10}(Re_1)}, \quad \text{(E.12)}
\]
\[
T_1 = T_1' \left(1.0958 - 0.018066 \log_{10}(Re_1)\right). \quad \text{(E.13)}
\]

In region 1, where the wall contains a rib (and is therefore treated as a rough wall), the rough wall function based on \( y_k^+ \) is used:
\[
U_1^+ = \frac{1}{\kappa} \ln(y/h) + R(h^+). \quad \text{(E.14)}
\]

In region 2, the wall is smooth and the smooth wall function is used with a variable slope, \( A_S \), as
\[
U_2^+ = A_S \ln(y_0^+) + 5.5. \quad \text{(E.15)}
\]
The Maubach (1972) transformation uses \( A_S = 1/\kappa \).

When Equations (E.14) and (E.15) are integrated over regions 1 and 2, respectively, the result is
\[
\sqrt{2} \frac{f_2}{f_1} = \frac{1}{\kappa} \ln \left( \frac{R_0 - R_1}{h} \right) + R(h^+) - G_1, \quad \text{(E.16)}
\]
and
\[ \sqrt{\frac{2}{f_2}} = A_S \ln \left( \frac{R_2 - R_0}{\nu_2} \sqrt{\frac{\tau_0}{\rho_2}} \right) + 5.5 - G_2, \] (E.17)
where \( G_1 \) and \( G_2 \) are given by the empirical expressions
\[
\begin{align*}
G_1 &= \frac{3.75 + 1.25\gamma}{1 + \gamma} , \\
G_2 &= \frac{3 + \beta}{2(1 + \beta)} A_S .
\end{align*}
\] (E.18) (E.19)

The velocity in the annulus reaches its maximum at \( r = R_0 \). This value must be computed by both Equations (E.14) and (E.15) at \( R_0 \), which provides a useful link between the two equations. This ignores the experimental observation that, in annular flows, the positions of maximum velocity and zero shear stress are different. Since the pressure gradient, \( dP/dz \) is the same in both regions 1 and 2, a force balance can be used to find a useful equation,
\[ \frac{\tau}{d_e} = \frac{\tau_1}{d_1} = \frac{\tau_2}{d_2} , \] (E.20)
where \( \tau_1 \) and \( \tau_2 \) are the wall shear stresses on the inner and outer walls, respectively, and \( \tau \) is the average wall shear stress,
\[ \tau = \frac{R_1\tau_1 + R_2\tau_2}{R_1 + R_2} . \] (E.21)
These relations can be re-written in terms of \( \alpha \), \( \beta \) and \( \gamma \) as
\[
\begin{align*}
\frac{\tau_1}{\tau} &= \frac{\beta^2 - \alpha^2}{\alpha(1 - \alpha)} , \\
\frac{\tau_2}{\tau} &= \frac{1 - \beta^2}{1 - \alpha} , \\
\frac{\tau_1}{\tau_2} &= \frac{\beta^2 - \alpha^2}{\alpha(1 - \beta^2)} .
\end{align*}
\] (E.22) (E.23) (E.24)
Due to the definition of \( f \), the following relation is valid in regions 1, 2, and the bulk (appropriate subscripts would be added in regions 1 and 2):
\[ \sqrt{\frac{\tau}{\rho}} = U \sqrt{\frac{f}{2}} . \] (E.25)
Another useful equation comes from the continuity equation, which states that
\[ U_1 S_1 + U_2 S_2 = US , \] (E.26)
where \( S \) is the surface area of the flow in the respective region.

These equations are used to derive the following equations, which are solved iteratively and simultaneously (Maubach, 1972; Dalle Donne and Meerwald, 1970; Dalle Donne and Meyer, 1977). Equation (E.30) is the empirical correlation from Warburton (1974) and Equa-
tion (E.31) is the Prandtl correlation for the friction factor in a smooth pipe.

\[
\sqrt{\frac{2}{f}} = \frac{\beta^2 - \alpha^2}{1 - \alpha} \sqrt{\frac{\beta^2 - \alpha^2}{\alpha(1 - \alpha)}} \sqrt{\frac{\rho_1}{\rho}} \left( \sqrt{\frac{\rho_1}{\rho_2}} \sqrt{\frac{(1 - \beta^2)\alpha}{\beta^2 - \alpha^2}} A - G_1 \right) \tag{E.27}
\]

\[
A = A_S \ln \left( \frac{1 - \beta}{2(1 - \alpha)} \nu \frac{\rho}{\rho_2} \left( \frac{1 - \beta^2}{1 - \alpha} \sqrt{\frac{Re}{f}} \right) \right) + 5.5 \tag{E.28}
\]

\[
\sqrt{\frac{2}{f_1}} = \frac{A_S}{\sqrt{\frac{\beta^2 - \alpha^2}{\alpha(1 - \beta^2)}}} \tag{E.29}
\]

\[
f_2 = f_0 \left( 1.056 + 0.005 \frac{f_1}{f_2} \right), \tag{E.30}
\]

\[
f_0^{-1/2} = 4 \log_{10} \left( Re \frac{f_0^{1/2}}{f_2} \right) - 0.4, \tag{E.31}
\]

\[
Re_1 = Re \frac{\nu}{\nu_1} \sqrt{\frac{f_1}{f_2}} \left( \frac{\beta^2 - \alpha^2}{\alpha(1 - \beta^2)} \right)^{3/2} \tag{E.32}
\]

\[
Re_2 = Re \frac{\nu}{\nu_2} \sqrt{\frac{f_1}{f_2}} \left( \frac{1 - \beta^2}{1 - \alpha} \right)^{3/2} \tag{E.33}
\]

\[
A_S = \sqrt{\frac{2}{f_2}} - 5.5 \tag{E.34}
\]

\[
R(h_+^+) = \sqrt{\frac{2}{f_2}} - \frac{1}{\kappa} \ln \left( \frac{R_1(\beta - \alpha)}{\alpha h} \right) + G_1. \tag{E.35}
\]

It is now possible to calculate \( h_+^+ \) as

\[
h_+^+ = \frac{h}{d_e} \frac{Re}{\nu} \sqrt{\frac{f_1}{f_2}} \left( \frac{\beta^2 - \alpha^2}{\alpha(1 - \beta^2)} \right)^{3/2} \tag{E.36}
\]

However, it can also be evaluated in terms of the properties at the wall, which defines \( h_{r,W}^+ \) as

\[
h_{r,W}^+ = h_+^+ \frac{\nu_1}{\nu_W} \sqrt{\frac{\rho_1}{\rho_W}}. \tag{E.37}
\]

In order to build a correlation for \( R(h_+^+) \), a parameter \( \hat{y} \) is introduced, which is defined as

\[
\hat{y} = R_0 - R_1, \tag{E.38}
\]

which is equal to the distance from the inner wall to the surface of zero shear. Then, \( R(h_+^+) \) is reduced to its value at \( h/\hat{y} = 0.01 \) and stripped of its temperature dependence to produce

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Appendix E. The correlation of Dalle Donne and Meyer (1977)

a value \( R(h_r^+)_{1\%} \):

\[
R(h_r^+)_{1\%} = R(h_r^+) - 0.4 \ln \left( \frac{h/\hat{y}}{0.01} \right) - \frac{5}{\sqrt{h_r^+T_B}} \left( \frac{T_W}{T_B} - 1 \right)^2.
\]  
(E.39)

For \( h_r^+,W \geq 70 \), \( R(h_r^+)_{1\%} \) is approximately constant, and is written as

\[
R(\infty)_{01} = R(h_r^+)_{1\%} \text{ for } h_r^+,W \geq 70.
\]  
(E.40)

The experimental results of 19 authors were used to build the following correlation for \( R(\infty)_{01} \):

\[
R(\infty)_{01} = \begin{cases} 
9.3 \left( \frac{W-w}{h} \right)^{-0.73} - \left( 2 - \frac{7h}{W-w} \right) \log_{10} \left( \frac{h}{w} \right) & \text{for } 2 \leq \frac{W-w}{h} \leq 6.3, \\
1.04 \left( \frac{W-w}{h} \right)^{0.46} - \left( 2 - \frac{7h}{W-w} \right) \log_{10} \left( \frac{h}{w} \right) & \text{for } 6.3 < \frac{W-w}{h} \leq 20,
\end{cases}
\]  
(E.41)

where \( W \) is the rib pitch and \( w \) is the rib width in the axial direction. Equation (E.41) is valid for

\[
0.25 \leq h/w \leq 2,
\]  
(E.42)

\[
0.008 \leq h/\hat{y} \leq 0.235.
\]  
(E.43)

For \( h/\hat{y} > 0.235 \) the rib can no longer be considered as a roughness element and the flow is better-approximated as an orifice plate (Dalle Donne and Meyer, 1977).

Note that in Dalle Donne and Meyer (1977), \( R(h_r^+) \) is sometimes written as \( R(h_{r,W}^+) \) to emphasise its dependence on \( T_W \). However, in this report the terminology \( R(h_r^+) \) is always used, since this is what appears in Equation (E.35). The parameter \( h_{r,W}^+ \) is only used to remove the effect of the temperature from \( R(h_r^+) \). Dalle Donne and Meyer (1977), tested two methods of doing this:

\[
R(h_r^+) = 0.8 \left( \frac{T_W}{T_1} - 1 \right)^{1.3},
\]  
(E.44)

and

\[
R(h_{r,W}^+) = \frac{5}{h_{r,W}^+} \left( \frac{T_W}{T_1} - 1 \right)^2.
\]  
(E.45)

The second of method performed better, as is shown in Figures 30 and 31 of Dalle Donne and Meyer (1977).

---

1Since the rib is on the wall, it is strictly \( h_{r,W}^+ \) rather than \( h_r^+ \) that determines whether or not the wall is hydrodynamically rough.