Mathematics, Numerics, Derivations and OpenFOAM®

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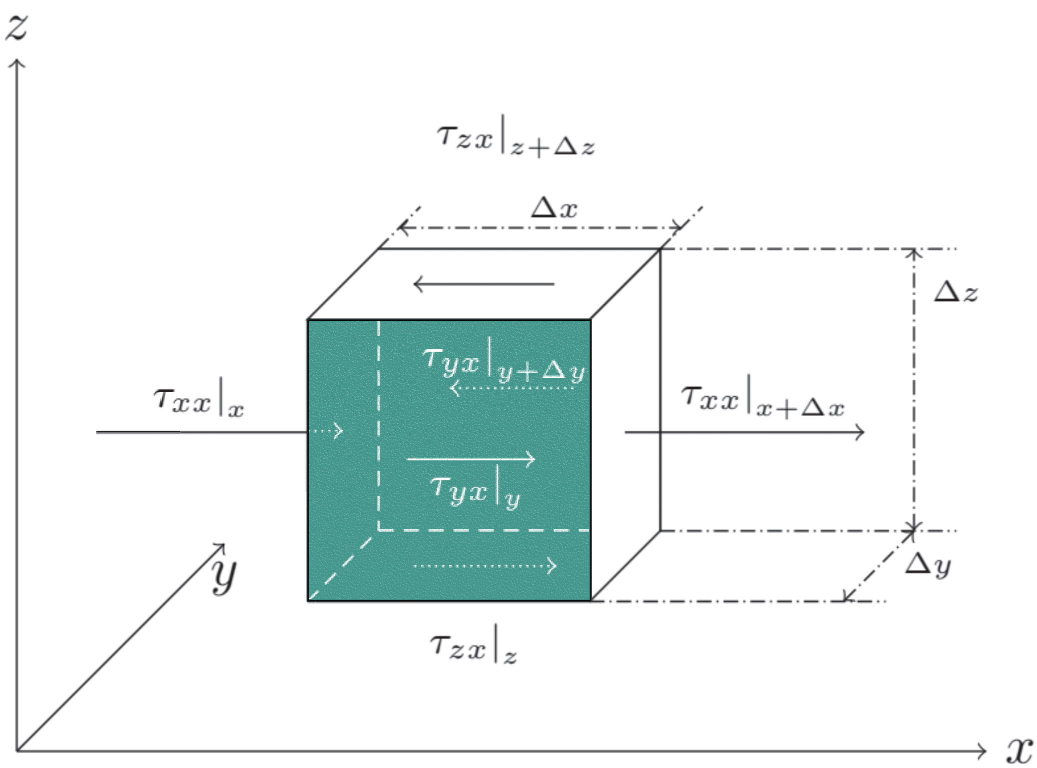
MATHEMATICS, NUMERICS, DERIVATIONS AND OPENFOAM®

The Basics for Numerical Simulations.



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***D**edidcated to the OpenFOAM® community and especially to all colleagues and people who support me. The ambition of writing the book is to give an introduction to computational fluid dynamics, show interesting equations and relations that are not given in most of the literature and prepare you for all the tasks that you may focus in your personal career, hopefully with OpenFOAM®.*

***T**he book is also available as soft-cover. If you are interested to have on, just ask me for a copy.*

***Y**ou can register for free on my homepage to get the latest updates about the book and all of my work or just follow me on Twitter, Facebook, Linkedin, XING or Youtube.*

***E**ach feedback and all critics are taken into considerations. Please let me know if you find mistakes or if you think some special topic is missing.*

What is this book about

This book collects many aspects of mathematics, numerics and derivations that are used in the field of CFD and OpenFOAM®.

Thanksgiving

I would thank Dr. Alexander Vakhrushev for all the interesting discussions and the help in the topics of mathematics and programming in OpenFOAM®.

Furthermore, I would like to thank Sergei (Zappo) from the cfd-online platform and Vigneshkumar for the useful remarks and corrections. In addition I thank my sister Michaela Holzmann for further improvements and Andrea Jall for the beautiful cover page and all the support in my life.

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Outline

This book gives an introduction to the basic mathematics that are used in the field of computational fluid dynamics. After knowing the mathematic aspects, all conservation equations are derived using a finite volume element, $\mathrm{d}V$. It is shown how the mass and momentum equation can be derived. After that all different kinds of energy equations are discussed in all details. Here, the distinguish between the kinetic, the internal, the total energy and the enthalpy equation is done. Based on the nature of the equations, the general governing equation is introduced and it is shown how other equations can be derived out of this one. In a separated chapter the definition of the shear-rate tensor $\boldsymbol{\tau}$ for Newtonian fluids is given which is followed by a discussion that shows the analogy between the Cauchy stress tensor $\boldsymbol{\sigma}$, the shear-rate tensor $\boldsymbol{\tau}$ and the pressure p. The equations are summed up with a *one page summary* of all all equations.

Due to the fact that the flow pattern for engineering applications are mostly turbulent, the Reynolds-Averaging methods are explained. After that the incompressible Reynolds-Averaged-Navier-Stokes equations are derived and finally the closure problem is discussed. Here, we investigate into the Reynolds-Stress equation and the analogy to the Cauchy stress tensor is shown. During the introduction of the eddy-viscosity theory, the equation for the turbulent kinetic energy k, dissipation ϵ are deducted and it is shown how the turbulence modeling is applied. The topic ends with a brief description about the derivation for the compressible equations and its difficulties.

At the end of the book, the implementation of the shear-rate tensor $\boldsymbol{\tau}$ in OpenFOAM® is given and discussed. Here, the main focus is based on the investigation into the C++ code and the numerical stabilization. Finally, a more general discussion of the different pressure-momentum coupling algorithms is performed and it is explained how to use the `PIMPLE` algorithm in a correct way using OpenFOAM®.

The last chapter is related to OpenFOAM® tutorials and some further useful information.

Contents

Chapter 1

Basic Mathematics

In the field of computational fluid dynamics, it is essential to understand the equations and the mathematics. This will be helpful especially if we are going to implement, reorder or manipulate equations within a software or toolbox. There are a lot of ways to represent equations and thus a brief collection of the most essential mathematics are given in this chapter. The beauty of mathematics are also described in Greenshields [2015], Dantzig and Rappaz [2009], Jasak [1996] and Moukalled et al. [2015].

In the field of numerical simulations we are dealing with `tensors` $\mathbf{T}^n$ of rank n. A `tensor` stands for any kind of field like a scalar, a vector or the classical known tensor that represents a matrix (normally a 3 by 3 matrix) and is of rank two. To keep things clear we use the following definition:

Zero rank `tensor` $\mathbf{T}^0$:= scalar a

First rank `tensor` $\mathbf{T}^1$:= vector $\mathbf{a}$

Second rank `tensor` $\mathbf{T}^2$:= tensor $\mathbf{T}$ (matrix of 3x3)

Third rank `tensor` $\mathbf{T}^3$:= tensor T_{ijk}

A tensor that is of higher order than rank zero is `always` given in bold symbol. Tensors higher than second order are only needed during the derivation of the Reynolds-Stress equation.

1.1 Basic Rules of Derivatives

The governing conservation equations in fluid dynamics are partial differential equations. Thats why we briefly summarize the rules that are needed when we deal with this kind of equations. Considering the sum of two quantities ϕ and χ that are derived respectively to τ, we can split the derivative:

$$\frac{\partial(\phi+\chi)}{\partial\tau} = \frac{\partial\phi}{\partial\tau} + \frac{\partial\chi}{\partial\tau} \ . \tag{1.1}$$

If we have to derive the product of the two quantities, we need to use the `product rule` to split the term. In other words, we have to keep one quantity constant whereas we derive the other one:

$$\frac{\partial\phi\chi}{\partial\tau} = \chi\frac{\partial\phi}{\partial\tau} + \phi\frac{\partial\chi}{\partial\tau} \ . \tag{1.2}$$

A constant quantity C can be taken inside or outside of a derivative:

$$\frac{\partial\, C\,\phi\chi}{\partial\tau} = C\,\frac{\partial\phi\chi}{\partial\tau} \ . \tag{1.3}$$

1.2 Einsteins Summation Convention

For vector and tensor equations there are several options of notations. The longest but clearest notation is the Cartesian one. This notation can be abbreviated using the Einsteins summation convention. In general, we are using this convention mostly for vector and tensor quantities. Assuming the sum of derivatives of the arbitrary variable ϕ_i (like the momentum) in x, y and z direction, the Cartesian form is written as:

$$\frac{\partial\phi_x}{\partial x} + \frac{\partial\phi_y}{\partial y} + \frac{\partial\phi_z}{\partial z} \ . \tag{1.4}$$

To simplify this equation, we can use the Einsteins summation convention. Commonly we neglect the summation sign $\sum$ to keep things clear and short:

$$\sum_i \frac{\partial\phi_i}{\partial x_i} = \frac{\partial\phi_i}{\partial x_i} \qquad i = x, y, z \ . \tag{1.5}$$

A more complex example that demonstrates the advantage of the Einsteins summation convention would be the convective term of the momentum equation (till now we do not need to know what this equation means and hence, we do not think about the meaning). Due to the fact that the momentum is a vector quantity, we get three equations:

$$\frac{\partial u_x u_x}{\partial x} + \frac{\partial u_y u_x}{\partial y} + \frac{\partial u_z u_x}{\partial z} \ , \tag{1.6}$$

$$\frac{\partial u_x u_y}{\partial x} + \frac{\partial u_y u_y}{\partial y} + \frac{\partial u_z u_y}{\partial z} \ , \tag{1.7}$$

$$\frac{\partial u_x u_z}{\partial x} + \frac{\partial u_y u_z}{\partial y} + \frac{\partial u_z u_z}{\partial z} \ . \tag{1.8}$$

By using the Einsteins convention we can simplify the three equations into one:

$$\sum_i \frac{\partial u_i u_j}{\partial x_i} = \frac{\partial u_i u_j}{\partial x_i} \qquad i = x, y, z; \ j = x, y, z \ . \tag{1.9}$$

The Einsteins summation convention is widely used in literatures. Hence, we should keep in mind what it stand for and how we have to apply it.

1.3 General Tensor Mathematics

A common and easy way to deal with equations is using the vector notation instead of the Einsteins summation convention. The vector notation require knowledge of special mathematics. We will familiarize different operations that act on scalars, vectors and tensors. For that purpose we introduce a scalar ϕ, two vectors $\mathbf{a}$ and $\mathbf{b}$ and a tensor $\mathbf{T}$:

$$\mathbf{a} = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \ , \qquad \mathbf{b} = \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \ ,$$

$$\mathbf{T} = \begin{bmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{yx} & T_{yy} & T_{yz} \\ T_{zx} & T_{zy} & T_{zz} \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix} \ .$$

Depending on the operation we are investigating, we use either the numeric indices $(1, 2, 3)$ or the space components (x, y, z). Furthermore, we need the unit vectors

e_i and the identity matrix $\mathbf{I}$:

$$e_1 = e_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \ , \quad e_2 = e_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \ , \quad e_3 = e_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ , \quad \mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \ .$$

Simple Operations

- The multiplication of a scalar ϕ by a vector $\mathbf{b}$ results in a vector and is commutative and associative. This is also valid for the multiplication of a scalar ϕ and a tensor $\mathbf{T}$:

$$\phi\mathbf{b} = \begin{pmatrix} \phi b_x \\ \phi b_y \\ \phi b_z \end{pmatrix} , \qquad \phi\mathbf{T} = \begin{bmatrix} \phi T_{xx} & \phi T_{xy} & \phi T_{xz} \\ \phi T_{yx} & \phi T_{yy} & \phi T_{yz} \\ \phi T_{zx} & \phi T_{zy} & \phi T_{zz} \end{bmatrix} . \tag{1.10}$$

The Inner Product

- The inner product of two vectors $\mathbf{a}$ and $\mathbf{b}$ produces a scalar ϕ and is commutative. This operation is indicated by the dot sign $\bullet$:

$$\phi = \mathbf{a} \bullet \mathbf{b} = \mathbf{a}^T\mathbf{b} = \sum_{i=1}^{3} a_i b_i \ . \tag{1.11}$$

- The inner product of a vector $\mathbf{a}$ and a tensor $\mathbf{T}$ produces a vector $\mathbf{b}$ and is non-commutative if the tensor is non-symmetric:

$$\mathbf{b} = \mathbf{T} \bullet \mathbf{a} = \sum_{i=1}^{3}\sum_{j=1}^{3} T_{ij} a_j e_i = \begin{pmatrix} T_{11}a_1 & + & T_{12}a_2 & + & T_{13}a_3 \\ T_{21}a_1 & + & T_{22}a_2 & + & T_{23}a_3 \\ T_{31}a_1 & + & T_{32}a_2 & + & T_{33}a_3 \end{pmatrix} . \tag{1.12}$$

$$\mathbf{b} = \mathbf{a} \bullet \mathbf{T} = \mathbf{T}^T \bullet \mathbf{a} = \sum_{i=1}^{3}\sum_{j=1}^{3} a_j T_{ji} e_i = \begin{pmatrix} a_1T_{11} & + & a_2T_{21} & + & a_3T_{31} \\ a_1T_{12} & + & a_2T_{22} & + & a_3T_{32} \\ a_1T_{13} & + & a_2T_{23} & + & a_3T_{33} \end{pmatrix} , \tag{1.13}$$

  A symmetric tensor is given, if $\mathbf{T}_{ij} = \mathbf{T}_{ji}$ and hence, $\mathbf{a} \bullet \mathbf{T} = \mathbf{T} \bullet \mathbf{a}$.

The Double Inner Product

- The double inner product of two tensors $\mathbf{T}$ and $\mathbf{S}$ results in a scalar ϕ and is commutative. It will be indicated by the colon $\boldsymbol{:}$ sign:

$$\phi = \mathbf{T}\colon \mathbf{S} = \sum_{i=1}^{3}\sum_{j=1}^{3} T_{ij}S_{ij} = T_{11}S_{11} + T_{12}S_{12} + T_{13}S_{13} + T_{21}S_{21} + T_{22}S_{22} + T_{23}S_{23} + T_{31}S_{31} + T_{32}S_{32} + T_{33}S_{33} \ . \tag{1.14}$$

The Outer Product

- The outer product of two vectors **a** and **b**, also known as dyadic product, results in a tensor, is non-commutative and is expressed by the dyadic sign $\otimes$:

$$\mathbf{T} = \mathbf{a} \otimes \mathbf{b} = \mathbf{a}\mathbf{b}^T = \begin{bmatrix} a_x b_x & a_x b_y & a_x b_z \\ a_y b_x & a_y b_y & a_y b_z \\ a_z b_x & a_z b_y & a_z b_z \end{bmatrix} . \tag{1.15}$$

In most of the literatures the dyadic sign $\otimes$ is neglected for brevity as shown below:

$$\mathbf{ab} \ . \tag{1.16}$$

Keep in mind, that both variants are used in literature whereas the last one is more common but the first one is more clear. In this book we use the definition of equation (1.15), to be more consistent with the mathematics.

Differential Operators

In vector notation, the spatial derivatives of a variable (scalar, vector or tensor) is made using the Nabla operator ∇. It contains the three space derivatives of x, y and z in a Cartesian coordinate system:

$$\nabla = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{pmatrix} .$$

Gradient Operator

- The gradient of a scalar ϕ results in a vector **a**:

$$\mathrm{grad}\,\phi = \nabla\phi = \begin{pmatrix} \frac{\partial \phi}{\partial x} \\ \frac{\partial \phi}{\partial y} \\ \frac{\partial \phi}{\partial z} \end{pmatrix} . \tag{1.17}$$

- The gradient of a vector $\mathbf{b}$ results in a tensor $\mathbf{T}$:

$$\operatorname{grad}\mathbf{b} = \nabla \otimes \mathbf{b} = \begin{bmatrix} \frac{\partial}{\partial x}b_x & \frac{\partial}{\partial x}b_y & \frac{\partial}{\partial x}b_z \\ \frac{\partial}{\partial y}b_x & \frac{\partial}{\partial y}b_y & \frac{\partial}{\partial y}b_z \\ \frac{\partial}{\partial z}b_x & \frac{\partial}{\partial z}b_y & \frac{\partial}{\partial z}b_z \end{bmatrix} . \tag{1.18}$$

We see that this operation is actually the outer product of the Nabla operator (special vector) and an arbitrary vector $\mathbf{b}$. Hence, it is commonly written as:

$$\nabla\mathbf{b} \ . \tag{1.19}$$

In this book we use the first notation (with the dyadic sign) to be more consistent within the mathematics.

Note: The gradient operation increase the rank of the `tensor` by one and hence, we can apply it to any `tensor` field.

Divergence Operator

- The divergence of a vector $\mathbf{b}$ results in a scalar ϕ and is expressed by the combination of the Nabla operator and the dot sign, $\nabla\bullet$:

$$\operatorname{div}\mathbf{b} = \nabla \bullet \mathbf{b} = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} b_i = \frac{\partial b_1}{\partial x_1} + \frac{\partial b_2}{\partial x_2} + \frac{\partial b_3}{\partial x_3} \ . \tag{1.20}$$

- The divergence of a tensor $\mathbf{T}$ results in a vector $\mathbf{b}$:

$$\operatorname{div}\mathbf{T} = \nabla \bullet \mathbf{T} = \sum_{i=1}^{3}\sum_{j=1}^{3} \frac{\partial}{\partial x_j} T_{ji} e_i = \begin{bmatrix} \frac{\partial T_{11}}{\partial x_1} & + & \frac{\partial T_{21}}{\partial x_2} & + & \frac{\partial T_{31}}{\partial x_3} \\ \frac{\partial T_{12}}{\partial x_1} & + & \frac{\partial T_{22}}{\partial x_2} & + & \frac{\partial T_{32}}{\partial x_3} \\ \frac{\partial T_{13}}{\partial x_1} & + & \frac{\partial T_{23}}{\partial x_2} & + & \frac{\partial T_{33}}{\partial x_3} \end{bmatrix} . \tag{1.21}$$

Note: The divergence operation decrease the rank of the `tensor` by one. Hence, it does not make sense to apply this operator on a `scalar`.

The Product Rule within the Divergence Operator

If we have a product within a divergence term, we can split the term using the product rule. Based on the `tensor` ranks inside the divergence, we have to apply different rules, which are given now.

- The divergence of the product of a vector $\mathbf{a}$ and a scalar ϕ can be split as follow and results in a scalar:

$$\nabla \bullet (\mathbf{a}\phi) = \underbrace{\mathbf{a} \bullet \nabla\phi}_{\text{Eqn. (1.11)}} + \underbrace{\phi\nabla \bullet \mathbf{a}}_{\text{simple multiplication}} \quad . \tag{1.22}$$

- The divergence of the outer product (dyadic product) of two vectors $\mathbf{a}$ and $\mathbf{b}$ can be split as follow and results in a vector:

$$\nabla \bullet (\mathbf{a} \otimes \mathbf{b}) = \underbrace{\mathbf{a} \bullet \nabla \otimes \mathbf{b}}_{\text{Eqn. (1.13)}} + \underbrace{\mathbf{b}\nabla \bullet \mathbf{a}}_{\text{Eqn. (1.10)}} \quad . \tag{1.23}$$

- The divergence of the inner product of a tensor $\mathbf{T}$ and a vector $\mathbf{b}$ can be split as follow and results in a scalar:

$$\nabla \bullet (\mathbf{T} \bullet \mathbf{b}) = \underbrace{\mathbf{T} \colon \nabla \otimes \mathbf{b}}_{\text{Eqn. (1.14)}} + \underbrace{\mathbf{b} \bullet \nabla \bullet \mathbf{T}}_{\text{Eqn. (1.11)}} \quad . \tag{1.24}$$

If you think that the product rule for the inner product of two vectors is missing, just think about the result of the inner product of two vectors and how this `tensor` will change (rank) if we apply the divergence operator. Hopefully you will figure out, that the divergence of a scalar does not make sense.

1.3.1 The Total Derivative

The definition of the total derivative of an arbitrary quantity ϕ – in the field of fluid dynamics – is defined as:

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} = \frac{\partial\phi}{\partial t} + \underbrace{\mathbf{U} \bullet \nabla\phi}_{\text{inner product}} \quad , \tag{1.25}$$

where $\mathbf{U}$ represents the velocity vector. The last term in equation (1.25) denotes the inner product. Depending on the quantity ϕ (scalar, vector, tensor, and so on), we have to use the correct mathematical expressions for the second term on the right hand side. Example given:

- If ϕ is a scalar, we have to use equation (1.11),
- If ϕ is a vector, we have to use equation (1.13).

Short Outline for the Total Derivative

The total derivative is used to represent non-conserved equations. In other words, each conserved equation can be changed into a non-conserved equation using the continuity equation. In literature people start to derive equations using the total derivative and using the continuity equation to extend the non-conservative equation to the conserved one. The better way would be to derive *first* the conserved equation and *then* using the continuity equation to get the non-conserved form. *Why*? It is easier to understand. The difference between both equations is the frame of reference. In the conserved representation, we have the Euler expression, for non-conserved equations it is the Lagrange expression.

If you have literature that start with the non-conservation equations, this would help to understand the following extension (at the moment we do not need to understand this equations, it is just an example):

- Incompressible:

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} = \underbrace{\frac{\partial \phi}{\partial t} + \mathbf{U} \bullet \nabla \phi}_{\text{non}-\text{conserved}} \quad \boxed{+ \ \phi \ \underbrace{(\nabla \bullet (\mathbf{U}))}_{\text{continuity } = \ 0}} \ . \tag{1.26}$$

- Compressible:

$$\rho \frac{\mathrm{D}\phi}{\mathrm{D}t} = \underbrace{\rho \left[\frac{\partial \phi}{\partial t} + \mathbf{U} \bullet \nabla \phi \right]}_{\text{non}-\text{conserved}} \quad \boxed{+ \ \phi \underbrace{\left(\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{U}) \right)}_{\text{continuity } = \ 0}} \ . \tag{1.27}$$

The reason we multiply the continuity equation (second term on the right hand side) by the quantity ϕ comes from the product rule, that is applied to the convective term. After the momentum equation is derived and the conservative form is transformed into the non-conserved one, this will get clear.

1.3.2 Matrix Algebra, Deviatoric and Hydrostatic Part

In the field of numerical simulations we are dealing with quantities that are represented by matrices like the stress tensor. Thats why we need to introduce some basics here. Each matrix $\mathbf{A}$ can be split into a deviatoric $\mathbf{A}^{\text{dev}}$ and hydrostatic $\mathbf{A}^{\text{hyd}}$ part:

$$\mathbf{A} = \mathbf{A}^{\text{hyd}} + \mathbf{A}^{\text{dev}} \ . \tag{1.28}$$

The hydrostatic part can be expressed as scalar or matrix and is defined by using the trace operator. If we want to get the scalar, we use the following definition:

$$A^{\text{hyd}} = \frac{1}{3}\,\text{tr}(\mathbf{A}) = \frac{1}{3}\sum_{i=1}^{n}(a_{ii}) \; . \tag{1.29}$$

The operator `tr` denotes the trace operator and is applied on the matrix. This operator is simply the sum of the diagonal elements. The matrix notation of the hydrostatic part given by:

$$\mathbf{A}^{\text{hyd}} = A^{\text{hyd}}\mathbf{I} = \frac{1}{3}\,\text{tr}(\mathbf{A})\mathbf{I} = \frac{1}{3}\sum_{i=1}^{n}(a_{ii})\mathbf{I} \; . \tag{1.30}$$

The deviatoric part $\mathbf{A}^{\text{dev}}$ is given as:

$$\mathbf{A}^{\text{dev}} = \mathbf{A} - \mathbf{A}^{\text{hyd}} = \mathbf{A} - \frac{1}{3}\,\text{tr}(\mathbf{A})\mathbf{I} \; . \tag{1.31}$$

Note: The deviatoric part of a matrix is *traceless*. Hence, $\text{tr}(\mathbf{A}^{\text{dev}}) = 0$; The trace operator is zero not the diagonal elements.

1.3.3 The Gauss Theorem

To transform any equation from the differential form to the integral one (or vice versa), it is necessary to know the Gauss theorem. This theorem allows us to establish a relation between the *fluxes through the surface* of an arbitrary volume element and the *divergence operator on the volume element*:

$$\oint \mathbf{a} \cdot \mathbf{n}\mathrm{d}S = \int (\nabla \bullet \mathbf{a})\mathrm{d}V \; . \tag{1.32}$$

In equation (1.32), $\mathbf{n}$ represents the surface normal vector pointing outwards, dS the integration with respect to the surface and dV the integration with respect to the volume.

Note: The small dot $\cdot$ denotes the inner product of two vectors (1.11). In the following book, we use the small dot in all integrals to sign that we calculate the inner product of a vector $\mathbf{a}$ and the *surface normal vector* $\mathbf{n}$. Keep in mind that the small dot expresses exact the same as the bullet.

Chapter 2

Derivations of the Governing Equations

The following chapter demonstrates how to derive the continuity, momentum, total energy, mechanical (kinetic) energy, thermo (internal) energy and enthalpy equation using a small volume element $\mathrm{d}V$. The equations are derived using the Cartesian coordinate system. A complete summary of all equations is given on page 49. The structure of this chapter is (mainly) as follows:

- Express the phenomena that act on the volume element using finite differences,
- Transform the finite difference equation to a partial differential equation,
- Manipulate the equation to get the common form,
- Transform the Cartesian notation into the vector notation,
- Proof that the vector notation results in the Cartesian notation,
- Transform the equation into the integral and non-conserved form.

The main references that are used within this chapter are Greenshields [2015], Dantzig and Rappaz [2009], Jasak [1996], Ferziger and Perić [2008], Bird et al. [1960], Versteeg and Malalasekera [1995], Schwarze [2013] and Moukalled et al. [2015].

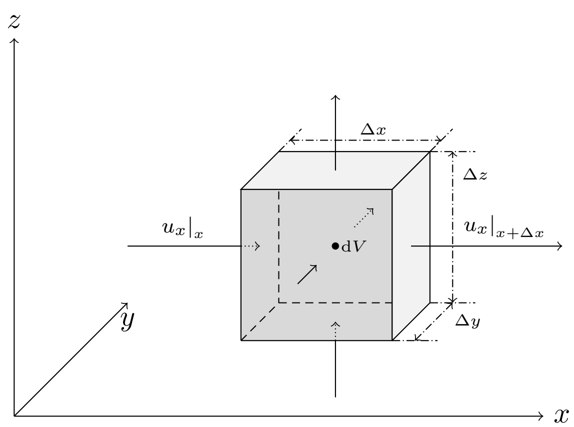
2.1 The Continuity Equation

In the following section we are going to derive the continuity equation. This equation is simply a mass balance of an arbitrary volume element.

Consider the mass flow through a small control volume element $\mathrm{d}V$, using the constrain that mass is not transformed into energy or vice versa, a mass balance has to be fulfilled for the volume element. That means, that the mass flow that enters or leaves the volume element through its surfaces has to be equal. Furthermore, we have to take the rate of mass accumulation into account:

$$\begin{bmatrix}\text{rate of mass}\\\text{accumulation}\end{bmatrix} = \begin{bmatrix}\text{rate of mass}\\\text{entering the volume}\end{bmatrix} - \begin{bmatrix}\text{rate of mass}\\\text{leaving the volume}\end{bmatrix}. \tag{2.1}$$

To make things clearer, we analyze figure 2.1. It is obvious that the mass is transported through the surface by the velocity. This transport phenomenon is called convection or sometimes named advection and happens for all three space directions x (u_x), y (u_y) and z (u_z). Additionally a mass change inside the element can occur due to compression or expansion phenomena; that means the density will change.



Mass inside x : $(\rho u_x)|_x \Delta y \Delta z$

Mass outside x : $(\rho u_x)|_{x+\Delta x} \Delta y \Delta z$

Mass inside y : $(\rho u_y)|_y \Delta x \Delta z$

Mass outside y : $(\rho u_y)|_{y+\Delta y} \Delta x \Delta z$

Mass inside z : $(\rho u_z)|_z \Delta x \Delta y$

Mass outside z : $(\rho u_z)|_{z+\Delta z} \Delta x \Delta y$

Figure 2.1: Mass balance in a small volume element $\mathrm{d}V$.

Having a closer look on figure 2.1, we can see that it shows the velocity vectors normal to the faces. The rate of mass that enters or leaves the volume element through the surface is called mass flux and is simply the density times the velocity with respect to the area of the face. For the derivation of the mass conservation equation we have to build the balance of the fluxes at the surfaces of the volume element. In other words, everything that is going inside has to go out if we assume that there is no mass accumulation inside the volume (incompressible). The single terms that describe the fluxes at the surfaces are given on the right side of figure 2.1.

If we have a compressible fluid, the rate of change for the density ρ is related to the volume, **mass per unit volume**, and will only change with respect to time. Therefore, we can write the rate of change of the density as:

$$\frac{\Delta\rho}{\Delta t} \ . \tag{2.2}$$

Rewriting equation (2.1) by using the mathematical expressions of figure 2.1 and equation (2.2), it follows:

$$\begin{aligned}\frac{\Delta\rho}{\Delta t}\Delta x\Delta y\Delta z = &\left((\rho u_x)|_x - (\rho u_x)|_{x+\Delta x}\right)\Delta y\Delta z\\ &+\left((\rho u_y)|_y - (\rho u_y)|_{y+\Delta y}\right)\Delta x\Delta z\\ &+\left((\rho u_z)|_z - (\rho u_z)|_{z+\Delta z}\right)\Delta x\Delta y \ .\end{aligned} \tag{2.3}$$

Dividing the equation by the volume $\Delta V = \Delta x\Delta y\Delta z$, we get:

$$\begin{aligned}\frac{\Delta\rho}{\Delta t} = &\frac{(\rho u_x)|_x - (\rho u_x)|_{x+\Delta x}}{\Delta x}\\ &+\frac{(\rho u_y)|_y - (\rho u_y)|_{y+\Delta y}}{\Delta y}\\ &+\frac{(\rho u_z)|_z - (\rho u_z)|_{z+\Delta z}}{\Delta z} \ .\end{aligned} \tag{2.4}$$

Introducing the assumption of an infinitesimal small volume element – which means that we decrease the distance between the corners of the volume element and therefore Δ goes to zero:

$$\frac{\Delta}{\Delta x} \quad\longrightarrow\quad \lim_{\Delta x\to 0}\frac{\Delta}{\Delta x} = \frac{\partial}{\partial x} \ , \tag{2.5}$$

and also an infinitesimal small time range:

$$\frac{\Delta}{\Delta t} \quad\longrightarrow\quad \lim_{\Delta t\to 0}\frac{\Delta}{\Delta t} = \frac{\partial}{\partial t} \ , \tag{2.6}$$

we can transform the finite difference equation to a partial differential equation. For that, we have to apply equation (2.5) and (2.6) to (2.4). It follows:

$$\frac{(\rho u_x)|_x - (\rho u_x)|_{x+\Delta x}}{\Delta x} = \frac{-\Delta(\rho u_x)}{\Delta x} \longrightarrow -\frac{\partial}{\partial x}(\rho u_x) \ , \tag{2.7}$$

$$\frac{(\rho u_y)|_y - (\rho u_y)|_{y+\Delta y}}{\Delta y} = \frac{-\Delta(\rho u_y)}{\Delta y} \longrightarrow -\frac{\partial}{\partial y}(\rho u_y) \ , \tag{2.8}$$

$$\frac{(\rho u_z)|_z - (\rho u_x)|_{z+\Delta z}}{\Delta z} = \frac{-\Delta(\rho u_z)}{\Delta z} \longrightarrow -\frac{\partial}{\partial z}(\rho u_z) \ , \tag{2.9}$$

$$\frac{\Delta \rho}{\Delta t} \rightarrow \frac{\partial \rho}{\partial t} \ , \tag{2.10}$$

and the general mass conservation (continuity) equation is given by:

$$\boxed{\frac{\partial \rho}{\partial t} = -\left(\frac{\partial}{\partial x}(\rho u_x) + \frac{\partial}{\partial y}(\rho u_y) + \frac{\partial}{\partial z}(\rho u_z)\right)} \ . \tag{2.11}$$

If we use the Nabla-Operator ∇ and the velocity vector $\mathbf{U}$, the equation can be rewritten in vector notation:

$$\boxed{\frac{\partial \rho}{\partial t} = -\nabla \bullet (\rho \mathbf{U})} \ . \tag{2.12}$$

However, if we focus on incompressible fluids, we could assume that the density is constant and therefore the quantity ρ can be taken out of the derivatives and we are allowed to divide by ρ. It is obvious that the time derivative will vanish because of the fact that the density is a constant and will not change with respect to time. One may also try to explain it in the following way: if we assume constant density, there is no expansion or compression phenomena and therefore the time derivative can be canceled to zero. Hence, only the mass flux that enters and/or leaves the volume element at its surface has to be taken into account.

Remark: In many cases incompressibility means that there is no expansion and/or compression phenomena. However, the fluid density can still be temperature depended. In such a case we have to be careful which mass conservation equation we are using (incompressible or compressible). In general, if the density is not a constant value, we are not allowed to use the simplified mass conservation equation (2.13) due to the fact that it is not possible anymore to push the density out of the derivative.

If the density change is really small, we are allowed to use the simplified mass conservation equation with limitations. The reason for that is based on numerics and the interaction with the momentum conservation equation.

For the incompressible case, the density for the fluid is constant and thus we can simplify the mass conservation equation to:

$$\boxed{\nabla \bullet \mathbf{U} = 0} \,. \tag{2.13}$$

For the simple mass conservation equation it is obvious that the vector notation results in the Cartesian form. Thats why the transformation is not demonstrated here. If you want to check it ourself, you just need to use equation (1.20).

2.1.1 Integral Form of the Conserved Continuity Equation

For the completeness, the integral form of the mass conservation equation will be given now. Using the Gauss theorem (1.32), we can transform the divergence term (that acts on the volume) to a surface integral. The accumulation of density in the element is a simple volume integral. Furthermore, the volume element itself is not changing with respect to time (fixed finite volume - the discrete volumes are not changing during the simulation; static meshes). Thus, we end up with:

Compressible:

$$\boxed{\frac{\partial}{\partial t} \int \rho \mathrm{d}V = - \oint \rho \mathbf{U} \cdot \mathbf{n} \mathrm{d}S} \,. \tag{2.14}$$

Incompressible:

$$\boxed{\oint \mathbf{U} \cdot \mathbf{n} \mathrm{d}S = 0} \,. \tag{2.15}$$

The surface integral means nothing more than taking the balance of the fluxes on the surface of volume element; what is going in and out. Depending on the shape of the volume, we have to evaluate more or less faces. The integral form of the continuity equation leads to the so called finite volume method (FVM). This method is conservative and we can apply this method to each arbitrary volume (hexaeder, tetraeder, prisms, wedges and so on) which makes this method popular.

2.1.2 Continuity Equation and the Total Derivative

Using the total derivative formulation (1.25), we are able to rewrite the continuity equation (2.12) by applying the product rule (1.22) to the divergence term:

$$\nabla \bullet (\rho \mathbf{U}) = \mathbf{U} \bullet \nabla \rho + \rho \nabla \bullet \mathbf{U} \ . \tag{2.16}$$

Substituting this expression into equation (2.12), we get:

$$\frac{\partial \rho}{\partial t} = -\mathbf{U} \bullet \nabla \rho - \rho \nabla \bullet \mathbf{U} \ . \tag{2.17}$$

Finally, we put all terms to the LHS:

$$\underbrace{\frac{\partial \rho}{\partial t} + \mathbf{U} \bullet \nabla \rho}_{\text{Total derivative}} + \rho \nabla \bullet \mathbf{U} = 0 \ . \tag{2.18}$$

The result is:

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho \nabla \bullet \mathbf{U} = 0 \ . \tag{2.19}$$

This equation is not common but could be found in Anderson [1995].

OpenFOAM®

In OpenFOAM® we are using this equation (integral one) to calculate the fluxes at the faces of each cell. The flux field is named `phi` in and is created by the call of one of the two header files in each solver:

- createPhi.H
- compressibleCreatePhi.H

Due to the fact that we store the density and the velocity at the cell center, we need to interpolate the values to the face centers. This is done by calling the function `interpolate(rho*U)`. This will simply calculate the product of the density and the velocity vector at the cell center and interpolate it to the face center by including the neighbor cell information with respect to the face we are going to evaluate. To get the fluxes, the interpolated values are then multiplied by the surface normal vector (area) using the inner product of two vectors denoted by the ampersand sign `&` in OpenFOAM®.

2.2 The Conserved Momentum Equation

For the derivation of the conserved momentum equation, we are going to use the volume element $\mathrm{d}V$ again. The main difference in the momentum equation compared to the mass conservation equation is, that we have to consider more phenomena that can transport and change the momentum inside the volume element and that this quantity is not a scalar; it is a vector (velocity in x, y and z direction).

Generally we are allowed to say that the momentum can be transported and changed by the following aspects:

$$\begin{bmatrix} \text{rate of} \\ \text{momentum} \\ \text{accumulation} \end{bmatrix} = \begin{bmatrix} \text{rate of} \\ \text{momentum} \\ \text{entering the} \\ \text{volume} \end{bmatrix} - \begin{bmatrix} \text{rate of} \\ \text{momentum} \\ \text{leaving the} \\ \text{volume} \end{bmatrix} + \begin{bmatrix} \text{sum of forces} \\ \text{that act on} \\ \text{the volume} \end{bmatrix} . \tag{2.20}$$

Figure 2.2 shows the volume element like in 2.1 but now showing another transport phenomenon that acts **only** on the surfaces. The phenomenon transports the momentum based on molecular effects. This molecular transport acts normal and tangential to the surface and is an outcome or property of the vector quantity.

Other phenomena that change the momentum are given as a sum of forces acting on the volume element $\mathrm{d}V$. For example we could have the gravitational acceleration and the pressure force.

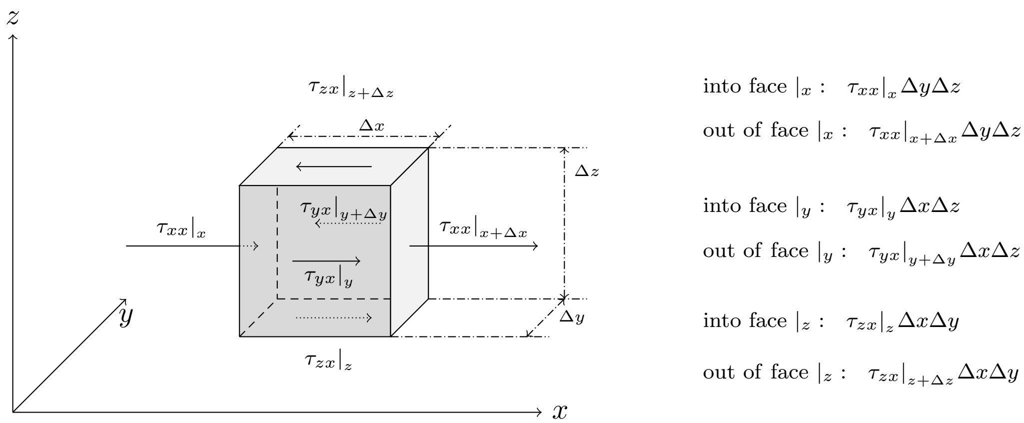


Figure 2.2: Molecular transport of the momentum in x-direction in an arbitrary small volume element $\mathrm{d}V$.

On the right side of figure 2.2, the terms that transport the x-component of the momentum through the surfaces by the molecular transport effect are given.

Convection of the Momentum in x-Direction

The x-component of the momentum is transported by convection into the volume element through all six faces that is also an outcome related to the vector quantity. Therefore, the convection of the momentum can be derived similarly to the convective transport of the mass. But now we have to take care about the **vector** quantity. Thus, the momentum in x-direction enters the volume at the face $|_x$ and leaves the volume through the face $|_{x+\Delta x}$; identical to the continuity equation. But now it is also possible that the x-component of the momentum is transported through the faces in y and z direction. Hence, we can write the transport of the momentum due to convection; it is simply the velocity in x-direction multiplied by the **flux** through the face we are looking at (Newtons second law):

$$
\begin{aligned}
\text{into face } |_x : \quad & (\rho u_x) u_x|_x \ , \\
\text{out of face } |_{x+\Delta x} : \quad & (\rho u_x) u_x|_{x+\Delta x} \ , \\
\text{into face } |_y : \quad & (\rho u_y) u_x|_y \ , \\
\text{out of face } |_{y+\Delta y} : \quad & (\rho u_y) u_x|_{y+\Delta y} \ , \\
\text{into face } |_z : \quad & (\rho u_z) u_x|_z \ , \\
\text{out of face } |_{z+\Delta z} : \quad & (\rho u_z) u_x|_{z+\Delta z} \ .
\end{aligned}
$$

After combining the terms and using the face areas, we get:

$$
\begin{aligned}
& \left((\rho u_x) u_x|_x - (\rho u_x) u_x|_{x+\Delta x} \right) \Delta y \Delta z \\
+ & \left((\rho u_y) u_x|_y - (\rho u_y) u_x|_{y+\Delta y} \right) \Delta x \Delta z \\
+ & \left((\rho u_z) u_x|_z - (\rho u_z) u_x|_{z+\Delta z} \right) \Delta x \Delta y \ .
\end{aligned}
$$

Molecular Transport of the Momentum in x-Direction

Additionally, the x-component of the momentum is transported due to the molecular phenomenon as demonstrated in figure 2.2. The effect is based on velocity differences (velocity gradients). As we can see in figure 2.2, we have different kind of terms: the normal component τ_{xx} and the tangential components τ_{yx}, τ_{zx}. Therefore, the molecular transport of the x-momentum through the surfaces can be written as:

$$
\begin{aligned}
&\left(\tau_{xx}\big|_x - \tau_{xx}\big|_{x+\Delta x}\right)\Delta y \Delta z \\
+ &\left(\tau_{yx}\big|_y - \tau_{yx}\big|_{y+\Delta y}\right)\Delta x \Delta z \\
+ &\left(\tau_{zx}\big|_z - \tau_{zx}\big|_{z+\Delta z}\right)\Delta x \Delta y \ .
\end{aligned}
$$

These terms represent additional fluxes of momentum through the surface. We consider these fluxes as stresses. τ_{xx} denotes the stress perpendicular to the direction we are looking at (here face $|_x$ and face $|_{x+\Delta x}$) and τ_{yx}, τ_{zx} denote the x-directed tangential stresses which act on the faces with respect to the indices. All these stresses are known as shear stresses due to the fact that they are generated with respect to velocity gradients that introduce shearing.

Additional Forces that Influence the Momentum

In most problems, the only important forces that influence the momentum are the pressure and gravity force. The pressure acts on the surface whereat the gravitational force acts on the volume of the element. Hence, we are able to derive the change of the x-momentum based on the pressure and gravitational force:

$$\left(p\big|_x - p\big|_{x+\Delta x}\right)\Delta y \Delta z + \rho g_x \Delta x \Delta y \Delta z \ .$$

Conserved Momentum Equation

After we have all terms, we can reconstruct equation (2.20) with the mathematic expressions. Of course the accumulation of the momentum inside an arbitrary volume element is given by:

$$\frac{\Delta}{\Delta t}\rho u_x \Delta x \Delta y \Delta z \ .$$

Thus, for the momentum in x-direction we can write:

$$
\begin{aligned}
\frac{\Delta}{\Delta t}\rho u_x \Delta x \Delta y \Delta z = & \left((\rho u_x) u_x|_x - (\rho u_x) u_x|_{x+\Delta x} \right) \Delta y \Delta z \\
& + \left((\rho u_y) u_x|_y - (\rho u_y) u_x|_{y+\Delta y} \right) \Delta x \Delta z \\
& + \left((\rho u_z) u_x|_z - (\rho u_z) u_x|_{z+\Delta z} \right) \Delta x \Delta y \\
& + \left(\tau_{xx}|_x - \tau_{xx}|_{x+\Delta x} \right) \Delta y \Delta z \\
& + \left(\tau_{yx}|_y - \tau_{yx}|_{y+\Delta y} \right) \Delta x \Delta z \\
& + \left(\tau_{zx}|_z - \tau_{zx}|_{z+\Delta z} \right) \Delta x \Delta y \\
& + \left(p|_x - p|_{x+\Delta x} \right) \Delta y \Delta z \\
& + \rho g_x \Delta x \Delta y \Delta z \ .
\end{aligned}
\tag{2.21}
$$

Now, by dividing the whole equation by the volume $\mathrm{d}V$, it follows:

$$
\begin{aligned}
\frac{\Delta}{\Delta t}\rho u_x = & \frac{(\rho u_x) u_x|_x - (\rho u_x) u_x|_{x+\Delta x}}{\Delta x} + \frac{(\rho u_y) u_x|_y - (\rho u_y) u_x|_{y+\Delta y}}{\Delta y} \\
& + \frac{(\rho u_z) u_x|_z - (\rho u_z) u_x|_{z+\Delta z}}{\Delta z} + \frac{\tau_{xx}|_x - \tau_{xx}|_{x+\Delta x}}{\Delta x} + \frac{\tau_{yx}|_y - \tau_{yx}|_{y+\Delta y}}{\Delta y} \\
& + \frac{\tau_{zx}|_z - \tau_{zx}|_{z+\Delta z}}{\Delta z} + \frac{p|_x - p|_{x+\Delta x}}{\Delta x} + \rho g_x \ .
\end{aligned}
\tag{2.22}
$$

Finally we use the assumption of an infinitesimal small volume element (2.5) and time range (2.6) to rewrite the x-component of the momentum equation above. The other two space directions can be derived in the same way and is not shown in details.

The x-component of the momentum is then written as:

$$
\boxed{
\begin{aligned}
\frac{\partial}{\partial t}\rho u_x = & -\left(\frac{\partial}{\partial x}\rho u_x u_x + \frac{\partial}{\partial y}\rho u_y u_x + \frac{\partial}{\partial z}\rho u_z u_x \right) \\
& -\left(\frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{yx} + \frac{\partial}{\partial z}\tau_{zx} \right) - \frac{\partial p}{\partial x} + \rho g_x
\end{aligned}
} \ .
\tag{2.23}
$$

For the y-component of the momentum, we get:

$$
\boxed{
\begin{aligned}
\frac{\partial}{\partial t}\rho u_y = & -\left(\frac{\partial}{\partial x}\rho u_x u_y + \frac{\partial}{\partial y}\rho u_y u_y + \frac{\partial}{\partial z}\rho u_z u_y \right) \\
& -\left(\frac{\partial}{\partial x}\tau_{xy} + \frac{\partial}{\partial y}\tau_{yy} + \frac{\partial}{\partial z}\tau_{zy} \right) - \frac{\partial p}{\partial y} + \rho g_y
\end{aligned}
} \ ,
\tag{2.24}
$$

and for the z-component we achieve:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\rho u_z = &-\left(\frac{\partial}{\partial x}\rho u_x u_z + \frac{\partial}{\partial y}\rho u_y u_z + \frac{\partial}{\partial z}\rho u_z u_z\right)\\ &-\left(\frac{\partial}{\partial x}\tau_{xz} + \frac{\partial}{\partial y}\tau_{yz} + \frac{\partial}{\partial z}\tau_{zz}\right) - \frac{\partial p}{\partial z} + \rho g_z\end{aligned}}\ . \tag{2.25}$$

Introducing the gravitational acceleration vector $\mathbf{g}$, the gradient of the pressure ∇p and the shear-rate tensor $\boldsymbol{\tau}$ that are defined as

$$\nabla p = \begin{pmatrix}\frac{\partial p}{\partial x}\\ \frac{\partial p}{\partial y}\\ \frac{\partial p}{\partial z}\end{pmatrix}, \qquad \boldsymbol{\tau} = \begin{bmatrix}\tau_{xx} & \tau_{xy} & \tau_{xz}\\ \tau_{yx} & \tau_{yy} & \tau_{yz}\\ \tau_{zx} & \tau_{zy} & \tau_{zz}\end{bmatrix}, \qquad \mathbf{g} = \begin{pmatrix}g_x\\ g_y\\ g_z\end{pmatrix},$$

we are able to write the momentum equation in vector form. **Note**, that the negative sign of the shear-rate tensor will change, if we introduce the definition of the shear-rate tensor $\boldsymbol{\tau}$ later on.

$$\boxed{\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U}\otimes\mathbf{U}) - \nabla \bullet \boldsymbol{\tau} - \nabla p + \rho\mathbf{g}} \tag{2.26}$$

2.2.1 The Proof of the Transformation

The following section will proof that equation (2.26) results in (2.23), (2.24) and (2.25). For clearance, we will focus on each term separately. Starting with the first term, the time derivative, we get:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = \begin{pmatrix}\frac{\partial}{\partial t}\rho u_x\\ \frac{\partial}{\partial t}\rho u_y\\ \frac{\partial}{\partial t}\rho u_z\end{pmatrix} \stackrel{!}{=} \begin{cases}\frac{\partial}{\partial t}\rho u_x & \text{of } x-\text{momentum}\\ \frac{\partial}{\partial t}\rho u_y & \text{of } y-\text{momentum}\\ \frac{\partial}{\partial t}\rho u_z & \text{of } z-\text{momentum}\end{cases}\ . \tag{2.27}$$

As we see the time derivative term results in the the same three terms that we have in the Cartesian formulation. The second term embrace the transport of momentum due to convection by the flux $\rho\mathbf{U}$. To evaluate the term, we need the mathematics (1.15) and (1.21):

$$-\nabla\bullet(\rho\mathbf{U}\otimes\mathbf{U}) = -\nabla\bullet\left\{\rho\begin{pmatrix}u_x\\ u_y\\ u_z\end{pmatrix}\otimes\begin{pmatrix}u_x\\ u_y\\ u_z\end{pmatrix}\right\} = -\nabla\bullet\left\{\rho\begin{bmatrix}u_xu_x & u_xu_y & u_xu_z\\ u_yu_x & u_yu_y & u_yu_z\\ u_zu_x & u_zu_y & u_zu_z\end{bmatrix}\right\}$$

$$= -\nabla \bullet \begin{bmatrix} \rho u_x u_x & \rho u_x u_y & \rho u_x u_z \\ \rho u_y u_x & \rho u_y u_y & \rho u_y u_z \\ \rho u_z u_x & \rho u_z u_y & \rho u_z u_z \end{bmatrix} = -\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \begin{bmatrix} \rho u_x u_x & \rho u_x u_y & \rho u_x u_z \\ \rho u_y u_x & \rho u_y u_y & \rho u_y u_z \\ \rho u_z u_x & \rho u_z u_y & \rho u_z u_z \end{bmatrix}$$

$$= -\begin{bmatrix} \frac{\partial}{\partial x}\rho u_x u_x + \frac{\partial}{\partial y}\rho u_y u_x + \frac{\partial}{\partial z}\rho u_z u_x \\ \frac{\partial}{\partial x}\rho u_x u_y + \frac{\partial}{\partial y}\rho u_y u_y + \frac{\partial}{\partial z}\rho u_z u_y \\ \frac{\partial}{\partial x}\rho u_x u_z + \frac{\partial}{\partial y}\rho u_y u_z + \frac{\partial}{\partial z}\rho u_z u_z \end{bmatrix} \stackrel{!}{=} \begin{cases} -\left(\frac{\partial}{\partial x}\rho u_x u_x + \frac{\partial}{\partial y}\rho u_y u_x + \frac{\partial}{\partial z}\rho u_z u_x\right) \\ -\left(\frac{\partial}{\partial x}\rho u_x u_y + \frac{\partial}{\partial y}\rho u_y u_y + \frac{\partial}{\partial z}\rho u_z u_y\right) \\ -\left(\frac{\partial}{\partial x}\rho u_x u_z + \frac{\partial}{\partial y}\rho u_y u_z + \frac{\partial}{\partial z}\rho u_z u_z\right) \end{cases} .$$

Again, it can be seen that the terms are equal and we end up with the same set of equations. Now we investigate into the third term that describes shearing due to the gradients of the velocities. Using the convention (1.21) for the shear-rate tensor $\boldsymbol{\tau}$, we get:

$$-\nabla \bullet \boldsymbol{\tau} = -\nabla \bullet \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} =$$

$$-\begin{bmatrix} \frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{yx} + \frac{\partial}{\partial z}\tau_{zx} \\ \frac{\partial}{\partial x}\tau_{xy} + \frac{\partial}{\partial y}\tau_{yy} + \frac{\partial}{\partial z}\tau_{zy} \\ \frac{\partial}{\partial x}\tau_{xz} + \frac{\partial}{\partial y}\tau_{yz} + \frac{\partial}{\partial z}\tau_{zz} \end{bmatrix} \stackrel{!}{=} \begin{cases} -\left(\frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{yx} + \frac{\partial}{\partial z}\tau_{zx}\right) & \text{of } x \text{ momentum} \\ -\left(\frac{\partial}{\partial x}\tau_{xy} + \frac{\partial}{\partial y}\tau_{yy} + \frac{\partial}{\partial z}\tau_{zy}\right) & \text{of } y \text{ momentum} \\ -\left(\frac{\partial}{\partial x}\tau_{xz} + \frac{\partial}{\partial y}\tau_{yz} + \frac{\partial}{\partial z}\tau_{zz}\right) & \text{of } z \text{ momentum} \end{cases} .$$

It was already clear, that we end up with the same terms. At last the pressure and gravitational acceleration term is analyzed. For the pressure term we need the definition of equation (1.17) and for the gravitational term equation (1.10). It follows:

$$-\nabla p = -\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} p = -\begin{pmatrix} \frac{\partial p}{\partial x} \\ \frac{\partial p}{\partial y} \\ \frac{\partial p}{\partial z} \end{pmatrix} \stackrel{!}{=} \begin{cases} -\frac{\partial p}{\partial x} & \text{of } x \text{ momentum} \\ -\frac{\partial p}{\partial y} & \text{of } y \text{ momentum} \\ -\frac{\partial p}{\partial z} & \text{of } z \text{ momentum} \end{cases} ,$$

$$\rho \mathbf{g} = \rho \begin{pmatrix} g_x \\ g_y \\ g_z \end{pmatrix} = \begin{pmatrix} \rho g_x \\ \rho g_y \\ \rho g_z \end{pmatrix} \stackrel{!}{=} \begin{cases} \rho g_x \text{ of } x \text{ momentum} \\ \rho g_y \text{ of } y \text{ momentum} \\ \rho g_z \text{ of } z \text{ momentum} \end{cases} .$$

As we `proofed` now, the vector form ends up in the Cartesian form.

If we want to solve this equation now, it is necessary to know the shear-rate tensor $\boldsymbol{\tau}$. We are going to investigate into that quantity in chapter 5. Further representations of the momentum equation can be found in chapter 7. The implementation of the momentum equation in OpenFOAM® will be discussed in chapter 9; especially the treatment of the diffusion term. Keep in mind that equation (2.26) includes *only* the gravitational acceleration and pressure force. If there are further phenomena (forces) influencing the momentum equation, these terms have to be taken into account.

2.2.2 Integral Form of the Conserved Momentum Equation

The integral form of the momentum equation (2.26) can be obtained by using the Gauss theorem (1.32). It follows:

$$\boxed{\frac{\partial}{\partial t}\int \rho \mathbf{U} \mathrm{d}V = -\oint (\rho \mathbf{U} \otimes \mathbf{U}) \cdot \mathbf{n} \mathrm{d}S - \oint \boldsymbol{\tau} \cdot \mathbf{n} \mathrm{d}S - \int p \mathrm{d}V + \int \rho \mathbf{g} \mathrm{d}V} \ . \tag{2.28}$$

2.2.3 Non-Conserved Momentum Equation

We can manipulate the conserved momentum equation with the continuity equation (2.12) to get a non-conservative form. For that, we consider equation (2.26) first and split the time and convection term by using the product rule. The time derivative becomes:

$$\frac{\partial}{\partial t}\rho \mathbf{U} = \rho \frac{\partial}{\partial t}\mathbf{U} + \mathbf{U}\frac{\partial}{\partial t}\rho \ , \tag{2.29}$$

and the convection term can be rewritten using equation (1.23). It follows:

$$\nabla \bullet (\rho \mathbf{U} \otimes \mathbf{U}) = \underbrace{\rho \mathbf{U} \bullet \underbrace{\nabla \otimes \mathbf{U}}_{\text{gradient}}}_{\text{inner product}} + \mathbf{U} \underbrace{\nabla \bullet (\rho \mathbf{U})}_{\text{divergence}} \ . \tag{2.30}$$

Replacing these terms into equation (2.26) and put the convection terms to the LHS, we end up with:

$$\rho \frac{\partial}{\partial t}\mathbf{U} + \mathbf{U}\frac{\partial}{\partial t}\rho + \rho \mathbf{U} \bullet \nabla \otimes \mathbf{U} + \mathbf{U}\nabla \bullet (\rho \mathbf{U}) = \dots \tag{2.31}$$

After analyzing the equation, we see that we can take out ρ and $\mathbf{U}$:

$$\rho \left[\frac{\partial}{\partial t}\mathbf{U} + \mathbf{U} \bullet \nabla \otimes \mathbf{U}\right] + \mathbf{U} \underbrace{\cancel{\left[\frac{\partial}{\partial t}\rho + \nabla \bullet (\rho \mathbf{U})\right]}}_{\text{continuity}} = \dots \tag{2.32}$$

It is clear that the second term is zero due to the continuity equation. Applying the definition of the total derivative (1.25), we can write the non-conservative form of the momentum equation as:

$$\rho \frac{\mathrm{D}\mathbf{U}}{\mathrm{D}t} = -\nabla \bullet \boldsymbol{\tau} - \nabla p + \rho \mathbf{g} \tag{2.33}$$

Remark: As already mentioned before, the negative sign of the first term on the RHS will vanish after we introduced the definition of the shear-rate components τ_{ii}.

2.3 The Conserved Total Energy Equation

This section will show the derivation of the total energy equation. The total energy includes the internal (thermal) and kinetic (mechanical) energy. In general, the change of the total energy can be described in an arbitrary volume element dV by:

$$\begin{aligned} &\begin{bmatrix} \text{rate of internal} \\ \text{and kinetic} \\ \text{energy accumulation} \end{bmatrix} = \begin{bmatrix} \text{rate of internal} \\ \text{and kinetic energy} \\ \text{entering the volume} \end{bmatrix} - \begin{bmatrix} \text{rate of internal} \\ \text{and kinetic energy} \\ \text{leaving the volume} \end{bmatrix} \\ &+ \begin{bmatrix} \text{net rate of} \\ \text{heat addition by} \\ \text{conduction} \end{bmatrix} - \begin{bmatrix} \text{net rate of} \\ \text{work done by} \\ \text{system on surroundings} \end{bmatrix} + \begin{bmatrix} \text{net rate of} \\ \text{additional} \\ \text{heat sources} \end{bmatrix}. \end{aligned} \tag{2.34}$$

This is the first law of thermodynamics written for an open and unsteady state system with the extension of additional heat sources which was also stated by Bird et al. [1960]. The statement is not complete because no transport of energy can be done due to nuclear, radiative and electromagnetic phenomena but as we already mentioned, we assume that energy can not be transfered into mass and vice versa.

In the equation above, internal, kinetic and work energy are included and therefore unsteady behavior is allowed. The kinetic energy (`by unit volume`) is given by $\frac{1}{2}\rho|\mathbf{U}|^2$ where $|\mathbf{U}|$ denotes the magnitude of the local velocity. The internal energy e (`by unit volume`) can be interpreted as the energy associated with the random translation and internal motion of molecules plus the energy of interaction between them. Therefore, the internal energy is temperature and density depended.

The Accumulation of Total Energy during Time

Now we write the above equation explicit for a finite volume element dV. The accumulation in time is clear (like in the other equations before):

$$\Delta x \Delta y \Delta z \frac{\partial}{\partial t}(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2) \ . \tag{2.35}$$

The Convection of Total Energy

To get the net rate of total energy – that enters and leaves the volume element based on the convection phenomenon –, we simply have to multiply the internal and kinetic energy by the velocity respectively to the face it acts on (compare figure 2.1):

$$\begin{aligned}
&\Delta y \Delta z \left[u_x(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_x - u_x(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_{x+\Delta x} \right] \\
&+\Delta x \Delta z \left[u_y(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_y - u_y(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_{y+\Delta y} \right] \\
&+\Delta x \Delta y \left[u_z(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_z - u_z(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_{z+\Delta z} \right] \ .
\end{aligned} \tag{2.36}$$

If we take out the density, we clearly see the mass flux; e.g. $\Delta y \Delta z u_x \rho$.

The Change of Total Energy due to Conduction

The next term that influences the energy is based on the conduction phenomenon. For this we introduce the heat flux vector $\mathbf{q}$, that is used later on:

$$\begin{aligned}
&\Delta y \Delta z \left[q_x|_x - q_x|_{x+\Delta x} \right] \\
&+\Delta x \Delta z \left[q_y|_y - q_y|_{y+\Delta y} \right] \\
&+\Delta x \Delta y \left[q_z|_z - q_z|_{z+\Delta z} \right] \ .
\end{aligned} \tag{2.37}$$

The quantities q_x, q_y and q_z are the single components of the heat flux vector $\mathbf{q}$.

The Change of Total Energy due to Work against its Surroundings

The work done by the fluid against its surroundings can be split into two parts:

- The work against the volume forces (like gravity),
- The work against the surface forces (like pressure or viscous forces).

Some recall:

- (Work) = (Force) x (Distance in the direction of the force),

- (rate of doing work) = (Force) x (Velocity in the direction of the force).

Hence, the rate of doing work against the components of the gravitational acceleration can be written as:

$$-\rho\Delta x\Delta y\Delta z\left(u_x g_x + u_y g_y + u_z g_z\right)\ , \tag{2.38}$$

and the rate of doing work against the pressure p (static pressure) at the faces of the volume element is:

$$\begin{aligned}&\Delta y\Delta z\left[-(pu_x)|_x + (pu_x)|_{x+\Delta x}\right]\\ &+\Delta x\Delta z\left[-(pu_y)|_y + (pu_y)|_{y+\Delta y}\right]\\ &+\Delta x\Delta y\left[-(pu_z)|_z + (pu_z)|_{z+\Delta z}\right]\ .\end{aligned} \tag{2.39}$$

In a similar way, the rate of doing work against the viscous forces is:

$$\begin{aligned}&\Delta y\Delta z\left[-(\tau_{xx}u_x + \tau_{xy}u_y + \tau_{xz}u_z)|_x + (\tau_{xx}u_x + \tau_{xy}u_y + \tau_{xz}u_z)|_{x+\Delta x}\right]\\ &+\Delta x\Delta z\left[-(\tau_{yx}u_x + \tau_{yy}u_y + \tau_{yz}u_z)|_y + (\tau_{yx}u_x + \tau_{yy}u_y + \tau_{yz}u_z)|_{y+\Delta y}\right]\\ &+\Delta x\Delta y\left[-(\tau_{zx}u_x + \tau_{zy}u_y + \tau_{zz}u_z)|_z + (\tau_{zx}u_x + \tau_{zy}u_y + \tau_{zz}u_z)|_{z+\Delta z}\right]\ .\end{aligned} \tag{2.40}$$

Additional Heat Source

Additional heat sources or sinks can be taken into account by simply defining a source term:

$$Q_{\mathrm{S}} = \Delta x\Delta y\Delta z\rho\mathrm{S}\ . \tag{2.41}$$

Here Q_{S} denotes the heat source term. The subscript S stands for *Source* or *Sink*.

Now we have all terms and are able to rewrite equation (2.22):

$$
\begin{aligned}
\Delta x \Delta y \Delta z \frac{\partial}{\partial t}(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2) = \Delta y \Delta z &\left[u_x(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_x - u_x(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_{x+\Delta x} \right] \\
&+\Delta x \Delta z \left[u_y(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_y - u_y(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_{y+\Delta y} \right] \\
&+\Delta x \Delta y \left[u_z(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_z - u_z(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2)|_{z+\Delta z} \right] \\
&+\Delta y \Delta z \left[q_x|_x - q_x|_{x+\Delta x} \right] + \Delta x \Delta z \left[q_y|_y - q_y|_{y+\Delta y} \right] \\
&+\Delta x \Delta y \left[q_z|_z - q_z|_{z+\Delta z} \right] \\
&+\rho \Delta x \Delta y \Delta z \left(u_x g_x + u_y g_y + u_z g_z \right) \\
&-\Delta y \Delta z \left[-(p u_x)|_x + (p u_x)|_{x+\Delta x} \right] \\
&-\Delta x \Delta z \left[-(p u_y)|_y + (p u_y)|_{y+\Delta y} \right] \\
&-\Delta x \Delta y \left[-(p u_z)|_z + (p u_z)|_{z+\Delta z} \right] \\
&-\Delta y \Delta z \left[-(\tau_{xx} u_x + \tau_{xy} u_y + \tau_{xz} u_z)|_x + (\tau_{xx} u_x + \tau_{xy} u_y + \tau_{xz} u_z)|_{x+\Delta x} \right] \\
&-\Delta x \Delta z \left[-(\tau_{yx} u_x + \tau_{yy} u_y + \tau_{yz} u_z)|_y + (\tau_{yx} u_x + \tau_{yy} u_y + \tau_{yz} u_z)|_{y+\Delta y} \right] \\
&-\Delta x \Delta y \left[-(\tau_{zx} u_x + \tau_{zy} u_y + \tau_{zz} u_z)|_z + (\tau_{zx} u_x + \tau_{zy} u_y + \tau_{zz} u_z)|_{z+\Delta z} \right] \\
&+\Delta x \Delta y \Delta z \rho \mathrm{S} \ . \qquad (2.42)
\end{aligned}
$$

As before, we divide everything by the volume $\mathrm{d}V$ and use the assumption (2.5). Please keep in mind, that we have derivatives of $(\phi|_x - \phi|_{x+\Delta x})$ that end up with a negative sign and $(\phi|_{x+\Delta x} - \phi|_x)$ that end up with a positive sign. Hence, we get:

$$
\begin{aligned}
&\frac{\partial}{\partial t}(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2) = \\
&-\frac{\partial}{\partial x}\left[u_x(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2) \right] - \frac{\partial}{\partial y}\left[u_y(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2) \right] - \frac{\partial}{\partial z}\left[u_z(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2) \right] \\
&-\frac{\partial}{\partial x}\left[q_x \right] - \frac{\partial}{\partial y}\left[q_y \right] - \frac{\partial}{\partial z}\left[q_z \right] + \rho \left(u_x g_x + u_y g_y + u_z g_z \right) \\
&-\frac{\partial}{\partial x}\left[p u_x \right] - \frac{\partial}{\partial y}\left[p u_y \right] - \frac{\partial}{\partial z}\left[p u_z \right] + \frac{\partial}{\partial x}\left[-(\tau_{xx} u_x + \tau_{xy} u_y + \tau_{xz} u_z) \right] \\
&+\frac{\partial}{\partial y}\left[-(\tau_{yx} u_x + \tau_{yy} u_y + \tau_{yz} u_z) \right] + \frac{\partial}{\partial z}\left[-(\tau_{zx} u_x + \tau_{zy} u_y + \tau_{zz} u_z) \right] \\
&+\rho \mathrm{S} \ . \qquad (2.43)
\end{aligned}
$$

After taking out the minus signs and sort the equation, we get the conserved total energy equation as:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}(\rho e+\frac{1}{2}\rho|\mathbf{U}|^2) = -\Bigg\{\frac{\partial}{\partial x}\left[u_x(\rho e+\frac{1}{2}\rho|\mathbf{U}|^2)\right]+\frac{\partial}{\partial y}\left[u_y(\rho e+\frac{1}{2}\rho|\mathbf{U}|^2)\right]\\ +\frac{\partial}{\partial z}\left[u_z(\rho e+\frac{1}{2}\rho|\mathbf{U}|^2)\right]\Bigg\}-\left\{\frac{\partial}{\partial x}q_x+\frac{\partial}{\partial y}q_y+\frac{\partial}{\partial z}q_z\right\}+\rho\left(u_x g_x+u_y g_y+u_z g_z\right)\\ -\left\{\frac{\partial}{\partial x}pu_x+\frac{\partial}{\partial y}pu_y+\frac{\partial}{\partial z}pu_z\right\}-\Bigg\{\frac{\partial}{\partial x}(\tau_{xx}u_x+\tau_{xy}u_y+\tau_{xz}u_z)\\ +\frac{\partial}{\partial y}(\tau_{yx}u_x+\tau_{yy}u_y+\tau_{yz}u_z)+\frac{\partial}{\partial z}(\tau_{zx}u_x+\tau_{zy}u_y+\tau_{zz}u_z)\Bigg\}+\rho S\end{aligned}} . \tag{2.44}$$

To get a more visible and readable equation, we use the vector notation. The total energy equation then can be written in the following form and the terms can be described more precisely:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}(\rho e+\frac{1}{2}\rho|\mathbf{U}|^2) = &\underbrace{-\nabla\bullet\left(\rho\mathbf{U}(e+\frac{1}{2}|\mathbf{U}|^2)\right)}_{\text{convection}}\quad\underbrace{-\nabla\bullet\mathbf{q}}_{\text{conduction}}\quad\underbrace{+\rho\left(\mathbf{U}\bullet\mathbf{g}\right)}_{\text{gravity}}\\ &\underbrace{-\nabla\bullet(p\mathbf{U})}_{\text{pressure}}\quad\underbrace{-\nabla\bullet[\boldsymbol{\tau}\bullet\mathbf{U}]}_{\text{viscous forces}}\quad\underbrace{+\rho S}_{\text{heat source}}\end{aligned}} . \tag{2.45}$$

All terms on the RHS denote the inner product of two vectors. Hence, for a implementation into a software toolbox we need to use equation (1.11) and (1.12).

Remark: Till now no word is said about the potential energy. This will not be discussed here. If you need information about that, you will find all necessary information in Bird et al. [1960] p. 314. The reason why we do not mention this, is the fact that in most of the engineering cases, the potential energy is not of interest or is in a neglect-able range.

2.3.1 The Proof of the Vector Transformation

The next sites will convert the vector form of the total energy equation back into the Cartesian coordinate system. Hence, equation (2.45) will be used and transformed into (2.44). This is done step by step but not for each term. The terms of interest are the *gravity* and *viscous force* term. To manipulate the gravity term we need the mathematical law of equation (1.11). For the viscous force term we need equation (1.12) and (1.21).

It follows that the gravity term can be changed as:

$$\rho(\mathbf{U} \bullet \mathbf{g}) = \rho \left[\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} \bullet \begin{pmatrix} g_x \\ g_y \\ g_z \end{pmatrix} \right] \stackrel{!}{=} \rho \left(u_x g_x + u_y g_y + u_z g_z \right) \ . \tag{2.46}$$

The viscous force term can be changed as follows:

$$\begin{aligned} - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] &= -\nabla \bullet \left(\begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} \bullet \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} \right) \\ &= -\nabla \bullet \begin{bmatrix} \tau_{xx} u_x + \tau_{xy} u_y + \tau_{xz} u_z \\ \tau_{yx} u_x + \tau_{yy} u_y + \tau_{yz} u_z \\ \tau_{zx} u_x + \tau_{zy} u_y + \tau_{zz} u_z \end{bmatrix} = - \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \begin{bmatrix} \tau_{xx} u_x + \tau_{xy} u_y + \tau_{xz} u_z \\ \tau_{yx} u_x + \tau_{yy} u_y + \tau_{yz} u_z \\ \tau_{zx} u_x + \tau_{zy} u_y + \tau_{zz} u_z \end{bmatrix} \\ &\stackrel{!}{=} - \left\{ \frac{\partial}{\partial x} \left(\tau_{xx} u_x + \tau_{xy} u_y + \tau_{xz} u_z \right) + \frac{\partial}{\partial y} \left(\tau_{yx} u_x + \tau_{yy} u_y + \tau_{yz} u_z \right) \right. \\ &\qquad \left. + \frac{\partial}{\partial z} \left(\tau_{zx} u_x + \tau_{zy} u_y + \tau_{zz} u_z \right) \right\} \ . \end{aligned} \tag{2.47}$$

As we may already might had the feeling, the terms are equal of both notations. The other terms that are not discussed above are similar to the momentum equation and it is easy to demonstrate that each term of the vector notation represents the corresponding terms in the Cartesian equation. Due to that, we will not demonstrate it here again.

2.3.2 Integral Form of the Conserved Total Energy Equation

To obtain the integral form of the total energy equation (2.54), we use the Gauss theorem. It follows:

$$\boxed{\begin{aligned} \frac{\partial}{\partial t} \int \rho (e + \frac{1}{2} |\mathbf{U}|^2) \mathrm{d}V &= - \oint \rho \mathbf{U} (e + \frac{1}{2} |\mathbf{U}|^2) \cdot \mathbf{n} \mathrm{d}S - \oint \mathbf{q} \cdot \mathbf{n} \mathrm{d}S \\ &+ \int \rho \mathbf{U} \bullet \mathbf{g} \mathrm{d}V - \oint p \mathbf{U} \cdot \mathbf{n} \mathrm{d}S - \oint (\boldsymbol{\tau} \bullet \mathbf{U}) \cdot \mathbf{n} \mathrm{d}S + \int \rho S \mathrm{d}V \end{aligned}} \ . \tag{2.48}$$

2.3.3 Non-Conserved Total Energy Equation

As before, the mass conservation equation can be used to manipulate the conserved total energy equation. The transformation lead to the non-conservative form. For that, we first need to break the time and convective term of equation (2.45) by using the product rule. Hence, the time derivative can be rewritten as:

$$\frac{\partial}{\partial t}(\rho e+\frac{1}{2}\rho|\mathbf{U}|^2) = \frac{\partial}{\partial t}\left[\rho(e+\frac{1}{2}|\mathbf{U}|^2)\right] = \rho\frac{\partial}{\partial t}(e+\frac{1}{2}|\mathbf{U}|^2)+(e+\frac{1}{2}|\mathbf{U}|^2)\frac{\partial}{\partial t}\rho\,. \quad (2.49)$$

and the convective term will be transformed to:

$$\nabla\bullet\rho\mathbf{U}(e+\frac{1}{2}|\mathbf{U}|^2) = \underbrace{\rho\mathbf{U}\bullet\underbrace{\nabla(e+\frac{1}{2}|\mathbf{U}|^2)}_{\text{gradient}}}_{\text{inner product}}+(e+\frac{1}{2}|\mathbf{U}|^2)\underbrace{\nabla\bullet(\rho\mathbf{U})}_{\text{divergence}}\,. \quad (2.50)$$

The next step is replacing the above terms into equation (2.45) and put the terms that are related to the convective part to the LHS:

$$\rho\frac{\partial}{\partial t}(e+\frac{1}{2}|\mathbf{U}|^2)+(e+\frac{1}{2}|\mathbf{U}|^2)\frac{\partial}{\partial t}\rho+\rho\mathbf{U}\bullet\nabla(e+\frac{1}{2}|\mathbf{U}|^2)+(e+\frac{1}{2}|\mathbf{U}|^2)\nabla\bullet(\rho\mathbf{U}) = \ldots \quad (2.51)$$

After taking out the density and the term $(e+\frac{1}{2}|\mathbf{U}|^2)$, we get:

$$\rho\left[\frac{\partial}{\partial t}(e+\frac{1}{2}|\mathbf{U}|^2)+\mathbf{U}\bullet\nabla(e+\frac{1}{2}|\mathbf{U}|^2)\right]+(e+\frac{1}{2}|\mathbf{U}|^2)\underbrace{\cancel{\left[\frac{\partial}{\partial t}\rho+\nabla\bullet(\rho\mathbf{U})\right]}}_{\text{continuity}} = \ldots \quad (2.52)$$

We can observe that the second term on the LHS is equal to zero due to the continuity equation. Based on that, we can simplify the equation and end up with:

$$\rho\left[\frac{\partial}{\partial t}(e+\frac{1}{2}|\mathbf{U}|^2)+\mathbf{U}\bullet\nabla(e+\frac{1}{2}|\mathbf{U}|^2)\right] = \ldots \quad (2.53)$$

By using the definition of the total derivative (1.25), we finally are able to rewrite the equation in the non-conservative form:

$$\boxed{\rho\frac{\mathrm{D}}{\mathrm{D}t}(e+\frac{1}{2}|\mathbf{U}|^2) = -\nabla\bullet\mathbf{q}+\rho\mathbf{U}\bullet\mathbf{g}-\nabla\bullet p\mathbf{U}-\nabla\bullet[\boldsymbol{\tau}\bullet\mathbf{U}]+\rho\mathrm{S}}\,. \quad (2.54)$$

2.3.4 Kinetic Energy and Internal Energy

The total energy equation is the sum of the kinetic energy and internal energy. After we have either the kinetic or internal energy equation, we can simply subtract that equation from the total energy equation to get the other one. In your case we will derive the mechanical (kinetic) energy equation first and get the internal energy equation by subtracting the kinetic energy from the total energy equation.

The answer why we derive the mechanical (kinetic) energy equation instead of the internal energy equation is simple. The derivation of the kinetic energy equation can be done simply by multiplying the momentum equation by the velocity again.

2.4 The Conserved Mechanical Energy Equation

As mentioned before, we will derive the mechanical (kinetic) energy equation using the momentum equation. To be consistent with the derivations before, we will split the derivation into two parts. The first part will use the finite volume element $\mathrm{d}V$ to derive the first part of the conserved kinetic energy equation without explaining the meaning of the source terms. After that we use the source terms of the momentum equation to get the source terms for the mechanical (kinetic) energy equation. At that stage it is easier to analyze the meaning of the different terms.

In general we can define the change of kinetic energy in an arbitrary volume element $\mathrm{d}V$ as:

$$\begin{bmatrix}\text{rate of kinetic}\\ \text{energy accumulation}\end{bmatrix} = \begin{bmatrix}\text{rate of kinetic energy}\\ \text{entering the volume}\end{bmatrix} - \begin{bmatrix}\text{rate of kinetic energy}\\ \text{leaving the volume}\end{bmatrix} + \begin{bmatrix}\text{sum of additional}\\ \text{source terms}\end{bmatrix} \tag{2.55}$$

Using the definition of the kinetic energy `per unit mass` (divided by ρ):

$$e_{\text{kin}} = \frac{1}{2}|\mathbf{U}|^2 \ , \tag{2.56}$$

we can simply derive the accumulation of the kinetic energy as:

$$\Delta x \Delta y \Delta z \frac{\Delta}{\Delta t}\rho e_{\text{kin}} = \Delta x \Delta y \Delta z \frac{\Delta}{\Delta t}\rho \frac{1}{2}|\mathbf{U}|^2 \ . \tag{2.57}$$

The Convection of Kinetic Energy

The kinetic energy that enters or leaves the volume element is transported due to fluxes and can be derived analogous to the convective transport of the total energy or momentum:

$$
\begin{aligned}
\text{into face } |_x : &\quad (\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_x \ , \\
\text{out of face } |_{x+\Delta x} : &\quad (\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_{x+\Delta x} \ , \\
\text{into face } |_y : &\quad (\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_y \ , \\
\text{out of face } |_{y+\Delta y} : &\quad (\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_{y+\Delta y} \ , \\
\text{into face } |_z : &\quad (\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_z \ , \\
\text{out of face } |_{z+\Delta z} : &\quad (\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_{z+\Delta z} \ .
\end{aligned}
$$

With the expressions above, it is possible to rewrite the transport of the kinetic energy due to convection as:

$$
\begin{aligned}
&\left((\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_x - (\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_{x+\Delta x}\right)\Delta y \Delta z \\
+&\left((\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_y - (\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_{y+\Delta y}\right)\Delta x \Delta z \\
+&\left((\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_z - (\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_{z+\Delta z}\right)\Delta x \Delta y \ .
\end{aligned}
$$

Defining the sum of additional source terms that act on the volume by the quantity e_S and put the new evaluated terms into equation (2.55), we get:

$$
\begin{aligned}
\Delta x \Delta y \Delta z \frac{\partial}{\partial t}\rho\frac{1}{2}|\mathbf{U}|^2 = &\left((\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_x - (\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_{x+\Delta x}\right)\Delta y \Delta z \\
+&\left((\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_y - (\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_{y+\Delta y}\right)\Delta x \Delta z \\
+&\left((\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_z - (\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_{z+\Delta z}\right)\Delta x \Delta y \\
+&e_\mathrm{S}\Delta x \Delta y \Delta z \ .
\end{aligned} \tag{2.58}
$$

To get to a partial differential equation, we will divide the whole equation by the volume of the element $\mathrm{d}V$. Thus, we get:

$$\begin{aligned}\frac{\partial}{\partial t}\rho\frac{1}{2}|\mathbf{U}|^2 =& \frac{(\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_x - (\rho u_x)\frac{1}{2}|\mathbf{U}|^2|_{x+\Delta x}}{\Delta x} \\ &+ \frac{(\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_y - (\rho u_y)\frac{1}{2}|\mathbf{U}|^2|_{y+\Delta y}}{\Delta y} \\ &+ \frac{(\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_z - (\rho u_z)\frac{1}{2}|\mathbf{U}|^2|_{z+\Delta z}}{\Delta z} + e_{\mathrm{S}}\ . \end{aligned} \tag{2.59}$$

The next step is to use the assumption of equation (2.5) and (2.6). Therefore, we get the first part of the kinetic energy equation without any explicit mentioned source term:

$$\boxed{\frac{\partial}{\partial t}\rho\frac{1}{2}|\mathbf{U}|^2 = -\frac{\partial}{\partial x}(\rho u_x\frac{1}{2}|\mathbf{U}|^2) - \frac{\partial}{\partial y}(\rho u_y\frac{1}{2}|\mathbf{U}|^2) - \frac{\partial}{\partial z}(\rho u_z\frac{1}{2}|\mathbf{U}|^2) + e_{\mathrm{S}}}\ . \tag{2.60}$$

The vector notation for this equation is:

$$\boxed{\frac{\partial}{\partial t}\frac{1}{2}|\mathbf{U}|^2 = -\nabla \bullet (\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2) + e_{\mathrm{S}}}\ . \tag{2.61}$$

Equation (2.61) can also be derived using the momentum equation and forming the scalar product of the local velocity and equation (2.26).

Source Terms of the Kinetic Energy

The kinetic energy can be changed by several phenomena. These sources (terms) act on the volume element. To get the different source terms we will use the momentum equation (2.26). The terms e_{S} are simply the source terms in the momentum equation (2.26) multiplied by the velocity.

Recall: The source terms of the equation of motion are:

- Pressure (surface) ,
- Shear-rate (surface) ,
- Gravity (volume) .

Using this information, we can replace the quantity e_S by:

$$e_S = -(\nabla \bullet \boldsymbol{\tau}) \bullet \mathbf{U} - (\nabla p) \bullet \mathbf{U} + \underbrace{(\rho \mathbf{g}) \bullet \mathbf{U}}_{\text{work done by gravity}} \quad . \tag{2.62}$$

Note: The multiplication with the velocity results in the inner product.

If we insert the source term e_S into equation (2.61), we get the conserved mechanical (kinetic) energy equation with the source terms.

$$\boxed{\frac{\partial}{\partial t}\frac{1}{2}|\mathbf{U}|^2 = -\nabla \bullet (\rho \mathbf{U}\frac{1}{2}|\mathbf{U}|^2) - (\nabla \bullet \boldsymbol{\tau}) \bullet \mathbf{U} - (\nabla p) \bullet \mathbf{U} + (\rho \mathbf{g}) \bullet \mathbf{U}} \quad . \tag{2.63}$$

Analyzing the new equation, we already know the meaning of the term on the LHS and the the first and last term on the RHS. Thinking about the second and third term on the RHS is not so clear till now. Therefore, we will replace these terms by manipulating both by applying the product rule. The term that denotes the viscous force, can be rewritten as:

$$\nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] = \underbrace{\boldsymbol{\tau} \boldsymbol{:} \underbrace{(\nabla \otimes \mathbf{U})}_{\text{gradient}}}_{\text{double inner product}} + \underbrace{\mathbf{U} \bullet \underbrace{(\nabla \bullet \boldsymbol{\tau})}_{\text{divergence}}}_{\text{inner product}} \quad . \tag{2.64}$$

The pressure term can be manipulated like:

$$\nabla \bullet (p\mathbf{U}) = \underbrace{\mathbf{U} \bullet \underbrace{\nabla p}_{\text{gradient}}}_{\text{inner product}} + p \underbrace{\nabla \bullet \mathbf{U}}_{\text{divergence}} \quad . \tag{2.65}$$

Now we rearrange these equations:

$$\mathbf{U} \bullet (\nabla \bullet \boldsymbol{\tau}) = \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] - \boldsymbol{\tau} \boldsymbol{:} (\nabla \otimes \mathbf{U}) \ , \tag{2.66}$$

$$\mathbf{U} \bullet \nabla p = \nabla \bullet (p\mathbf{U}) - p \nabla \bullet \mathbf{U} \ , \tag{2.67}$$

and insert both into equation (2.62). The resulting equation gives us the possibility to get a better physical base for the meaning of the single terms. Hence, we get for the source terms the following expression:

$$\boxed{\begin{aligned} e_S = & \underbrace{-\nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}]}_{\substack{\text{work done} \\ \text{by viscous force}}} - \underbrace{(-\boldsymbol{\tau} : (\nabla \otimes \mathbf{U}))}_{\substack{\text{irreversibe conversion} \\ \text{to internal energy} \\ \text{(shear-heating)}}} \quad \underbrace{-\nabla \bullet (p\mathbf{U})}_{\substack{\text{work done by} \\ \text{pressure of sourroundings}}} \\ & - \underbrace{p(-\nabla \bullet \mathbf{U})}_{\substack{\text{reversible conversion} \\ \text{to internal energy}}} + \underbrace{(\rho \mathbf{g}) \bullet \mathbf{U}}_{\substack{\text{work done} \\ \text{by gravity}}} \end{aligned}} . \tag{2.68}$$

Finally, we use the new evaluated sources e_S to get a more understandable and readable kinetic energy equation:

$$\boxed{\begin{aligned} \frac{\partial}{\partial t} \frac{1}{2} \rho |\mathbf{U}|^2 = -\nabla \bullet (\rho \mathbf{U} \frac{1}{2} |\mathbf{U}|^2) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] - (-\boldsymbol{\tau} : (\nabla \otimes \mathbf{U})) \\ -\nabla \bullet (p\mathbf{U}) - p(-\nabla \bullet \mathbf{U}) + (\rho \mathbf{g}) \bullet \mathbf{U} \end{aligned}} . \tag{2.69}$$

The Meaning of Some Terms

- $(-\boldsymbol{\tau} : \nabla \mathbf{U})$: as stated by Bird et al. [1960], this term is always positive for Newtonian fluids and describes that motion energy is irreversibly exchanged into thermal energy and therefore no real processes are reversible. This term will heat up the fluid internally. The heating due to this term will only be measurable if the speed of the fluid is very high (large velocity gradients); e.g. high-speed flight or rapid extrusion.

- $p(-\nabla \bullet \mathbf{U})$: this term will cool or heat the fluid internally due to sudden expansion or compression phenomena; e.g. turbines or shock-tubes.

2.4.1 Integral Form of the Conserved Mechanical Energy Equation

The integral form of the kinetic energy equation (2.69) can be achieved by using the Gauss theorem (1.32) as before. Hence, we get:

$$\boxed{\begin{aligned} & \frac{\partial}{\partial t} \int \frac{1}{2} \rho |\mathbf{U}|^2 \mathrm{d}V = - \oint \rho \mathbf{U} \frac{1}{2} |\mathbf{U}|^2 \cdot \mathbf{n} \mathrm{d}S - \oint [\boldsymbol{\tau} \bullet \mathbf{U}] \cdot \mathbf{n} \mathrm{d}S \\ & - \int (-\boldsymbol{\tau} : (\nabla \otimes \mathbf{U})) \mathrm{d}V - \oint p\mathbf{U} \cdot \mathbf{n} \mathrm{d}S - \int p(-\nabla \bullet \mathbf{U}) \mathrm{d}V + \int (\rho \mathbf{g}) \bullet \mathbf{U} \mathrm{d}V \end{aligned}} . \tag{2.70}$$

2.4.2 Non-Conserved Mechanical Energy Equation

As before, we are able to use the continuity equation, to change the conserved kinetic energy equation into the non-conservative form. Therefore, we have to split the time derivative and convection term using the product rule again. In addition we have to put the convective term to the LHS of equation (2.69). Thus, the time derivative will change to:

$$\frac{\partial}{\partial t}\rho\frac{1}{2}|\mathbf{U}|^2 = \rho\frac{\partial}{\partial t}\frac{1}{2}|\mathbf{U}|^2 + \frac{1}{2}|\mathbf{U}|^2\frac{\partial}{\partial t}\rho \ , \tag{2.71}$$

and the convection term to:

$$\nabla \bullet \left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right) = \rho\mathbf{U} \bullet \nabla\frac{1}{2}|\mathbf{U}|^2 + \frac{1}{2}|\mathbf{U}|^2\nabla \bullet (\rho\mathbf{U}) \ . \tag{2.72}$$

We end up with:

$$\rho\frac{\partial}{\partial t}\frac{1}{2}|\mathbf{U}|^2 + \frac{1}{2}|\mathbf{U}|^2\frac{\partial}{\partial t}\rho + \rho\mathbf{U} \bullet \nabla\frac{1}{2}|\mathbf{U}|^2 + \frac{1}{2}|\mathbf{U}|^2\nabla \bullet (\rho\mathbf{U}) = \dots \tag{2.73}$$

After we exclude ρ and $\frac{1}{2}|\mathbf{U}|^2$ from the equations, we get:

$$\rho\left[\frac{\partial}{\partial t}\frac{1}{2}|\mathbf{U}|^2 + \mathbf{U} \bullet \nabla\frac{1}{2}|\mathbf{U}|^2\right] + \frac{1}{2}|\mathbf{U}|^2\underbrace{\cancel{\left[\frac{\partial}{\partial t}\rho + \nabla \bullet (\rho\mathbf{U})\right]}}_{\text{continuity}} = \dots \tag{2.74}$$

As we can see, the second term on the LHS is zero due to continuity and therefore we get the non-conserved kinetic energy equation by using the definition of the total derivative (1.25):

$$\boxed{\rho\frac{\mathrm{D}\frac{1}{2}|\mathbf{U}|^2}{\mathrm{D}t} = -\nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] - (-\boldsymbol{\tau} : (\nabla \otimes \mathbf{U})) - \nabla \bullet (p\mathbf{U}) - p(-\nabla \bullet \mathbf{U}) + (\rho\mathbf{g}) \bullet \mathbf{U}} \ . \tag{2.75}$$

Remark: It should be obvious that we can use equation (2.64) and (2.65) to change/eliminate some terms again.

2.5 The Conserved Thermo Energy Equation

After we have the total energy and the kinetic energy equation, we can simply get the equation for the thermo (internal) energy equation by subtracting equation (2.69) from (2.45). To get the internal energy equation, we will split the time and convection term of equation (2.45) first. This is done to separate the single quantities. Hence, we get:

$$\frac{\partial}{\partial t}\left(\rho e + \frac{1}{2}\rho|\mathbf{U}|^2\right) = -\nabla \bullet \left(\rho\mathbf{U}(e + \frac{1}{2}|\mathbf{U}|^2)\right) + \ldots \tag{2.76}$$

$$\frac{\partial}{\partial t}(\rho e) + \underline{\frac{\partial}{\partial t}\left(\frac{1}{2}\rho|\mathbf{U}|^2\right)} = -\nabla \bullet (\rho\mathbf{U}e) - \nabla \bullet \left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right) + \ldots \tag{2.77}$$

The next step is to replace the underlined term by the conserved kinetic energy equation (2.69).

$$\begin{aligned}
&\frac{\partial}{\partial t}(\rho e) - \nabla \bullet \left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] - (-\boldsymbol{\tau} \colon (\nabla \otimes \mathbf{U})) - \nabla \bullet (p\mathbf{U}) \\
&- p(-\nabla \bullet \mathbf{U}) + (\rho\mathbf{g}) \bullet \mathbf{U} = -\nabla \bullet (\rho\mathbf{U}e) - \nabla \bullet \left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right) \\
&- \nabla \bullet \mathbf{q} + \rho\mathbf{U} \bullet \mathbf{g} - \nabla \bullet p\mathbf{U} - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] + \rho \mathrm{S}\ .
\end{aligned} \tag{2.78}$$

We can see that the second, third, fifth and seventh term on the LHS cancel with the second, fourth, fifth and sixth term on the RHS. Note that $\rho\mathbf{U} \bullet \mathbf{g} = (\rho\mathbf{g}) \bullet \mathbf{U}$. Hence, we get the following equation for the kinetic (internal) energy equation:

$$\frac{\partial}{\partial t}(\rho e) - (-\boldsymbol{\tau} \colon (\nabla \otimes \mathbf{U})) - p(-\nabla \bullet \mathbf{U}) = -\nabla \bullet (\rho\mathbf{U}e) - \nabla \bullet \mathbf{q} + \rho \mathrm{S}\ . \tag{2.79}$$

After sorting the equation we get the final form:

$$\boxed{\frac{\partial}{\partial t}(\rho e) = \underbrace{-\nabla \bullet (\rho\mathbf{U}e)}_{\substack{\text{transport by}\\ \text{convection}}} \quad \underbrace{-(\boldsymbol{\tau} \colon (\nabla \otimes \mathbf{U}))}_{\substack{\text{irreversible}\\ \text{energy by}\\ \text{viscous dissipation}\\ \text{shear-heating}}} \quad \underbrace{-p(\nabla \bullet \mathbf{U})}_{\substack{\text{reversible}\\ \text{energy by}\\ \text{compression}}} \quad \underbrace{-\nabla \bullet \mathbf{q}}_{\substack{\text{energy input}\\ \text{by conduction}}} \quad \underbrace{+\rho \mathrm{S}}_{\text{heat source}}}\ . \tag{2.80}$$

2.5.1 Integral Form of the Thermo Energy Equation

The integral form of the internal energy equation (2.80) is observed using the Gauss theorem (1.32):

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\int \rho e \mathrm{d}V = -\oint \rho \mathbf{U} e \cdot \mathbf{n} \mathrm{d}S - \int (\boldsymbol{\tau} \boldsymbol{:} (\nabla \otimes \mathbf{U}))\mathrm{d}V \\ - \int p(\nabla \bullet \mathbf{U})\mathrm{d}V - \oint \mathbf{q} \cdot \mathbf{n}\mathrm{d}S + \int \rho \mathrm{S} \mathrm{d}V\end{aligned}} \ . \tag{2.81}$$

2.5.2 Non-Conserved Thermo (Internal) Energy Equation

As before, we can rewrite the conserved internal energy equation into a non-conserved form using the continuity equation. For that we split the time and convective terms again. As before, the terms look always similar. The time derivative will be manipulated to:

$$\frac{\partial}{\partial t}(\rho e) = \rho \frac{\partial e}{\partial t} + e \frac{\partial \rho}{\partial t} \ , \tag{2.82}$$

and the convective term to:

$$\nabla \bullet (\rho \mathbf{U} e) = \rho \mathbf{U} \bullet \nabla e + e \nabla \bullet (\rho \mathbf{U}) \ . \tag{2.83}$$

After inserting the two terms into equation (2.80), we get:

$$\rho \frac{\partial e}{\partial t} + e \frac{\partial \rho}{\partial t} + \rho \mathbf{U} \bullet \nabla e + e \nabla \bullet (\rho \mathbf{U}) = \dots \tag{2.84}$$

Now we extract ρ and e:

$$\underbrace{\rho \left[\frac{\partial e}{\partial t} + \mathbf{U} \bullet \nabla e\right]}_{\text{total derivative}} + \underbrace{e \left[\cancel{\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{U})}\right]}_{\text{continuity}} = \dots \tag{2.85}$$

Due to the continuity equation, we can cancel out the second term and write the non-conserved internal energy equation as:

$$\boxed{\rho \frac{\mathrm{D}e}{\mathrm{D}t} = -(\boldsymbol{\tau} \boldsymbol{:} (\nabla \otimes \mathbf{U})) - p(\nabla \bullet \mathbf{U}) - \nabla \bullet \mathbf{q} + \rho \mathrm{S}} \ . \tag{2.86}$$

2.6 The Conserved Enthalpy Equation

The next equation that we are going to derive is the conserved enthalpy equation. For that we will use the total energy equation (2.45) and the definition of the enthalpy h, that is simply the sum of the internal energy plus the kinematic pressure:

$$h = e + \frac{p}{\rho} \ . \tag{2.87}$$

If we replace e in equation (2.45) with the new expression, we get:

$$\begin{aligned}\frac{\partial}{\partial t}\left\{\rho\left[h-\frac{p}{\rho}\right]+\frac{1}{2}\rho|\mathbf{U}|^2\right\} = &-\nabla\bullet\left(\rho\mathbf{U}\left\{\left[h-\frac{p}{\rho}\right]+\frac{1}{2}|\mathbf{U}|^2\right\}\right)-\nabla\bullet\mathbf{q}+\rho\left(\mathbf{U}\bullet\mathbf{g}\right)\\ &-\nabla\bullet\left(p\mathbf{U}\right)-\nabla\bullet\left[\boldsymbol{\tau}\bullet\mathbf{U}\right]+\rho\mathrm{S}\ .\end{aligned}\tag{2.88}$$

For further simplification, we split the time and convective term:

$$\begin{aligned}\frac{\partial}{\partial t}\rho h-\frac{\partial}{\partial t}\rho\frac{p}{\rho}+\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2 = &-\nabla\bullet\left(\rho\mathbf{U}h\right)\underline{+\nabla\bullet\left(\rho\mathbf{U}\frac{p}{\rho}\right)}-\nabla\bullet\left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right)-\nabla\bullet\mathbf{q}\\ &+\rho\left(\mathbf{U}\bullet\mathbf{g}\right)\underline{-\nabla\bullet\left(p\mathbf{U}\right)}-\nabla\bullet\left[\boldsymbol{\tau}\bullet\mathbf{U}\right]+\rho\mathrm{S}\ .\end{aligned}\tag{2.89}$$

The terms that are underlined are equal and cancel out as well as the density in the second term of the LHS. Thus, we get the conserved enthalpy equation as:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\rho h-\frac{\partial}{\partial t}p+\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2 = -\nabla\bullet\left(\rho\mathbf{U}h\right)-\nabla\bullet\left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right)-\nabla\bullet\mathbf{q}\\ +\rho\left(\mathbf{U}\bullet\mathbf{g}\right)-\nabla\bullet\left[\boldsymbol{\tau}\bullet\mathbf{U}\right]+\rho\mathrm{S}\end{aligned}}\ . \tag{2.90}$$

2.6.1 Integral Form of the Conserved Enthalpy Equation

The integral form of the conserved enthalpy equation (mechanical energy included) is constructed by using the Gauss theorem. Hence, equation (2.90) can be rewritten like:

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\int\rho h\mathrm{d}V-\frac{\partial}{\partial t}\int p\mathrm{d}V+\int\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2\mathrm{d}V = -\oint\left(\rho\mathbf{U}h\right)\cdot\mathbf{n}\mathrm{d}S+\int\rho\left(\mathbf{U}\bullet\mathbf{g}\right)\mathrm{d}V\\ &-\oint\left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right)\cdot\mathbf{n}\mathrm{d}S-\oint\mathbf{q}\cdot\mathbf{n}\mathrm{d}S-\oint\left[\boldsymbol{\tau}\bullet\mathbf{U}\right]\cdot\mathbf{n}\mathrm{d}S+\int\rho\mathrm{S}\mathrm{d}V\end{aligned}}\ . \tag{2.91}$$

2.6.2 Non-conserved Enthalpy Equation

As for each conserved equation, it is possible to change equation (2.90) to a non-conservative form by using the continuity equation. To manipulate the conserved equation, we first have to split the time and convection terms of the enthalpy equation. Hence, the time derivation can be re-ordered as:

$$\frac{\partial}{\partial t}\rho h = \rho\frac{\partial}{\partial t}h + h\frac{\partial}{\partial t}\rho \; . \tag{2.92}$$

The convection term will be manipulated to:

$$\nabla \bullet (\rho \mathbf{U} h) = \rho \mathbf{U} \bullet \nabla h + h \nabla \bullet (\rho \mathbf{U}) \; . \tag{2.93}$$

Finally, we replace the split term in equation (2.90) and move the convective term to the LHS. The result is:

$$\rho\frac{\partial}{\partial t}h + h\frac{\partial}{\partial t}\rho - \frac{\partial}{\partial t}p + \frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2 + \rho\mathbf{U}\bullet\nabla h + h\nabla\bullet(\rho\mathbf{U}) = \dots \tag{2.94}$$

By taking out the density ρ and enthalpy h of the terms of interest:

$$\rho\left[\frac{\partial}{\partial t}h + \rho\mathbf{U}\bullet\nabla h +\right] + h\underbrace{\cancel{\left[\frac{\partial}{\partial t}\rho + \nabla\bullet(\rho\mathbf{U})\right]}}_{\text{continuity}} + \frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2 - \frac{\partial}{\partial t}p = \dots \tag{2.95}$$

and sort the equation, we get the non-conserved enthalpy equation:

$$\boxed{\begin{aligned}\rho\frac{\mathrm{D}h}{\mathrm{D}t} = -\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2 + \frac{\partial}{\partial t}p - \nabla\bullet\left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right) - \nabla\bullet\mathbf{q} + \rho\left(\mathbf{U}\bullet\mathbf{g}\right)\\ -\nabla\bullet[\boldsymbol{\tau}\bullet\mathbf{U}] + \rho\mathrm{S}\end{aligned}} \; . \tag{2.96}$$

2.6.3 The Conserved Enthalpy Equation (only Thermo)

In many literatures we find another enthalpy equation. The difference is, that the mechanical energy is removed and we only have the thermo energy included. Therefore, we need to subtract equation (2.90) with (2.69) and use (2.65):

$$\left\{\frac{\partial}{\partial t}\rho h - \frac{\partial}{\partial t}p + \frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2\right\} - \left\{\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2\right\} = \dots$$

≫*continues on next site*

$$\ldots \left\{ -\nabla \bullet (\rho \mathbf{U} h) - \nabla \bullet \left(\rho \mathbf{U} \frac{1}{2} |\mathbf{U}|^2 \right) - \nabla \bullet \mathbf{q} + \rho (\mathbf{U} \bullet \mathbf{g}) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] + \rho \mathrm{S} \right\}$$

$$- \Big\{ -\nabla \bullet (\rho \mathbf{U} \frac{1}{2} |\mathbf{U}|^2) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] - (-\boldsymbol{\tau} \colon (\nabla \otimes \mathbf{U})) \\ -\nabla \bullet (p\mathbf{U}) - p(-\nabla \bullet \mathbf{U}) + (\rho \mathbf{g}) \bullet \mathbf{U} \} \ . \qquad (2.97)$$

The outcome of the subtraction is, that a lot of terms can be canceled out. Furthermore, the 10th and 11th term on the RHS can be combined using the product rule. Thus, we are allowed to rewrite this term as $-\mathbf{U} \bullet \nabla p$. The equation we get is very common and can be found in many literatures.

$$\boxed{\frac{\partial}{\partial t} \rho h - \frac{\partial}{\partial t} p = -\nabla \bullet (\rho \mathbf{U} h) - \nabla \bullet \mathbf{q} + \rho \mathrm{S} + (-\boldsymbol{\tau} \colon (\nabla \otimes \mathbf{U})) + \mathbf{U} \bullet \nabla p} \ . \qquad (2.98)$$

Furthermore, it is possible to modify this equation by putting the second term of the LHS to the RHS:

$$\frac{\partial}{\partial t} \rho h = -\nabla \bullet (\rho \mathbf{U} h) - \nabla \bullet \mathbf{q} + \rho \mathrm{S} + (-\boldsymbol{\tau} \colon (\nabla \otimes \mathbf{U})) + \underbrace{\frac{\partial}{\partial t} p + \mathbf{U} \bullet \nabla p}_{\text{Total derivative}} \ . \qquad (2.99)$$

This lead to the the total derivative on the RHS for the pressure and we can apply the rule given by equation (1.25). The modified equation is then given by:

$$\boxed{\frac{\partial}{\partial t} \rho h = -\nabla \bullet (\rho \mathbf{U} h) - \nabla \bullet \mathbf{q} + \rho \mathrm{S} + (-\boldsymbol{\tau} \colon (\nabla \otimes \mathbf{U})) + \frac{\mathrm{D}p}{\mathrm{D}t}} \ . \qquad (2.100)$$

Note: The equation above can be found in the following literatures Bird et al. [1960], Ferziger and Perić [2008], Schwarze [2013]. Keep in mind that we still did not introduce the definition of the shear-rate tensor $\boldsymbol{\tau}$. Therefore, we have a negative sign in front of $\boldsymbol{\tau}$.

Chapter 3

The Governing Equations for Engineers

Normally, it is sufficient enough (for engineers) to know the general conservation equation for an arbitrary quantity ϕ. Once the meaning of this equation is understood, we are able to – *probably* – derive any kind of equation. The general (governing) conservation equation of any quantity ϕ is given by:

$$\underbrace{\frac{\partial}{\partial t}\rho\phi}_{\text{time accumulation}} = - \underbrace{\nabla \bullet (\rho \mathbf{U} \phi)}_{\text{convective transport}} + \underbrace{\nabla \bullet (D \nabla \phi)}_{\text{diffusive transport}} + \underbrace{S_\phi}_{\text{source terms}} \, . \tag{3.1}$$

In the equation above, D stands for the diffusion coefficient, that can be a scalar or a vector and S_ϕ stands for any kind of sources or sinks that influence the quantity ϕ. Now we are able to simply derive the mass, momentum and other conservative equations out of this by replacing the quantity ϕ by the quantity of interest.

3.1 The Continuity Equation

To derive the mass conservation equation, we have to replace ϕ by 1. Furthermore, we have to know that the mass is not transfered by diffusion and we suggest that the mass is not transfered into energy or vice verse; no source terms. Thus, we get the continuity equation (2.12):

$$\frac{\partial}{\partial t}\rho = -\nabla \bullet (\rho \mathbf{U}) \, . \tag{3.2}$$

Of course, if we have an incompressible fluid we get equation (2.13).

3.2 The Momentum Equation

To get the momentum equation we replace ϕ by $\mathbf{U}$. In addition, we need to know the diffusion term and all other source terms that influence the momentum in the volume element. The diffusion term determines the transport of momentum due to molecular effects ($\boldsymbol{\tau}$). The source terms are: gravitational acceleration and the pressure force. Later on, we see a more general form of these equation.

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \boldsymbol{\tau} - \nabla p + \rho\mathbf{g} \tag{3.3}$$

Note: As we see, the shear-rate tensor $\boldsymbol{\tau}$ has a positive sign in this equation. In each equation before we had a negative sign. The sign change will be understood after we introduce the definition of the shear-rate components (all components are negative). In the equation above we already applied the definition of the shear-rate components and hence the sign has to change.

The momentum equation shows, that it is possible to use the governing conservation equation to derive other – more complex – equations. Doing so, we always have to know which source terms are important and how the diffusion term looks like. If we get more familiar with the equations especially with the stress-tensor and the source terms, it is very easy to use this equation and derive the one that is needed.

3.3 The Enthalpy Equation

To derive the enthalpy equation, we have to replace ϕ by h. This will lead to the internal energy equation. The diffusion term ($-\nabla \bullet \mathbf{q}$) can be expressed by the Fourier law $\mathbf{q} = -\lambda\nabla T$. In addition, the energy of a fluid can be changed by other sources like the pressure work, friction, and so on. These terms are given in the chapter before and are neglected now.

$$\frac{\partial}{\partial t}\rho h = -\nabla \bullet (\rho\mathbf{U}h) + \nabla \bullet (\lambda\nabla T) \qquad \underbrace{(+S_h)}_{\text{neglected}} \ . \tag{3.4}$$

It should be mentioned that the enthalpy equation has a special characteristic because is the necessity to know the temperature field T. The enthalpy equation is of interest, if we are solving compressible fluids. That can be also analyzed from the OpenFOAM® toolbox. For incompressible fluids, no temperature or enthalpy equation is used whereas for compressible fluid we solve the enthalpy equation. However we set the temperature field, we recalculate the enthalpy based on the temperature fluid and the fluid properties.

Temperature equation

The temperature equation can be derived using the thermodynamic relation:

$$dh = \int c_{\mathrm{p}} dT \ .$$

Assuming constant heat capacity and incompressibility, we can manipulate the enthalpy equation to get to the temperature equation:

$$c_{\mathrm{p}} \frac{\partial}{\partial t} \rho T = -c_{\mathrm{p}} \nabla \bullet (\rho \mathbf{U} T) + \nabla \bullet (\lambda \nabla T) \qquad \underbrace{(+S_h)}_{\text{neglected}} \ . \tag{3.5}$$

Depending on the field we are working on, we have to take care about the source terms. Example given: if friction, pressure work or the kinetic energy accumulation are really influencing the enthalpy equation, we have to take these phenomena into account. However, as already mentioned above, the temperature equation was derived with the assumptions of incompressibility and constant heat capacity. Therefore, we should be aware if the equation is valid in the case we are trying to solve. Solver crashes in OpenFOAM® are sometimes related to wrong coupled equations. One nice example would be, solving a fluid for incompressible fluids but using a temperature depended density. It can be shown mathematically that this case can cause troubles if the implementation is not done correct.

3.3.1 Common Source Terms

- Shear-heating – viscous dissipation

Shear-heating can be included to the enthalpy equation. Therefore, we have to add the term that describes the shear-heating; compare equation (2.80):

$$S_{\mathrm{sh}} = \boldsymbol{\tau} : (\nabla \otimes \mathbf{U}) \ . \tag{3.6}$$

- Pressure work

Pressure can also increase the enthalpy of a fluid during time. This can be expressed as; compare equation (2.90):

$$S_{\mathrm{pw}} = \frac{\partial p}{\partial t} \ . \tag{3.7}$$

Note: This term can be turned on and off in the enthalpy equation by using the `dpdt` keyword within the *thermophysicalProperties* file in OpenFOAM®. By default it is set to *yes*. The term was introduced in OpenFOAM® version 2.2.0.

- Additional pressure work

There is also an additional pressure work done by the divergence of the pressure and velocity; compare (2.68):

$$S_{\mathrm{apw}} = \nabla \bullet (\mathbf{U}p) \ . \tag{3.8}$$

If we are dealing with incompressible fluids, we are allowed to say that the additional pressure work is only done by the gradient of the pressure ∇p because we can split S_{apw} using the product rule. If follows:

$$S_{\mathrm{apw}} = \nabla \bullet (\mathbf{U}p) = \mathbf{U} \bullet \nabla p + p \underbrace{\nabla \bullet \mathbf{U}}_{\text{continuity}} = \mathbf{U} \bullet \nabla p \ . \tag{3.9}$$

Other source terms can be found in chapter 2 or in the literature that was given at the beginning of this chapter.

Chapter 4

Summary of the Equations

On the next site, all derived equations are given in a summary for a fast look-up. Depending on the problem we are focusing on, special terms can be neglected or has to be taken into account. Thus, we should be familiar with the toolbox and which equation is is solving.

There are more equations that could be included here; for example the equations for solid mechanics (stress calculation) and magneto hydrodynamics (Maxwell-equations). Due to the fact that we did not discuss these special kind of equations, they are not presented here.

Table 4.1: Conserved equations for pure fluids

Continuity	–	$\frac{\partial \rho}{\partial t} = -\nabla \bullet \rho \mathbf{U}$	For incompressible fluids we get $\nabla \bullet \mathbf{U} = 0$
Momentum	Forced Convection	$\frac{\partial}{\partial t} \rho \mathbf{U} = -\nabla \bullet (\rho \mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau} - \nabla p + \rho \mathbf{g}$	For $\boldsymbol{\tau} = 0$ we get the Euler equation
	Free Convection	$\frac{\partial}{\partial t} \rho \mathbf{U} = -\nabla \bullet (\rho \mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau} - \rho \beta \mathbf{g}(T - T_0)$	Approximate; $\nabla p = \bar{\rho} \mathbf{g}$ Bird et al. [1960]
Energy	Total Energy	$\frac{\partial}{\partial t}(\rho e + \frac{1}{2} \rho \lvert\mathbf{U}\rvert^2) = -\nabla \bullet \left(\rho \mathbf{U}(e + \frac{1}{2}\lvert\mathbf{U}\rvert^2)\right) - \nabla \bullet \mathbf{q}$ $+\rho\,(\mathbf{U} \bullet \mathbf{g}) - \nabla \bullet (p \mathbf{U}) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] + \rho \mathrm{S}$	Sum of thermo and mechanic energy
	Kinetic Energy	$\frac{\partial}{\partial t} \frac{1}{2} \rho \lvert\mathbf{U}\rvert^2 = -\nabla \bullet (\rho \mathbf{U} \frac{1}{2} \lvert\mathbf{U}\rvert^2) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] - (-\boldsymbol{\tau} : (\nabla \otimes \mathbf{U}))$ $-\nabla \bullet (p \mathbf{U}) - p(-\nabla \bullet \mathbf{U}) + (\rho \mathbf{g}) \bullet \mathbf{U}$	mechanical energy
	Internal Energy	$\frac{\partial}{\partial t}(\rho e) = -\nabla \bullet (\rho \mathbf{U} e) - (\boldsymbol{\tau} : (\nabla \otimes \mathbf{U})) - p(\nabla \bullet \mathbf{U}) - \nabla \bullet \mathbf{q} + \rho \mathrm{S}$	thermo energy
	Enthalpy	$\frac{\partial}{\partial t} \rho h - \frac{\partial}{\partial t} p = -\nabla \bullet (\rho \mathbf{U} h) - \nabla \bullet \mathbf{q} + (\mathbf{U} \bullet \nabla \mathbf{p}) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] + \rho \mathrm{S}$	$h = e + \frac{p}{\rho}$
	Temperature	$\frac{\partial}{\partial t} \rho c_{\mathrm{v}} T = -\nabla \bullet (\rho \mathbf{U} c_{\mathrm{v}} T) - \nabla \bullet \mathbf{q} - (\boldsymbol{\tau} : \nabla \otimes \mathbf{U}) - T \left(\frac{\partial p}{\partial T}\right)_\rho (\nabla \bullet \mathbf{U}) + \rho T \frac{\mathbf{D} c_{\mathrm{p}}}{\mathbf{D} t}$	in terms of c_{v} Bird et al. [1960]
	Temperature	$\frac{\partial}{\partial t} \rho c_{\mathrm{p}} T = -\nabla \bullet (\rho \mathbf{U} c_{\mathrm{p}} T) - \nabla \bullet \mathbf{q} - (\boldsymbol{\tau} : \nabla \otimes \mathbf{U}) + \left(\frac{\partial \ln V}{\partial \ln T}\right)_\rho \frac{\mathbf{D} p}{\mathbf{D} t} + \rho T \frac{\mathbf{D} c_{\mathrm{p}}}{\mathbf{D} t}$	in terms of c_{p} Bird et al. [1960]

Chapter 5

The Shear-rate Tensor and the Navier-Stokes Equations

The equations that we derived till now allow us to calculate the flow fields numerically. This enables the possibility to get a better insight into the physics and lead to a better understanding about the phenomena in the flow field which can be used to optimize designs or increase the efficiency of a special device. In addition, it is possible to extract quantities that are not measurable in reality – just imagine a liquid metal and measuring the pressure or velocity in a *simple* way. However, if we analyze the equations we figure out that some quantities are not known; for example the shear-rate components τ_{ij}. These unknown quantities have to be expressed by known one.

The shear-rate tensor is expressed by different equations which depend on the behavior of the liquid. Here we distinguish between *Newtonian* and *Non-Newtonian* fluids. In this chapter we introduce the shear-rate tensor $\boldsymbol{\tau}$ for Newtonian fluids. Further notes and information can be found in Ferziger and Perić [2008], Bird et al. [1960], Dantzig and Rappaz [2009].

5.1 Newtonian Fluids

If we investigating into Newtonian fluids, we use the Newtonian law for the shear-rate (viscose stress) tensor $\boldsymbol{\tau}$. It was shown that the nine components can be described as:

$$\tau_{xx} = -2\mu\frac{\partial u_x}{\partial x} + (\frac{2}{3}\mu - \kappa)(\nabla \bullet \mathbf{U}) \ , \tag{5.1}$$

$$\tau_{yy} = -2\mu\frac{\partial u_y}{\partial y} + (\frac{2}{3}\mu - \kappa)(\nabla \bullet \mathbf{U}) \ , \tag{5.2}$$

$$\tau_{zz} = -2\mu\frac{\partial u_z}{\partial z} + (\frac{2}{3}\mu - \kappa)(\nabla \bullet \mathbf{U}) \ , \tag{5.3}$$

$$\tau_{xy} = \tau_{yx} = -\mu\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right) \ , \tag{5.4}$$

$$\tau_{yz} = \tau_{zy} = -\mu\left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}\right) \ , \tag{5.5}$$

$$\tau_{zx} = \tau_{xz} = -\mu\left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}\right) \ . \tag{5.6}$$

The normal stress components have the bulk viscosity κ included. This viscosity is not really important for dense gases and liquids and can be neglected. That is the reason why we can not find this quantity in many literatures. In addition we find the value $\frac{2}{3}\mu$, that describes the secondary viscosity for Newtonian fluids and is related to the dilatation viscosity or first Lames coefficient λ. We will see that the following correlation is valid later on: $\lambda = -\frac{2}{3}\mu$.

If we insert the above mentioned definitions of the shear-rate components into the momentum equations (2.23), (2.24) and (2.25), we will get the momentum equations for Newtonian fluids also known as Navier-Stokes equations.

For the x-component of the Navier-Stokes equation we get:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\rho u_x = &- \left(\frac{\partial}{\partial x}\rho u_x u_x + \frac{\partial}{\partial y}\rho u_y u_x + \frac{\partial}{\partial z}\rho u_z u_x\right) \\ &- \left\{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial u_x}{\partial x} + (\frac{2}{3}\mu - \kappa)(\nabla \bullet \mathbf{U})\right] + \frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right]\right. \\ &\left. + \frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}\right)\right]\right\} \\ &- \frac{\partial p}{\partial x} + \rho g_x\end{aligned}} \ . \tag{5.7}$$

For the y-component of the Navier-Stokes equation we get:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\rho u_y = &-\left(\frac{\partial}{\partial x}\rho u_x u_y + \frac{\partial}{\partial y}\rho u_y u_y + \frac{\partial}{\partial z}\rho u_z u_y\right)\\ &-\left\{\frac{\partial}{\partial x}\left[-\mu\left(\frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[-2\mu\frac{\partial u_y}{\partial y}+(\frac{2}{3}\mu-\kappa)(\nabla\bullet\mathbf{U})\right]\right.\\ &\left.+\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial u_z}{\partial y}+\frac{\partial u_y}{\partial z}\right)\right]\right\}\\ &-\frac{\partial p}{\partial y}+\rho g_y\end{aligned}}\,, \tag{5.8}$$

and finally the z-component of the Navier-Stokes equation can be written as:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\rho u_z = &-\left(\frac{\partial}{\partial x}\rho u_x u_z + \frac{\partial}{\partial y}\rho u_y u_z + \frac{\partial}{\partial z}\rho u_z u_z\right)\\ &-\left\{\frac{\partial}{\partial x}\left[-\mu\left(\frac{\partial u_x}{\partial z}+\frac{\partial u_z}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial u_y}{\partial z}+\frac{\partial u_z}{\partial y}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial z}\left[-2\mu\frac{\partial u_z}{\partial z}+(\frac{2}{3}\mu-\kappa)(\nabla\bullet\mathbf{U})\right]\right\}\\ &-\frac{\partial p}{\partial z}+\rho g_z\end{aligned}}\,. \tag{5.9}$$

The three equations can be put together by using the Einsteins summation convention:

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\rho u_i = -\frac{\partial}{\partial x_j}(\rho u_j u_i) - \frac{\partial}{\partial x_i}&\left[-2\mu\left(\frac{1}{2}\left\{\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right\}\right)\right.\\ &\left.+\left(\frac{2}{3}\mu-\kappa\right)\frac{\partial u_i}{\partial x_i}\right] - \frac{\partial p}{\partial x_i}+\rho g_i\end{aligned}}\,. \tag{5.10}$$

Introducing the deformation rate (strain-rate) tensor $\mathbf{D}$,

$$\mathbf{D} = \frac{1}{2}\left[\nabla\otimes\mathbf{U} + (\nabla\otimes\mathbf{U})^T\right]\ , \tag{5.11}$$

where T stands for the transpose operation, that means $A_{ij}\to A_{ji}$, we are able to write the vector form of this equation:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla\bullet(\rho\mathbf{U}\otimes\mathbf{U}) - \nabla\bullet\left(-2\mu\mathbf{D}+\left[\frac{2}{3}\mu-\kappa\right](\nabla\bullet\mathbf{U})\mathbf{I}\right) - \nabla p + \rho\mathbf{g}\ . \tag{5.12}$$

Finally, we take the negative sign into the brackets of the second term on the RHS to get the general Navier-Stokes equation in vector notation:

$$\boxed{\frac{\partial}{\partial t}\rho\mathbf{U} + \nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) = \nabla \bullet \underbrace{\left(2\mu\mathbf{D} + \left[-\frac{2}{3}\mu + \kappa\right](\nabla \bullet \mathbf{U})\mathbf{I}\right)}_{\text{viscose stress tensor } \boldsymbol{\tau}} - \nabla p + \rho\mathbf{g}} . \tag{5.13}$$

The viscose stress tensor also named shear-rate or deformation rate tensor $\boldsymbol{\tau}$ can be defined as:

$$\boldsymbol{\tau} = \left(2\mu\mathbf{D} + \left[-\frac{2}{3}\mu + \kappa\right](\nabla \bullet \mathbf{U})\mathbf{I}\right) . \tag{5.14}$$

If we use $\kappa = 0$, we get the common Navier-Stokes equation as shown in almost all literatures:

$$\boxed{\frac{\partial}{\partial t}\rho\mathbf{U} + \nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) = \nabla \bullet \underbrace{\left(2\mu\mathbf{D} - \frac{2}{3}\mu(\nabla \bullet \mathbf{U})\mathbf{I}\right)}_{\text{viscose stress tensor } \boldsymbol{\tau}} - \nabla p + \rho\mathbf{g}} . \tag{5.15}$$

Another form of the momentum equation (5.13) can be achieved after pushing the pressure gradient into the viscose stress tensor:

$$\boxed{\frac{\partial}{\partial t}\rho\mathbf{U} + \nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) = \nabla \bullet \underbrace{\left(2\mu\mathbf{D} + \left\{\left[-\frac{2}{3}\mu + \kappa\right](\nabla \bullet \mathbf{U}) - p\right\}\mathbf{I}\right)}_{\text{Cauchy stress tensor } \boldsymbol{\sigma}} + \rho\mathbf{g}} . \tag{5.16}$$

The result of the bracket is called the Cauchy stress tensor $\boldsymbol{\sigma}$. A discussion about this quantity is given in chapter 6. Finally we can insert the dilatation viscosity λ, to get a more general form of the momentum equation:

$$\boxed{\frac{\partial}{\partial t}\rho\mathbf{U} + \nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) = \nabla \bullet (2\mu\mathbf{D} + \{[\lambda + \kappa](\nabla \bullet \mathbf{U}) + p\}\mathbf{I}) + \rho\mathbf{g}} . \tag{5.17}$$

Now it is obvious that the dilatation viscosity or first Lamés coefficient λ is equal to $-\frac{2}{3}\mu$.

The reason why we introduce the Lamés coefficient λ is related to the solid mechanics theory. If we replace the velocity vector $\mathbf{U}$ with the deformation vector $\mathbf{D}$ (do not mix with the deformation rate tensor here), we are able to derive stress equations for solid materials Jasak and Weller [1998].

5.1.1 The Proof of the Transformation

The following section discusses the transformation of the vector form into the Cartesian one. As before, we will investigate only into the terms that are not discussed till now. The terms that we are going to investigate are the viscose stress tensor $\boldsymbol{\tau}$ and the pressure gradient of equation (5.13).

$$\nabla \bullet \left(2\mu\mathbf{D} + \left[-\frac{2}{3}\mu + \kappa\right](\nabla \bullet \mathbf{U})\mathbf{I}\right) - \nabla p \ .$$

The first step is to split the terms:

$$\nabla \bullet (2\mu\mathbf{D}) + \nabla \bullet \left(\left[-\frac{2}{3}\mu + \kappa\right](\nabla \bullet \mathbf{U})\mathbf{I}\right) - \nabla p \ .$$

It is easy to demonstrate that the pressure gradient is equal to the terms in equation (5.7), (5.8) and (5.9). Additionally it is easy to show that the expression of $\nabla \bullet (p\mathbf{I})$ is equal to ∇p. For that, we are using the mathematic operation (1.21):

$$-\nabla \bullet (p\mathbf{I}) = -\nabla \bullet \left\{ p \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right\} = -\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \begin{bmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{bmatrix} \stackrel{!}{=} -\begin{pmatrix} \frac{\partial p}{\partial x} \\ \frac{\partial p}{\partial y} \\ \frac{\partial p}{\partial z} \end{pmatrix} = -\nabla p \ . \tag{5.18}$$

As we can see, the terms are equal for the pressure. The investigation into the first term that includes the deformation rate tensor $\mathbf{D}$, needs the mathematic operations (1.18) and (1.21):

$$\nabla \bullet (2\mu\mathbf{D}) = \nabla \bullet \left(2\mu\frac{1}{2}\left[\nabla \otimes \mathbf{U} + (\nabla \otimes \mathbf{U})^T\right]\right) \tag{5.19}$$

$$= \nabla \bullet \left(\mu \left[\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \otimes \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} + \left\{\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \otimes \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix}\right\}^T\right]\right) \tag{5.20}$$

$$= \nabla \bullet \left(\mu \left\{\begin{bmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_y}{\partial x} & \frac{\partial u_z}{\partial x} \\ \frac{\partial u_x}{\partial y} & \frac{\partial u_y}{\partial y} & \frac{\partial u_z}{\partial y} \\ \frac{\partial u_x}{\partial z} & \frac{\partial u_y}{\partial z} & \frac{\partial u_z}{\partial z} \end{bmatrix} + \begin{bmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_x}{\partial y} & \frac{\partial u_x}{\partial z} \\ \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} & \frac{\partial u_y}{\partial z} \\ \frac{\partial u_z}{\partial x} & \frac{\partial u_z}{\partial y} & \frac{\partial u_z}{\partial z} \end{bmatrix}\right\}\right) \tag{5.21}$$

$$= \nabla \bullet \left(\mu \begin{bmatrix} \frac{\partial u_x}{\partial x} + \frac{\partial u_x}{\partial x} & \frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} & \frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z} \\ \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} + \frac{\partial u_y}{\partial y} & \frac{\partial u_z}{\partial y} + \frac{\partial u_x}{\partial z} \\ \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} & \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} & \frac{\partial u_z}{\partial z} + \frac{\partial u_z}{\partial z} \end{bmatrix}\right) \tag{5.22}$$

$$
= \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \begin{bmatrix} \mu[\frac{\partial u_x}{\partial x} + \frac{\partial u_x}{\partial x}] & \mu[\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}] & \mu[\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}] \\ \mu[\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}] & \mu[\frac{\partial u_y}{\partial y} + \frac{\partial u_y}{\partial y}] & \mu[\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z}] \\ \mu[\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}] & \mu[\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}] & \mu[\frac{\partial u_z}{\partial z} + \frac{\partial u_z}{\partial z}] \end{bmatrix} \tag{5.23}
$$

$$
= \begin{bmatrix} \frac{\partial}{\partial x}\left(2\mu\frac{\partial u_x}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu[\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}]\right) + \frac{\partial}{\partial z}\left(\mu[\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}]\right) \\ \frac{\partial}{\partial x}\left(\mu[\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}]\right) + \frac{\partial}{\partial y}\left(2\mu\frac{\partial u_y}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu[\frac{\partial u_z}{\partial y} + \frac{\partial u_x}{\partial z}]\right) \\ \frac{\partial}{\partial x}\left(\mu[\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}]\right) + \frac{\partial}{\partial y}\left(\mu[\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}]\right) + \frac{\partial}{\partial z}\left(2\mu\frac{\partial u_z}{\partial z}\right) \end{bmatrix} \stackrel{!}{=} \left\{ \begin{array}{l} \text{of } x-\text{mom.} \\ \text{of } y-\text{mom.} \\ \text{of } z-\text{mom.} \end{array} \right. . \tag{5.24}
$$

Now we need to check if the terms are correct; of course equation (5.24) already shows that the terms have to be similar but we will demonstrate why. For that, we use the term within the brackets {...} of equation (5.7),

$$
-\left\{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial u_x}{\partial x} + (\frac{2}{3}\mu - \kappa)(\nabla \bullet \mathbf{U})\right] + \frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right] + \frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}\right)\right]\right\} , \tag{5.25}
$$

taking the minus sign into the brackets, split the x-derivative, we end up with:

$$
\underline{\frac{\partial}{\partial x}\left(2\mu\frac{\partial u_x}{\partial x}\right)} - \frac{\partial}{\partial x}\left((\frac{2}{3}\mu - \kappa)(\nabla \bullet \mathbf{U})\right) + \underline{\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right]} + \underline{\frac{\partial}{\partial z}\left[\mu\left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}\right)\right]} . \tag{5.26}
$$

Apply the same procedure on the terms of equation (5.8) and (5.9), we get the analyzed term of the y-momentum to:

$$
\underline{\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_x}{\partial y}\right)\right]} + \underline{\frac{\partial}{\partial y}\left(2\mu\frac{\partial u_y}{\partial y}\right)} - \frac{\partial}{\partial y}\left((\frac{2}{3}\mu - \kappa)(\nabla \bullet \mathbf{U})\right) + \underline{\frac{\partial}{\partial z}\left[\mu\left(\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z}\right)\right]} , \tag{5.27}
$$

and the term of the z-momentum is equal to:

$$\underline{\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial u_x}{\partial z}+\frac{\partial u_z}{\partial x}\right)\right]}+\underline{\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u_y}{\partial z}+\frac{\partial u_z}{\partial y}\right)\right]}$$
$$+\underline{\frac{\partial}{\partial z}\left(2\mu\frac{\partial u_z}{\partial z}\right)}-\frac{\partial}{\partial z}\left((\frac{2}{3}\mu-\kappa)(\nabla\bullet\mathbf{U})\right)\ . \tag{5.28}$$

The underlined terms occur in equations (5.24). That means, that the vector form and Cartesian one are similar for these term but there is one term missing in each derivative. This term comes from the last term that we neglected till now. The last term can be manipulated to:

$$-\nabla\bullet\left(\left[\frac{2}{3}\mu-\kappa\right](\nabla\bullet\mathbf{U})\mathbf{I}\right)=-\nabla\bullet\left[\left[\frac{2}{3}\mu-\kappa\right](\nabla\bullet\mathbf{U})\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\right] \tag{5.29}$$

$$=-\begin{pmatrix}\frac{\partial}{\partial x}\\\frac{\partial}{\partial y}\\\frac{\partial}{\partial z}\end{pmatrix}\bullet\begin{bmatrix}\left[\frac{2}{3}\mu-\kappa\right](\nabla\bullet\mathbf{U})&0&0\\0&\left[\frac{2}{3}\mu-\kappa\right](\nabla\bullet\mathbf{U})&0\\0&0&\left[\frac{2}{3}\mu-\kappa\right](\nabla\bullet\mathbf{U})\end{bmatrix} \tag{5.30}$$

$$=\begin{pmatrix}-\frac{\partial}{\partial x}[\frac{2}{3}\mu-\kappa](\nabla\bullet\mathbf{U})\\-\frac{\partial}{\partial y}[\frac{2}{3}\mu-\kappa](\nabla\bullet\mathbf{U})\\-\frac{\partial}{\partial z}[\frac{2}{3}\mu-\kappa](\nabla\bullet\mathbf{U})\end{pmatrix}\overset{!}{=}\begin{cases}\text{of } x \text{ mom}\\\text{of } y \text{ mom}\\\text{of } z \text{ mom}\end{cases}\ . \tag{5.31}$$

As demonstrated, all terms of the shear-rate tensor are similar and therefore the vector form is identical to the three single Cartesian ones.

5.1.2 The Dilatation Term

As mentioned at the beginning of this chapter, the second term $-\frac{2}{3}\mu$ is called dilatation term and represents expansion and compression phenomena. To demonstrate the meaning of the term and the correlation to expansion and compression phenomena, we will use the continuity equation to modify this equation. The mass conservation equation is given by:

$$\frac{\partial\rho}{\partial t}+\nabla\bullet(\rho\mathbf{U})=0\ . \tag{5.32}$$

After applying the product law (1.22), we get:

$$\frac{\partial \rho}{\partial t} + \rho \nabla \bullet \mathbf{U} + \mathbf{U} \bullet \nabla \rho = 0 \ , \tag{5.33}$$

$$\nabla \bullet \mathbf{U} = -\frac{1}{\rho} \left[\frac{\partial \rho}{\partial t} + \mathbf{U} \bullet \nabla \rho \right] \ . \tag{5.34}$$

This expression is now insert into the shear-rate tensor $\boldsymbol{\tau}$ of equation (5.13). The outcome is the following: We clearly see that the second term on the RHS is only related to the density change and thus, it is related to expansion and compression phenomena:

$$\boldsymbol{\tau} = 2\mu \mathbf{D} \underbrace{- \frac{2}{3}\mu \ \underbrace{\left\{ -\frac{1}{\rho} \left[\frac{\partial \rho}{\partial t} + \mathbf{U} \bullet \nabla \rho \right] \right\}}_{\text{expansion and compression}} \mathbf{I}}_{\text{dilatation term}} \ . \tag{5.35}$$

5.1.3 Further Simplifications

If we assume incompressibility of the fluid, $\rho =$ constant, we can use the continuity equation for a simplifying the shear-rate tensor. Hence, the second term in equation (5.35), the *dilatation term*, depends only on the density, this term will vanish based on the fact that the density will not change during time and the gradient of a constant number is zero. In addition, we are allowed to take out the density of all remaining derivatives. Thus, we can divide by this quantity to get rid of the density. The result of the shear-rate tensor is as follows ($\nu = \frac{\mu}{\rho}$):

$$\boldsymbol{\tau} = 2\nu \mathbf{D} \ . \tag{5.36}$$

If the dynamic viscosity ν can be assumed as constant, we further can simplify the equation by taking out the viscosity of the divergence operator:

$$\nabla \bullet \boldsymbol{\tau} = \nu \nabla \bullet (\underline{\nabla \otimes \mathbf{U} + (\nabla \otimes \mathbf{U})^T}) \ . \tag{5.37}$$

The underlined term results in a tensor that can be simplified by the continuity equation. Thus, we get the famous Laplace equation:

$$\nabla \bullet \boldsymbol{\tau} = \nu \nabla^2 \mathbf{U} = \nu \Delta \mathbf{U} \ . \tag{5.38}$$

Chapter 6

Relation between the Cauchy Stress Tensor, Shear-Rate Tensor and Pressure

In equation (5.16) we introduced the Cauchy stress tensor $\boldsymbol{\sigma}$. This stress tensor includes all stresses that act on the volume element $\mathrm{d}V$. That means, shear and pressure forces because both can related to stresses. How the total stress, shear-rate stress and pressure are related is briefly discussed in this chapter.

First we start with the introducing of the Cauchy stress tensor $\boldsymbol{\sigma}$:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zz} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \ . \tag{6.1}$$

As we know from chapter 1, we are able to split each matrix into a deviatoric and hydrostatic part. The definition is given in equation (1.28) and can be applied to the Cauchy stress tensor:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\text{hyd}} + \boldsymbol{\sigma}^{\text{dev}} \ . \tag{6.2}$$

The hydrostatic part of an arbitrary matrix $\mathbf{A}$ has the special meaning of the negative pressure p. Hence, equation (1.29) or (1.30) can be related to the pressure as:

$$-p = A^{\text{hyd}} = \frac{1}{3}\,\mathrm{tr}(\mathbf{A}) \ , \tag{6.3}$$

$$-\,p\mathbf{I} = A^{\mathrm{hyd}}\mathbf{I} = \frac{1}{3}\,\mathrm{tr}(\mathbf{A})\mathbf{I}\ . \tag{6.4}$$

Using the definition of the deviatoric part (1.31) and the above expression, we can rewrite equation (6.2):

$$\boldsymbol{\sigma} = -p\mathbf{I} + \underbrace{\left[\boldsymbol{\sigma} - \frac{1}{3}\,\mathrm{tr}(\boldsymbol{\sigma})\mathbf{I}\right]}_{\text{shear}-\text{rate tensor } \boldsymbol{\tau}}\ . \tag{6.5}$$

The deviatoric part is defined as the shear-rate stress and can be expressed by the shear-rate tensor $\boldsymbol{\tau}$:

$$\boldsymbol{\sigma}^{\mathrm{dev}} = \boldsymbol{\tau}\ , \tag{6.6}$$

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}\ . \tag{6.7}$$

Depending on the fluid we are using, $\boldsymbol{\tau}$ has to be replaced with the correct expressions.

Note: In fluid dynamics it is common to use the split Cauchy tensor to get the shear-rate tensor and pressure. In solid mechanics it is common to work with the full stress tensor $\boldsymbol{\sigma}$, compare Jasak and Weller [1998].

Chapter 7

Collection of Different Notations of the Momentum Equations

In literatures we find a lot of different notations for the momentum equation for Newtonian fluids. It is obvious that we can change the stress tensors as we want and play around with the mathematic laws to manipulate the equation as we like to have it.

- Common conserved momentum equation (2.26):

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau} - \nabla p + \rho\mathbf{g} \ . \tag{7.1}$$

- Conserved momentum equation with the shear-rate tensor:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \left(2\mu\mathbf{D} - \frac{2}{3}\mu(\nabla \bullet \mathbf{U})\mathbf{I}\right) - \nabla p + \rho\mathbf{g} \ . \tag{7.2}$$

- Conserved momentum equation with secondary viscosity:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet (2\mu\mathbf{D} + \lambda(\nabla \bullet \mathbf{U})\mathbf{I}) - \nabla p + \rho\mathbf{g} \ . \tag{7.3}$$

- Conserved momentum equation with bulk viscosity:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \left(2\mu\mathbf{D} + \left[-\frac{2}{3}\mu + \kappa\right](\nabla \bullet \mathbf{U})\mathbf{I}\right) - \nabla p + \rho\mathbf{g} \ . \tag{7.4}$$

- Conserved momentum equation with trace operator:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \left(2\mu\mathbf{D} + \left[-\frac{2}{3}\mu + \kappa\right] \mathrm{tr}(\mathbf{D})\mathbf{I}\right) - \nabla p + \rho\mathbf{g} \ . \quad (7.5)$$

- General conserved momentum equation with Cauchy stress tensor:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \boldsymbol{\sigma} + \rho\mathbf{g} \ . \quad (7.6)$$

- Non-conserved momentum equation with Cauchy stress tensor:

$$\rho\frac{\mathrm{D}\mathbf{U}}{\mathrm{D}t} = \nabla \bullet \boldsymbol{\sigma} + \rho\mathbf{g} \ . \quad (7.7)$$

- Integral form of momentum equation:

$$\frac{\partial}{\partial t}\int \rho\mathbf{U}\mathrm{d}V = -\oint (\rho\mathbf{U} \otimes \mathbf{U}) \cdot \mathbf{n}\mathrm{d}S - \oint \boldsymbol{\tau} \cdot \mathbf{n}\mathrm{d}S - \int p\mathrm{d}V + \int \rho\mathbf{g}\mathrm{d}V \ . \quad (7.8)$$

It should be obvious that we can transform all equations above into the non-conservative or integral form.

The Proof that the Trace Operator replaces the Divergence Operator

In one equation above we replaced the divergence operator by the trace operator. That the operation $\mathrm{tr}(\mathbf{D})$ results in $\nabla \bullet \mathbf{U}$ is shown now:

$$\nabla \bullet \mathbf{U} = \mathrm{tr}(\mathbf{D}) \ . \quad (7.9)$$

The demonstration is very simple:

$$\begin{aligned}\mathrm{tr}(\mathbf{D}) &= \mathrm{tr}\left(\frac{1}{2}\left[\nabla \otimes \mathbf{U} + (\nabla \otimes \mathbf{U})^T\right]\right) \\ &= \frac{1}{2}\left[2\frac{\partial u_x}{\partial x} + 2\frac{\partial u_y}{\partial y} + 2\frac{\partial u_z}{\partial z}\right] = \nabla \bullet \mathbf{U} \ . \quad (7.10)\end{aligned}$$

The divergence operator is evaluated by equation (1.20).

Chapter 8

Turbulence Modeling

In this chapter we focus on turbulent flow fields and the Reynolds-Averaging approach which was introduced by Osborne Reynolds. First we will investigate into different averaging approaches. Then we are going to derive the incompressible mass and momentum equation to show the closure problem. After that, we discuss some hypothesis that are used to get rid of the closure problem. That lead to the derivative of the Reynolds stress equation. The outcome of this equation is the analyze of the analogies to the Cauchy stress tensor and the derivation of the turbulent kinetic energy. Finally, we discuss the main problem if we want to average the compressible mass, momentum and energy equation and introduce the Favre averaging concept. The main literature that is used in this chapter is Ferziger and Perić [2008], Bird et al. [1960], Wilcox [1994].

8.1 Reynolds-Averaging

The investigation into flow fields are generally turbulent and hence, it is a challenging task to resolve the flow with all details – in other words, with all physics. Observing an arbitrary flow field, figure 7.1, we can analyze that the flow has a deterministic character. That means, the flow is chaotic and can be prescribed using a time independent mean value $\bar{\phi}$ and its fluctuation ϕ' that is oscillating around the mean value. This behavior is valid for each quantity we focus on like u_x, u_y, u_z, T, h, c and so on; for figure 8.1, ϕ would be the velocity u (in one direction) and could be expressed as:

$$\phi(t, x) = \bar{\phi}(x) + \phi'(t, x) \ . \tag{8.1}$$

Osborne Reynolds introduced several averaging concepts that are presented now:

- Time averaging ,
- Spacial averaging ,
- Ensemble averaging .

The **time averaging** method can be used for a statistic stationary turbulent flow (left figure of 8.1). Defining the instantaneous flow variable by $\phi(t,x)$ and the time averaged one by $\bar{\phi}(x)_{\mathrm{T}}$, the concept is defined by:

$$\bar{\phi}(x)_{\mathrm{T}} = \lim_{T\to\infty} \frac{1}{T} \int_{t}^{t+T} \phi(t,x)\mathrm{d}t \ . \tag{8.2}$$

In order to get good results, T should be chosen large enough compared to the time scale of the fluctuation ϕ'. That is the reason why we are interested in the case when T goes to ∞. As we observe in the figure and in the equation, the averaged value is no longer time depended.

The **spacial averaging** method is appropriate for homogeneous turbulent flows. This yields to a uniform turbulence in all space directions. Here we average over the volume. Renaming the averaged quantity to $\bar{\phi}(x)_{\mathrm{V}}$, we can write:

$$\bar{\phi}(x)_{\mathrm{V}} = \lim_{\mathrm{V}\to\infty} \int\int\int \phi(t,x)\mathrm{d}V \ . \tag{8.3}$$

The **ensemble averaging** method is the most general method. Think about a series of measurement with the number of N identical experiments where $\phi_n(t,x) = \phi(t,x)$ at the n^{th} series. The concept can be defined as follows; the averaged value is denoted by $\bar{\phi}(t,x)_{\mathrm{E}}$:

$$\bar{\phi}(t,x)_{\mathrm{E}} = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \phi_n(t,x) \ . \tag{8.4}$$

For turbulent flow fields that are stationary and homogeneous, all three concepts are similar and lead to the same result. This is also known as the *ergodic hypothesis*.

The averaging method that we choose for the further investigation is the *time averaging* method. The reason for that is based on the fact that things can be described easy and clear. Let us focus on the left part of figure 8.1 first. By

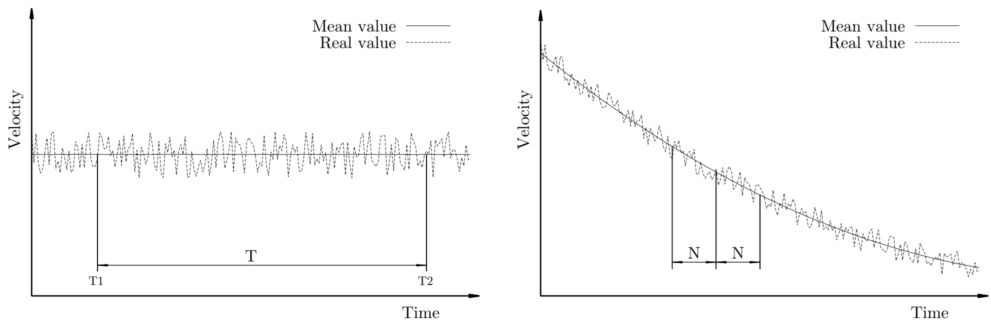


Figure 8.1: Averaging of a statistic stationary (left) and statistic non-stationary flow (right).

replacing the instantaneous variable in equation (8.2) by the definition (8.1), we get:

$$\bar{\phi}(x) = \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \left[\bar{\phi}(x) + \phi'(t,x)\right] \mathrm{d}t \ . \tag{8.5}$$

We observe that the time averaging of the mean and fluctuation quantity leads to the mean quantity again. Thus we can show, that the time average of an already averaged mean quantity is the mean quantity again:

$$\bar{\phi}(x) = \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \bar{\phi}(x) \mathrm{d}t \ . \tag{8.6}$$

In addition we can see that the time averaging of the fluctuation is zero. To demonstrate that, we use equation (8.1) and replace the mean quantity on the RHS of equation by (8.6):

$$\begin{aligned}
\lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \phi'(t,x) &= \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \left[\phi(t,x) - \bar{\phi}(x)\right] \mathrm{d}t \\
&= \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \phi(t,x) \mathrm{d}t - \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \bar{\phi}(x) \mathrm{d}t \\
&= \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \left[\bar{\phi}(x) + \phi'(t,x)\right] \mathrm{d}t - \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \bar{\phi}(x) \mathrm{d}t \\
&= \bar{\phi}(x) - \bar{\phi}(x) = 0 \ .
\end{aligned} \tag{8.7}$$

Some remarks of the validity of this method can be found in Wilcox [1994].

If we think about flows where the mean value of the instantaneous quantity is changing during time (non-stationary flows, figure 8.1; right), we have to modify equation (8.1) and (8.2) to:

$$\phi(t,x) = \bar{\phi}(t,x) + \phi'(t,x) \ , \tag{8.8}$$

$$\bar{\phi}(t,x) = \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \phi(t,x)\mathrm{d}t \ . \tag{8.9}$$

Some remarks and limits to equation (8.9) are given in Wilcox [1994].

Correlation for the Reynolds-Averaging

For the derivations of the Reynolds-Averaged conservation equations, we need some mathematic rules. For now we will use an *overline* to indicate that we use the Reynolds time-averaging concept instead of writing the integrals.

Linear Terms

Applying the average method (8.9) to linear terms lead to linear averaged terms. To demonstrate this, we will use two linear functions $f(t,x)$ and $g(t,x)$:

$$\begin{aligned}\overline{f(t,x)} = \frac{1}{T}\int_t^{t+T} f(t,x)\mathrm{d}t = \frac{1}{T}\int_t^{t+T} \left[\bar{f}(t,x) + f'(t,x)\right]\mathrm{d}t \\ = \underbrace{\overline{\bar{f}(t,x)}}_{\bar{f}(t,x)} + \underbrace{\overline{f'(t,x)}}_{=0} = \bar{f}(t,x)\end{aligned}$$

$$\begin{aligned}\overline{g(t,x)} = \frac{1}{T}\int_t^{t+T} g(t,x)\mathrm{d}t = \frac{1}{T}\int_t^{t+T} \left[\bar{g}(t,x) + g'(t,x)\right]\mathrm{d}t \\ = \underbrace{\overline{\bar{g}(t,x)}}_{\bar{\bar{g}}(t,x)} + \underbrace{\overline{g'(t,x)}}_{=0} = \bar{g}(t,x)\end{aligned}$$

Note: The result can be time dependent or not. This behavior is related to the problems we are looking at. For stationary problems we will end up with $\bar{f}(x), \bar{g}(x)$, whereas for non-stationary problems we get the terms we derived above.

If we have the sum of two linear terms $f(t,x)+g(t,x)$, we get:

$$\begin{aligned}
\overline{f(t,x)+g(t,x)} &= \frac{1}{T}\int_t^{t+T}\left[f(t,x)+g(t,x)\right]\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T} f(t,x)\mathrm{d}t + \frac{1}{T}\int_t^{t+T} g(t,x)\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T}\left[\bar{f}(t,x)+f'(t,x)\right]\mathrm{d}t + \frac{1}{T}\int_t^{t+T}\left[\bar{g}(t,x)+g'(t,x)\right]\mathrm{d}t \\
&= \overline{\bar{f}(t,x)} + \cancel{\overline{f'(t,x)}} + \overline{\bar{g}(t,x)} + \cancel{\overline{g'(t,x)}} \\
&= \bar{f}(t,x)+\bar{g}(t,x)\ .
\end{aligned} \tag{8.10}$$

Averaging linear terms end up with the same linear terms but now with the mean quantities. The fluctuation terms will vanish based on the proof we did above.

Non-Linear Terms

If we focus on non-linear terms like $f(t,x)g(t,x)$, we produce new additional terms during the averaging procedure. To demonstrate this, we will use the above term and average it. What we get is:

$$\begin{aligned}
\overline{f(t,x)g(t,x)} &= \frac{1}{T}\int_t^{t+T}\left[f(t,x)g(t,x)\right]\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T}\left[\left\{\bar{f}(t,x)+f'(t,x)\right\}\left\{\bar{g}(t,x)+g'(t,x)\right\}\right]\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T}\Big[\bar{f}(t,x)\bar{g}(t,x)+\bar{f}(t,x)g'(t,x) \\
&\qquad\qquad + f'(t,x)\bar{g}(t,x)+f'(t,x)g'(t,x)\Big]\mathrm{d}t \\
&= \overline{\bar{f}(t,x)\bar{g}(t,x)} + \cancel{\overline{\bar{f}(t,x)g'(t,x)}} \\
&\qquad\qquad + \cancel{\overline{f'(t,x)\bar{g}(t,x)}} + \overline{f'(t,x)g'(t,x)}\ .
\end{aligned} \tag{8.11}$$

Rewriting the whole equation, we get:

$$\overline{f(t,x)g(t,x)} = \bar{f}(t,x)\bar{g}(t,x) + \underbrace{\overline{f'(t,x)g'(t,x)}}_{\text{additional terms}} \tag{8.12}$$

The reason why the second and third term cancels out is due to the fact that the fluctuation is linear in this terms and hence equation (8.7) is valid. For the last term, there is no reason for the product of the fluctuations to vanish.

Constants

Finally, the Reynolds time-averaging concept does not affect constant quantities. Defining an arbitrary constant a, we get:

$$
\begin{aligned}
\overline{af(t,x)} &= \frac{1}{T}\int_t^{t+T} af(t,x)\mathrm{d}t \\
&= a\frac{1}{T}\int_t^{t+T} \left[\bar{f}(t,x) + f'(t,x)\right]\mathrm{d}t \\
&= a\overline{\bar{f}(t,x)} + a\cancel{\overline{f'(t,x)}} \\
&= a\bar{f}(t,x)\ . \qquad (8.13)
\end{aligned}
$$

8.2 Reynolds Time-Averaged Equations

The Navier-Stokes equations give us the possibility to resolve each vortex and hence all flow phenomena. Applying the equations to turbulent flow fields is a hard and challenging topic that requires extreme fine meshes and time steps and lead to high computational costs. Furthermore, engineers are commonly only interested in some averaged values and on some special physics. Hence, there is no need to resolve all details. Thus, we use the Reynolds-Averaging concept to simplify the flow equations; in other words, the whole turbulence behavior is approximated with models.

Considering incompressibility, the Reynolds time-averaged equations can be derived relatively easily compared to compressible flow fields. This will be discussed using the mass conservation equation now.

8.2.1 Incompressible Mass Conservation Equation

The start point for the derivation is the compressible mass conservation equation (2.12) in the form of Cartesian coordinates:

$$
\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_x)}{\partial x} + \frac{\partial(\rho u_y)}{\partial y} + \frac{\partial(\rho u_z)}{\partial z} = 0\ . \qquad (8.14)
$$

Assuming incompressibility of the fluid, we are allowed to put the density out of the derivatives; it is obvious that the time derivative will vanish and we end up with:

$$
\rho\frac{\partial u_x}{\partial x} + \rho\frac{\partial u_y}{\partial y} + \rho\frac{\partial u_z}{\partial z} = 0\ . \qquad (8.15)
$$

Replacing the values u_i by the assumption (8.1),

$$\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial x}+\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial y}+\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial z}=0\ , \tag{8.16}$$

and apply the Reynolds time-average concept,

$$\overline{\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial x}}+\overline{\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial y}}+\overline{\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial z}}=0\ , \tag{8.17}$$

we get the time-averaged incompressible mass conservation equation:

$$\boxed{\rho\frac{\partial\bar{u}_x}{\partial x}+\rho\frac{\partial\bar{u}_y}{\partial y}+\rho\frac{\partial\bar{u}_z}{\partial z}=\rho\nabla\bullet\bar{\mathbf{U}}=0}\ . \tag{8.18}$$

Of course we are allowed to divide the whole equation by the density.

8.2.2 Compressible Mass Conservation Equation

Doing the same average procedure with the compressible mass conservation equation lead to a more complex form because we also have to consider the density as a varying quantity. If follows:

$$\frac{\partial\rho}{\partial t}+\frac{\partial(\rho u_x)}{\partial x}+\frac{\partial(\rho u_y)}{\partial y}+\frac{\partial(\rho u_z)}{\partial z}=0\ , \tag{8.19}$$

$$\frac{\partial(\bar{\rho}+\rho')}{\partial t}+\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_x+u'_x)\right]}{\partial x}+\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_y+u'_y)\right]}{\partial y}+\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_z+u'_z)\right]}{\partial z}=0\ , \tag{8.20}$$

$$\overline{\frac{\partial(\bar{\rho}+\rho')}{\partial t}}+\overline{\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_x+u'_x)\right]}{\partial x}}+\overline{\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_y+u'_y)\right]}{\partial y}}+\overline{\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_z+u'_z)\right]}{\partial z}}=0\ , \tag{8.21}$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\overline{\bar{\rho}\bar{u}_x} + \cancel{\overline{\bar{\rho}u'_x}} + \cancel{\overline{\rho'\bar{u}_x}} + \overline{\rho' u'_x})}{\partial x} + \frac{\partial(\overline{\bar{\rho}\bar{u}_y} + \cancel{\overline{\bar{\rho}u'_y}} + \cancel{\overline{\rho'\bar{u}_y}} + \overline{\rho' u'_y})}{\partial y}$$
$$+ \frac{\partial(\overline{\bar{\rho}\bar{u}_z} + \cancel{\overline{\bar{\rho}u'_z}} + \cancel{\overline{\rho'\bar{u}_z}} + \overline{\rho' u'_z})}{\partial z} = 0 \ , \quad (8.22)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\bar{u}_x + \overline{\rho' u'_x})}{\partial x} + \frac{\partial(\bar{\rho}\bar{u}_y + \overline{\rho' u'_y})}{\partial y} + \frac{\partial(\bar{\rho}\bar{u}_z + \overline{\rho' u'_z})}{\partial z} = 0 \ , \quad (8.23)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i + \overline{\rho' u'_i}) = 0 \ . \quad (8.24)$$

Introducing a vector that contains the fluctuations of the velocities u'_x, u'_y, u'_z,

$$\mathbf{U}' = \begin{pmatrix} u'_x \\ u'_y \\ u'_z \end{pmatrix} \ , \quad (8.25)$$

we can rewrite the Reynolds time-averaged compressible mass conservation equation in vector notation:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \bullet \left(\bar{\rho}\bar{\mathbf{U}} + \overline{\rho'\mathbf{U}'}\right) = 0 \ . \quad (8.26)$$

Due to the fact that we have two quantities that have to be averaged, we get non-linear terms, that lead to new unknown $\rho' u'_i$. Due to this behavior, we will investigate into the incompressible flows fields first. Averaging the compressible equations will be discussed in section 8.13.

8.2.3 Incompressible Momentum Equation

The derivation of the time-averaged x-component of the momentum equation will be discussed now. For the derivation, we will use equation (5.7) and assume incompressibility of the fluid. For the y and z components, the equations (5.8) and (5.9) have to be used. Due to the fact that the derivations are identical, we only give the final equation for y and z without all steps. The x component is now analyzed and averaged in detail.

x-Component of Momentum

The incompressible momentum equation for the x-component is given by:

$$
\begin{aligned}
\rho\frac{\partial}{\partial t}u_x = &-\left(\rho\frac{\partial}{\partial x}u_x u_x + \rho\frac{\partial}{\partial y}u_y u_x + \rho\frac{\partial}{\partial z}u_z u_x\right) \\
&-\left\{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial u_x}{\partial x}\right] + \frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right]\right. \\
&\left. + \frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}\right)\right]\right\} - \frac{\partial p}{\partial x} + \rho g_x \ .
\end{aligned} \tag{8.27}
$$

This is the start point for the procedure. The first step is to replace the velocity quantities by equation (8.1) and apply the Reynolds time-averaging concept. For clearance, we will examine each term separately. Starting with the term on the LHS, we get:

$$
\overline{\rho\frac{\partial}{\partial t}(\bar{u}_x + u'_x)} = \rho\frac{\partial}{\partial t}\bar{u}_x \ . \tag{8.28}
$$

The first term on the RHS ends up as:

$$
-\left(\overline{\rho\frac{\partial}{\partial x}(\bar{u}_x + u'_x)(\bar{u}_x + u'_x)} + \overline{\rho\frac{\partial}{\partial y}(\bar{u}_y + u'_y)(\bar{u}_x + u'_x)} + \overline{\rho\frac{\partial}{\partial z}(\bar{u}_t + u'_t)(\bar{u}_x + u'_x)}\right) \ .
$$

To simplify the terms, we focus on each term separately. Therefore we get:

$$
\begin{aligned}
\overline{\rho\frac{\partial}{\partial x}(\bar{u}_x + u'_x)(\bar{u}_x + u'_x)} &= \rho\frac{\partial}{\partial x}\left[\overline{\bar{u}_x\bar{u}_x} + \cancel{\overline{\bar{u}_x u'_x}} + \cancel{\overline{u'_x\bar{u}_x}} + \overline{u'_x u'_x}\right] \\
&= \rho\frac{\partial}{\partial x}(\bar{u}_x\bar{u}_x) + \rho\frac{\partial}{\partial x}(\overline{u'_x u'_x}) \ ,
\end{aligned} \tag{8.29}
$$

$$
\begin{aligned}
\overline{\rho\frac{\partial}{\partial y}(\bar{u}_y + u'_y)(\bar{u}_x + u'_x)} &= \rho\frac{\partial}{\partial y}\left[\overline{\bar{u}_y\bar{u}_x} + \cancel{\overline{\bar{u}_y u'_x}} + \cancel{\overline{u'_y\bar{u}_x}} + \overline{u'_y u'_x}\right] \\
&= \rho\frac{\partial}{\partial y}\rho(\bar{u}_y\bar{u}_x) + \rho\frac{\partial}{\partial y}(\overline{u'_y u'_x}) \ ,
\end{aligned} \tag{8.30}
$$

$$
\begin{aligned}
\overline{\rho\frac{\partial}{\partial z}(\bar{u}_z + u'_z)(\bar{u}_x + u'_x)} &= \rho\frac{\partial}{\partial z}\left[\overline{\bar{u}_z\bar{u}_x} + \cancel{\overline{\bar{u}_z u'_x}} + \cancel{\overline{u'_z\bar{u}_x}} + \overline{u'_z u'_x}\right] \\
&= \rho\frac{\partial}{\partial z}\rho(\bar{u}_z\bar{u}_x) + \rho\frac{\partial}{\partial z}(\overline{u'_z u'_x}) \ .
\end{aligned} \tag{8.31}
$$

Finally, the first term on the RHS can be written as:

$$-\left(\rho\frac{\partial}{\partial x}(\bar{u}_x\bar{u}_x)+\rho\frac{\partial}{\partial x}(\overline{u'_x u'_x})+\rho\frac{\partial}{\partial y}(\bar{u}_y\bar{u}_x)\right.$$
$$\left.+\rho\frac{\partial}{\partial y}(\overline{u'_y u'_x})+\rho\frac{\partial}{\partial z}(\bar{u}_z\bar{u}_x)+\rho\frac{\partial}{\partial z}(\overline{u'_z u'_x})\right)\ .$$

After sorting the terms, we end up with:

$$-\underbrace{\left(\rho\frac{\partial}{\partial x}(\bar{u}_x\bar{u}_x)+\rho\frac{\partial}{\partial y}(\bar{u}_y\bar{u}_x)+\rho\frac{\partial}{\partial z}(\bar{u}_z\bar{u}_x)\right)}_{\text{identical convective terms}}$$
$$-\underbrace{\left(\rho\frac{\partial}{\partial x}(\overline{u'_x u'_x})+\rho\frac{\partial}{\partial y}(\overline{u'_y u'_x})+\rho\frac{\partial}{\partial z}(\overline{u'_z u'_x})\right)}_{\text{additonal terms; Reynolds-Stress}}\ .$$

The second term on the RHS of equation (8.27) will be discussed now. The term is given by:

$$-\left\{\underbrace{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial u_x}{\partial x}\right]}_{\text{Term 1}}+\underbrace{\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x}\right)\right]}_{\text{Term 2}}+\underbrace{\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial u_z}{\partial x}+\frac{\partial u_x}{\partial z}\right)\right]}_{\text{Term 3}}\right\}$$

By analyzing term one to term three step by step, we get for the first one the following expression:

$$\overline{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial(\bar{u}_x+u'_x)}{\partial x}\right]}=\frac{\partial}{\partial x}\left[-2\mu\frac{\partial\bar{u}_x}{\partial x}\right]\ , \tag{8.32}$$

for the second one this expression:

$$\overline{\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial(\bar{u}_x+u'_x)}{\partial y}+\frac{\partial(\bar{u}_y+u'_y)}{\partial x}\right)\right]}=\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial\bar{u}_x}{\partial y}+\frac{\partial\bar{u}_y}{\partial x}\right)\right]\ , \tag{8.33}$$

and for the third term this one:

$$\overline{\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial(\bar{u}_z+u'_z)}{\partial x}+\frac{\partial(\bar{u}_x+u'_x)}{\partial z}\right)\right]}=\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial\bar{u}_z}{\partial x}+\frac{\partial\bar{u}_x}{\partial z}\right)\right]\ . \tag{8.34}$$

Finally, after combining all three parts, we get the following expression for the second term on the RHS of equation (8.27):

$$-\left\{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial \bar{u}_x}{\partial x}\right]+\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial \bar{u}_x}{\partial y}+\frac{\partial \bar{u}_y}{\partial x}\right)\right]+\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial \bar{u}_z}{\partial x}+\frac{\partial \bar{u}_x}{\partial z}\right)\right]\right\} .$$

After we analyzed the first two terms, we will investigate into the last two terms on the RHS of equation (8.27). It follows:

$$-\overline{\frac{\partial p}{\partial x}}+\overline{\rho g_x}=-\overline{\frac{\partial(\bar{p}+p')}{\partial x}}+\rho g_x=-\frac{\partial \bar{p}}{\partial x}+\rho g_x . \tag{8.35}$$

Now we can rewrite the x-component of the momentum equation (8.27) as Reynolds time-averaged x-momentum equation:

$$\boxed{\begin{aligned}\rho\frac{\partial}{\partial t}\bar{u}_x = &-\left(\rho\frac{\partial}{\partial x}\bar{u}_x\bar{u}_x+\rho\frac{\partial}{\partial y}\bar{u}_y\bar{u}_x+\rho\frac{\partial}{\partial z}\bar{u}_z\bar{u}_x\right)\\ &-\left(\rho\frac{\partial}{\partial x}(\overline{u_x' u_x'})+\rho\frac{\partial}{\partial y}(\overline{u_y' u_x'})+\rho\frac{\partial}{\partial z}(\overline{u_z' u_x'})\right)\\ &-\left\{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial \bar{u}_x}{\partial x}\right]+\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial \bar{u}_x}{\partial y}+\frac{\partial \bar{u}_y}{\partial x}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial \bar{u}_z}{\partial x}+\frac{\partial \bar{u}_x}{\partial z}\right)\right]\right\}\\ &-\frac{\partial \bar{p}}{\partial x}+\rho g_x\end{aligned}} . \tag{8.36}$$

If we apply the same procedure to the y and z component of the momentum equation, we get the Reynolds time-averaged momentum equation for the y and z components respectively. These three Reynolds time-averaged equations are then called Reynolds-Averaged-Navier-Stokes equations (RANS).

y-Component of Momentum

$$\boxed{\begin{aligned}\rho\frac{\partial}{\partial t}\bar{u}_y = &-\left(\rho\frac{\partial}{\partial x}\bar{u}_x\bar{u}_y+\rho\frac{\partial}{\partial y}\bar{u}_y\bar{u}_y+\rho\frac{\partial}{\partial z}\bar{u}_z\bar{u}_y\right)\\ &-\left(\rho\frac{\partial}{\partial x}(\overline{u_x' u_y'})+\rho\frac{\partial}{\partial y}(\overline{u_y' u_y'})+\rho\frac{\partial}{\partial z}(\overline{u_z' u_y'})\right)\\ &-\left\{\frac{\partial}{\partial y}\left[-2\mu\frac{\partial \bar{u}_y}{\partial y}\right]+\frac{\partial}{\partial x}\left[-\mu\left(\frac{\partial \bar{u}_x}{\partial y}+\frac{\partial \bar{u}_y}{\partial x}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial \bar{u}_z}{\partial y}+\frac{\partial \bar{u}_y}{\partial z}\right)\right]\right\}-\frac{\partial \bar{p}}{\partial y}+\rho g_y\end{aligned}} . \tag{8.37}$$

z-Component of Momentum

$$\boxed{\begin{aligned}\rho\frac{\partial}{\partial t}\bar{u}_z = &-\left(\rho\frac{\partial}{\partial x}\bar{u}_x\bar{u}_z + \rho\frac{\partial}{\partial y}\bar{u}_y\bar{u}_z + \rho\frac{\partial}{\partial z}\bar{u}_z\bar{u}_z\right)\\ &-\left(\rho\frac{\partial}{\partial x}(\overline{u'_x u'_z}) + \rho\frac{\partial}{\partial y}(\overline{u'_y u'_z}) + \rho\frac{\partial}{\partial z}(\overline{u'_z u'_z})\right)\\ &-\left\{\frac{\partial}{\partial z}\left[-2\mu\frac{\partial \bar{u}_z}{\partial z}\right] + \frac{\partial}{\partial x}\left[-\mu\left(\frac{\partial \bar{u}_x}{\partial z} + \frac{\partial \bar{u}_z}{\partial x}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial \bar{u}_y}{\partial z} + \frac{\partial \bar{u}_z}{\partial y}\right)\right]\right\} - \frac{\partial \bar{p}}{\partial z} + \rho g_z\end{aligned}} \tag{8.38}$$

If we are using the vector of fluctuations $\mathbf{U}'$ (8.25), the definition of the deformation (strain) rate tensor $\mathbf{D}$ (5.11) and taking the convective terms to the LHS, we can rewrite the averaged momentum equation in vector form as:

$$\boxed{\underbrace{\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla \bullet (\bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \underbrace{(2\mu\bar{\mathbf{D}})}_{\bar{\boldsymbol{\tau}}} + \nabla\bar{p} + \rho\mathbf{g}}_{\text{Same as equation (5.13) (with } \rho\text{=const.)}} \underbrace{-\rho\nabla \bullet (\overline{\mathbf{U}' \otimes \mathbf{U}'})}_{\text{Reynolds}-\text{Stresses } \bar{\boldsymbol{\sigma}}_{\mathrm{t}}}} \,. \tag{8.39}$$

$\bar{\mathbf{D}}$ defines the Reynolds-Averaged (mean) deformation rate tensor, $\bar{\boldsymbol{\tau}}$ the mean shear-rate tensor and the last term the Reynolds-Stresses, denoted as Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_{\mathrm{t}}$; in many literatures we will find the greek symbol $\bar{\boldsymbol{\tau}}_{\mathrm{t}}$ to express the Reynolds-Stress tensor – this is omitted here because otherwise we are not able to show the analogies between the real stress tensor $\boldsymbol{\sigma}$ (Cauchy stress tensor) and the Reynolds-Stress tensor $\boldsymbol{\sigma}_{\mathrm{t}}$ clearly.

The Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_{\mathrm{t}}$ is defined as:

$$\bar{\boldsymbol{\sigma}}_{\mathrm{t}} = -\rho\overline{u'_i u'_j} = \begin{bmatrix} -\rho\overline{u'_x u'_x} & -\rho\overline{u'_y u'_x} & -\rho\overline{u'_z u'_x} \\ -\rho\overline{u'_x u'_y} & -\rho\overline{u'_y u'_y} & -\rho\overline{u'_z u'_y} \\ -\rho\overline{u'_x u'_z} & -\rho\overline{u'_y u'_z} & -\rho\overline{u'_z u'_z} \end{bmatrix} = \begin{bmatrix} \bar{\sigma}_{\mathrm{t}xx} & \bar{\sigma}_{\mathrm{t}yx} & \bar{\sigma}_{\mathrm{t}zx} \\ \bar{\sigma}_{\mathrm{t}xy} & \bar{\sigma}_{\mathrm{t}yy} & \bar{\sigma}_{\mathrm{t}zy} \\ \bar{\sigma}_{\mathrm{t}xz} & \bar{\sigma}_{\mathrm{t}yz} & \bar{\sigma}_{\mathrm{t}zz} \end{bmatrix} \,. \tag{8.40}$$

After we introduced the Reynolds-Stress tensor, we can rewrite the momentum equation in a more general form:

$$\boxed{\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla \bullet (\bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \bar{\boldsymbol{\tau}} + \nabla\bar{p} + \rho\mathbf{g} + \nabla \bullet \bar{\boldsymbol{\sigma}}_{\mathrm{t}}} \,. \tag{8.41}$$

Finally, we will use the relation between the Cauchy stress tensor, the shear-rate tensor and the pressure (6.7). Hence, we end up with the following equation:

$$\boxed{\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla \bullet (\bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \bar{\boldsymbol{\sigma}} + \rho\mathbf{g} + \nabla \bullet \bar{\boldsymbol{\sigma}}_{\mathrm{t}}}\,. \tag{8.42}$$

In section 2.2 we already showed and discussed that the vector form results in the Cartesian one. In the above equation there is only one term left that we should transformed to demonstrate that each term of the vector form represents the corresponding term in the Cartesian equation. Hence, we will only investigate into that one. The Reynolds-Stress term can be rewritten as:

$$-\rho\nabla \bullet (\overline{\mathbf{U}' \otimes \mathbf{U}'}) = -\rho \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \left[\overline{\begin{pmatrix} u'_x \\ u'_y \\ u'_z \end{pmatrix} \otimes \begin{pmatrix} u'_x \\ u'_y \\ u'_z \end{pmatrix}} \right] \tag{8.43}$$

$$= -\rho \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \left[\begin{pmatrix} \overline{u'_x u'_x} & \overline{u'_x u'_y} & \overline{u'_x u'_z} \\ \overline{u'_y u'_x} & \overline{u'_y u'_y} & \overline{u'_y u'_z} \\ \overline{u'_z u'_x} & \overline{u'_z u'_y} & \overline{u'_z u'_z} \end{pmatrix} \right] \tag{8.44}$$

$$= \begin{pmatrix} -\left[\rho\frac{\partial}{\partial x}\left(\overline{u'_x u'_x}\right) + \rho\frac{\partial}{\partial y}\left(\overline{u'_x u'_y}\right) + \rho\frac{\partial}{\partial z}\left(\overline{u'_x u'_z}\right)\right] \\ -\left[\rho\frac{\partial}{\partial x}\left(\overline{u'_y u'_x}\right) + \rho\frac{\partial}{\partial x}\left(\overline{u'_y u'_y}\right) + \rho\frac{\partial}{\partial x}\left(\overline{u'_y u'_z}\right)\right] \\ -\left[\rho\frac{\partial}{\partial y}\left(\overline{u'_z u'_x}\right) + \rho\frac{\partial}{\partial x}\left(\overline{u'_z u'_y}\right) + \rho\frac{\partial}{\partial z}\left(\overline{u'_z u'_z}\right)\right] \end{pmatrix} \stackrel{!}{=} \begin{cases} \text{of } x - \text{mom.} \\ \text{of } y - \text{mom.} \\ \text{of } z - \text{mom.} \end{cases} \tag{8.45}$$

As we can see – and already knew –, the terms are equal. In most literatures we will find the Reynolds time-averaged momentum equations in Cartesian form using the Einsteins summation convention. This lead to the following equation:

$$\boxed{\rho\frac{\partial}{\partial t}\bar{u}_i + \rho\frac{\partial}{\partial x_j}\left(\bar{u}_i\bar{u}_j\right) = \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial \bar{p}}{\partial x_i} + \rho g_i - \rho\frac{\partial}{\partial x_j}\left(\overline{u'_i u'_j}\right)}\,. \tag{8.46}$$

Furthermore, sometimes the Reynolds-Stress term is put into the convective term on the LHS. Hence, we get:

$$\boxed{\rho\frac{\partial}{\partial t}\bar{u}_i + \rho\frac{\partial}{\partial x_j}\left(\bar{u}_i\bar{u}_j + \overline{u'_i u'_j}\right) = \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial \bar{p}}{\partial x_i} + \rho g_i}\,. \tag{8.47}$$

The derivation of the Reynolds-Averaged momentum equations are done. The boxed equations above are known as Reynolds-Averaged-Navier-Stokes equations (RANS).

Note: It should be obvious that we can put the density in or out of the derivatives (it is a constant if we use the assumption of incompressibility). Hence, this formulation is also valid:

$$\boxed{\frac{\partial}{\partial t}\rho\bar{u}_i + \frac{\partial}{\partial x_j}\left(\rho\bar{u}_i\bar{u}_j + \rho\overline{u_i'u_j'}\right) = \frac{\partial\bar{\tau}_{ij}}{\partial x_j} + \frac{\partial\bar{p}}{\partial x_i} + \rho g_i}\ . \tag{8.48}$$

In addition it is clear, that we are allowed to divide the equations by the density ρ. For that, we just have to be sure to have the right quantities for the pressure and the dynamic viscosity μ. The dynamic viscosity will become the kinematic viscosity ν and the pressure is divided by the density. Furthermore we can think about the gravitational acceleration term ρg_i. If the density is constant, this term gets constant and can be neglected because it will not change the momentum in any case. If we still want to have a buoyancy term within the incompressible equations, we need to use some models like the Boussinesq approximation.

8.2.4 The (Incompressible) General Conservation Equation

After we derived the RANS equations, the derivation of all other conserved equations like the enthalpy, temperature or species equation can be done with the same procedure but is not demonstrated now. As we already know, we could use a general conservation equation to derive other equations. Therefore, we will derive the Reynolds time-averaged governing conserved equation (3.1) for incompressible fluids without any source terms. Hence, the starting point is:

$$\underbrace{\rho\frac{\partial}{\partial t}\phi}_{\text{time accumulation}} = \underbrace{-\rho\quad\nabla\bullet(\mathbf{U}\phi)}_{\text{convective transport}} + \underbrace{\nabla\bullet(D\nabla\phi)}_{\text{diffusive transport}}\ . \tag{8.49}$$

To show the transformation to the Reynolds time-averaged equation, we will switch this equation into the Cartesian form first by using the mathematics (1.20) and assume that the diffusion coefficient D represents a vector; like different thermal diffusivity coefficients in the three space directions (otherwise the derivation get simplified and is not worth do show):

$$\rho\frac{\partial}{\partial t}\phi = -\left(\rho\frac{\partial}{\partial x}(u_x\phi) + \rho\frac{\partial}{\partial y}(u_y\phi) + \rho\frac{\partial}{\partial z}(u_z\phi)\right) + \frac{\partial}{\partial x}\left(D_x\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial\phi}{\partial z}\right) \ . \quad (8.50)$$

The next step is to use the expression from equation (8.1) and apply it to ϕ, u_x, u_y and u_z – keep in mind that D are constant values and are not influenced by the averaging procedure. It follows:

$$\rho\frac{\partial}{\partial t}(\bar{\phi}+\phi') = -\left(\rho\frac{\partial}{\partial x}\left[(\bar{u}_x+u_x')(\bar{\phi}+\phi')\right] + \rho\frac{\partial}{\partial y}\left[(\bar{u}_y+u_y')(\bar{\phi}+\phi')\right] + \rho\frac{\partial}{\partial z}\left[(\bar{u}_z+u_z')(\bar{\phi}+\phi')\right]\right) \ , \quad (8.51)$$

$$\rho\frac{\partial}{\partial t}(\bar{\phi}+\phi') = +\frac{\partial}{\partial x}\left(D_x\frac{\partial}{\partial x}(\bar{\phi}+\phi')\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial}{\partial y}(\bar{\phi}+\phi')\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial}{\partial z}(\bar{\phi}+\phi')\right) \ . \quad (8.52)$$

To discuss the Reynolds-Averaging procedure, we will analyze each term separately of equation (8.52). Therefore, the time term results in:

$$\overline{\rho\frac{\partial}{\partial t}(\bar{\phi}+\phi')} = \rho\frac{\partial}{\partial t}\bar{\phi} \ . \quad (8.53)$$

The first term on the RHS,

$$-\left(\rho\frac{\partial}{\partial x}\left[(\bar{u}_x+u_x')(\bar{\phi}+\phi')\right] + \rho\frac{\partial}{\partial y}\left[(\bar{u}_y+u_y')(\bar{\phi}+\phi')\right] + \rho\frac{\partial}{\partial z}\left[(\bar{u}_z+u_z')(\bar{\phi}+\phi')\right]\right) \ ,$$

will be split to enable analyzing term by term. It follows:

$$\overline{\rho\frac{\partial}{\partial x}\left[(\bar{u}_x+u_x')(\bar{\phi}+\phi')\right]} = \rho\frac{\partial}{\partial x}\left[(\overline{\bar{u}_x\bar{\phi}} + \overline{\bar{u}_x\phi'} + \overline{u_x'\bar{\phi}} + \overline{u_x'\phi'})\right] = \rho\frac{\partial}{\partial x}(\bar{u}_x\bar{\phi}) + \frac{\partial}{\partial x}(\rho\overline{u_x'\phi'}) \ , \quad (8.54)$$

$$\overline{\rho\frac{\partial}{\partial y}\left[(\bar{u}_y + u'_y)(\bar{\phi} + \phi')\right]} = \rho\frac{\partial}{\partial y}\left[(\overline{\bar{u}_y\bar{\phi}} + \overline{\bar{u}_y\phi'} + \overline{u'_y\bar{\phi}} + \overline{u'_y\phi'})\right]$$
$$= \rho\frac{\partial}{\partial y}(\bar{u}_y\bar{\phi}) + \rho\frac{\partial}{\partial y}(\overline{u'_y\phi'}) \ , \quad (8.55)$$

$$\overline{\rho\frac{\partial}{\partial z}\left[(\bar{u}_z + u'_z)(\bar{\phi} + \phi')\right]} = \rho\frac{\partial}{\partial z}\left[(\overline{\bar{u}_z\bar{\phi}} + \overline{\bar{u}_z\phi'} + \overline{u'_z\bar{\phi}} + \overline{u'_z\phi'})\right]$$
$$= \rho\frac{\partial}{\partial z}(\bar{u}_z\bar{\phi}) + \rho\frac{\partial}{\partial z}(\overline{u'_z\phi'}) \ . \quad (8.56)$$

Hence, the first term on the RHS after sorting is:

$$-\left(\rho\frac{\partial}{\partial x}(\bar{u}_x\bar{\phi}) + \rho\frac{\partial}{\partial y}(\bar{u}_y\bar{\phi}) + \rho\frac{\partial}{\partial z}(\bar{u}_z\bar{\phi}) + \rho\frac{\partial}{\partial x}(\overline{u'_x\phi'}) + \rho\frac{\partial}{\partial y}(\overline{u'_y\phi'}) + \rho\frac{\partial}{\partial z}(\overline{u'_z\phi'})\right) \ .$$

The second, third and fourth term on the RHS will end up as:

$$\overline{\frac{\partial}{\partial x}\left(D_x\frac{\partial}{\partial x}(\bar{\phi} + \phi')\right)} = \frac{\partial}{\partial x}\left(D_x\frac{\partial\bar{\phi}}{\partial x}\right) \ , \quad (8.57)$$

$$\overline{\frac{\partial}{\partial y}\left(D_y\frac{\partial}{\partial y}(\bar{\phi} + \phi')\right)} = \frac{\partial}{\partial y}\left(D_y\frac{\partial\bar{\phi}}{\partial y}\right) \ , \quad (8.58)$$

$$\overline{\frac{\partial}{\partial z}\left(D_z\frac{\partial}{\partial z}(\bar{\phi} + \phi')\right)} = \frac{\partial}{\partial z}\left(D_z\frac{\partial\bar{\phi}}{\partial z}\right) \ . \quad (8.59)$$

To sum up, the general Reynolds-Averaged conservation equation can be written as:

$$\boxed{\begin{aligned}\rho\frac{\partial}{\partial t}\bar{\phi} = &-\left(\rho\frac{\partial}{\partial x}(\rho\bar{u}_x\bar{\phi}) + \rho\frac{\partial}{\partial y}(\bar{u}_y\bar{\phi}) + \rho\frac{\partial}{\partial z}(\bar{u}_z\bar{\phi})\right)\\ &+ \frac{\partial}{\partial x}\left(D_x\frac{\partial\bar{\phi}}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial\bar{\phi}}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial\bar{\phi}}{\partial z}\right)\\ &- \underbrace{\left(\rho\frac{\partial}{\partial x}(\overline{u'_x\phi'}) + \rho\frac{\partial}{\partial y}(\overline{u'_y\phi'}) + \rho\frac{\partial}{\partial z}(\overline{u'_z\phi'})\right)}_{\text{turbulent scalar flux}}\end{aligned}} \ , \quad (8.60)$$

and is given in vector form by:

$$\boxed{\underbrace{\rho\frac{\partial}{\partial t}\bar{\phi} = -\rho\nabla\bullet\left(\bar{\mathbf{U}}\bar{\phi}\right) + \nabla\bullet\left(D\nabla\bar{\phi}\right)}_{\text{same as before}} - \underbrace{\rho\nabla\bullet(\overline{\mathbf{U}'\phi'})}_{\text{turbulent scalar flux}}} \ . \quad (8.61)$$

Equation (8.61) allows us to derive each Reynolds-Averaged conservation equation by replacing ϕ with the quantity of interest (analogy to chapter 3).

As we already realized, after deriving the Reynolds-Averaged momentum equations, we get the same equations but with **additional terms**. These additional terms are called **Reynolds-Stresses** for the momentum equations and are named **additional turbulent scalar flux** for all other quantities. Finally – and if we want –, we can put the density inside the derivations and we end up with:

$$\boxed{\underbrace{\frac{\partial}{\partial t}\rho\bar{\phi} = -\nabla \bullet \left(\rho\bar{\mathbf{U}}\bar{\phi}\right) + \nabla \bullet \left(D\nabla\bar{\phi}\right)}_{\text{same as before}} - \underbrace{\nabla \bullet \left(\rho\overline{\mathbf{U}'\phi'}\right)}_{\text{turbulent scalar flux}}} \,. \tag{8.62}$$

Manipulating the equations should be familiar now. Thus, we can put the convective and the turbulent scalar flux terms together. In addition we add the arbitrary source term of ϕ. The resulting general Reynolds-Averaged conservation equation is then written as:

$$\boxed{\frac{\partial}{\partial t}\rho\bar{\phi} + \nabla \bullet \left(\rho\bar{\mathbf{U}}\bar{\phi} + \rho\overline{\mathbf{U}'\phi'}\right) = \nabla \bullet \left(D\nabla\bar{\phi}\right) + S_\phi} \,. \tag{8.63}$$

8.3 The Closure Problem

The Reynolds-Averaged procedure lead to the problem, that we create additional unknown quantities and no further equations. In other words, the terms $-\rho\overline{u_i'u_j'}$ and $-\rho\overline{u_i'\phi'}$ are not known and can not be calculated. Hence, the set of equations are not enough to close our problem and we cannot solve our system. This is known as *closure problem*. Therefore, we need approximations that correlate the unknown with known quantities.

Till today this problem is still **not solved** and we do not have a set of equations to get rid of the closure problem and therefore, we are **forced** to use approximations, if we use the Reynolds time-averaging procedure. The equations that are introduced by authors to get rid of the closure problem are known as turbulence models. Within this assumptions, we try to correlate the unknown quantities with known one.

For the **Reynolds-Stresses** and **turbulent scalar fluxes** we can use several theories that try approximate the unknown terms. The most popular methods are the Boussinesq's eddy viscosity, the Prandtl's mixing length or the Von-Kármán's similarity hypothesis. Further information about these theories (concept of higher viscosity) can be found in Ferziger and Perić [2008], Bird et al. [1960], Wilcox [1994].

Keywords: energy cascade, higher viscosity concept, eddy viscosity, dissipation and turbulent viscosity.

8.4 Boussinesq Eddy Viscosity

The most used hypothesis is the theory postulated by Joseph Boussinesq that simply relates the turbulence of a flow to a higher fluid viscosity. The thought behind is as follows: If we have a higher turbulence flow, the flow gets more chaotic and we get a lot of vortexes that can transport for example heat in addition to the already existing transport phenomena. Therefore, it is clear and of humans nature to say, that we could achieve that, if we increase the diffusion coefficient (the viscosity in the momentum equation) and keep the rest as it is. In other words, the molecular viscosity is increased by the so called eddy or turbulent viscosity. This assumption give us the possibility to model the smallest vortexes by using correlations and approximations and only resolve the larger eddies.

It is also possible to use the higher viscosity to describe or characterize the dissipation of kinetic energy (per unit mass) of the turbulence into heat – the higher the viscosity of the fluid, the higher the shearing and therefore we get higher mixing rates (additional transport) but although a larger dissipation of the kinetic energy into heat. Hence, we also could describe the theory vice versa: the higher the eddy viscosity, the higher the turbulence of the flow field.

Joseph Boussinesq related the Reynold-Stresses $-\rho\overline{u_i'u_j'}$ to the mean values of the velocities and the kinetic energy of the turbulence k as:

$$\underbrace{-\rho\overline{u_i'u_j'}}_{\bar{\boldsymbol{\sigma}}_\mathrm{t}} = \mu_t \underbrace{\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_x} - \frac{2}{3}\left(\nabla \bullet \bar{\mathbf{U}}\right)\delta_{ij}\right)}_{2\bar{\mathbf{D}} - \frac{2}{3}\,\mathrm{tr}(\bar{\mathbf{D}})} - \underbrace{\frac{2}{3}\rho\delta_{ij}k}_{\frac{2}{3}\rho\mathbf{I}k} \,, \tag{8.64}$$

$$\bar{\boldsymbol{\sigma}}_\mathrm{t} = \underline{2\mu_\mathrm{t}\bar{\mathbf{D}} - \frac{2}{3}\mu_\mathrm{t}\,\mathrm{tr}(\bar{\mathbf{D}})\mathbf{I}} - \frac{2}{3}\rho\mathbf{I}k \,, \tag{8.65}$$

$$\bar{\boldsymbol{\sigma}}_\mathrm{t} = \bar{\boldsymbol{\tau}}_\mathrm{t} - \frac{2}{3}\rho\mathbf{I}k \,. \tag{8.66}$$

In the equations above, we can see, that the underlined term is identical to the shear-rate tensor $\bar{\boldsymbol{\tau}}$, if we set the bulk viscosity κ to zero; cf. equation (5.14) with the difference that we use the turbulent eddy viscosity μ_t instead of the molecular viscosity μ, hence we mark it with the subscript t ($\bar{\boldsymbol{\tau}}_\mathrm{t}$). In addition we can say that the turbulent Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_\mathrm{t}$ equals to the shear-rate tensor $\bar{\boldsymbol{\tau}}_\mathrm{t}$ and an additional term $\frac{2}{3}\rho\delta_{ij}k$. *This term is necessary to guarantee the proper trace of the Reynolds-stress tensor* $\bar{\boldsymbol{\sigma}}_\mathrm{t}$ as mentioned by Ferziger and Perić [2008] and Wilcox [1994].

One may think about the term $\frac{2}{3}\rho\delta_{ij}k$ now. Where does it come from and why is this term necessary? As mentioned by Ferziger and Perić [2008] and Wilcox [1994], this term has to be added to get the proper trace of the Reynolds-stress tensor. To understand the meaning of the additional term, we simply have to take the trace of the Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_\mathrm{t}$ and the shear-rate tensor $\bar{\boldsymbol{\tau}}_\mathrm{t}$.

For that, we need to know the definition of the kinetic energy of the turbulence:

$$k = \frac{1}{2}\overline{u_i'u_i'} = \frac{1}{2}\left(\overline{u_x'u_x'} + \overline{u_y'u_y'} + \overline{u_z'u_z'}\right) \ . \tag{8.67}$$

New we need to take the trace of the Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_\mathrm{t}$ (8.40). It follows:

$$\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t}) = \mathrm{tr}(-\rho\overline{u_i'u_j'}) = \mathrm{tr}\left(\begin{bmatrix} -\rho\overline{u_x'u_x'} & -\rho\overline{u_y'u_x'} & -\rho\overline{u_z'u_x'} \\ -\rho\overline{u_x'u_y'} & -\rho\overline{u_y'u_y'} & -\rho\overline{u_z'u_y'} \\ -\rho\overline{u_x'u_z'} & -\rho\overline{u_y'u_z'} & -\rho\overline{u_z'u_z'} \end{bmatrix}\right) \ , \tag{8.68}$$

$$= \underbrace{(-\rho\overline{u_x'u_x'}) + (-\rho\overline{u_y'u_y'}) + (-\rho\overline{u_z'u_z'})}_{=\ -2\rho k} \ . \tag{8.69}$$

The result that we get is the following: The trace of the Reynolds-Stress tensor is twice the density multiplied by the kinetic energy of the turbulence, $-2\rho k$, and can be validated by substituting k by its definition (8.67):

$$-2\rho k = -2\rho\left[\frac{1}{2}\left(\overline{u_x'u_x'} + \overline{u_y'u_y'} + \overline{u_z'u_z'}\right)\right] = \underbrace{(-\rho\overline{u_x'u_x'}) + (-\rho\overline{u_y'u_y'}) + (-\rho\overline{u_z'u_z'})}_{\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t})} \ . \tag{8.70}$$

We demonstrated, that the trace of the Reynolds-Stress $\bar{\boldsymbol{\sigma}}_\mathrm{t}$ tensor has to be equal to $-2\rho k$. Therefore, the trace of the RHS of equation (8.66) has to be equal to $-2\rho k$ too. Otherwise the equation would not be correct in the mathematical point of view. Thus we get:

$$\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t}) = \mathrm{tr}\left(\bar{\boldsymbol{\tau}}_\mathrm{t} - \frac{2}{3}\rho\mathbf{I}k\right) = -2\rho k \ , \tag{8.71}$$

$$\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t}) = \mathrm{tr}\left(2\mu_\mathrm{t}\bar{\mathbf{D}} - \frac{2}{3}\mu_\mathrm{t}\,\mathrm{tr}(\bar{\mathbf{D}})\mathbf{I} - \frac{2}{3}\rho\mathbf{I}k\right) = -2\rho k\ . \tag{8.72}$$

If we use the definition of the deformation rate tensor (5.11) with respect to the mean quantities and apply the transformation (7.9), it follows:

$$\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t}) = \mathrm{tr}\left(\underbrace{2\mu_\mathrm{t}\left\{\frac{1}{2}\left[\nabla\otimes\bar{\mathbf{U}} + (\nabla\otimes\bar{\mathbf{U}})^T\right]\right\}}_{\text{Term 1}} - \underbrace{\frac{2}{3}\mu_\mathrm{t}\left(\nabla\bullet\bar{\mathbf{U}}\right)\mathbf{I}}_{\text{Term 2}} - \underbrace{\frac{2}{3}\rho\mathbf{I}k}_{\text{Term 3}}\right),$$

$$\begin{aligned}
&= \underbrace{\mu_\mathrm{t}\left[\begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix}\otimes\begin{pmatrix}\bar{u}_x\\ \bar{u}_y\\ \bar{u}_z\end{pmatrix} + \left\{\begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix}\otimes\begin{pmatrix}\bar{u}_x\\ \bar{u}_y\\ \bar{u}_z\end{pmatrix}\right\}^T\right]}_{\text{Term 1}}\\
&\underbrace{-\frac{2}{3}\mu_\mathrm{t}\begin{bmatrix}\frac{\partial\bar{u}_x}{\partial x}+\frac{\partial\bar{u}_y}{\partial y}+\frac{\partial\bar{u}_z}{\partial z} & 0 & 0\\ 0 & \frac{\partial\bar{u}_x}{\partial x}+\frac{\partial\bar{u}_y}{\partial y}+\frac{\partial\bar{u}_z}{\partial z} & 0\\ 0 & 0 & \frac{\partial\bar{u}_x}{\partial x}+\frac{\partial\bar{u}_y}{\partial y}+\frac{\partial\bar{u}_z}{\partial z}\end{bmatrix}}_{\text{Term 2}}\\
&\underbrace{-\begin{bmatrix}-\frac{2}{3}\rho k & 0 & 0\\ 0 & -\frac{2}{3}\rho k & 0\\ 0 & 0 & -\frac{2}{3}\rho k\end{bmatrix}}_{\text{Term 3}}.
\end{aligned}\tag{8.73}$$

Applying the dyadic product rule (1.15) to term 1, add both matrices and multiply everything by the eddy viscosity, we end up with term 1 as:

$$\begin{bmatrix}\mu_\mathrm{t}\frac{\partial u_x}{\partial x}+\mu_\mathrm{t}\frac{\partial u_x}{\partial x} & \mu_\mathrm{t}\frac{\partial u_y}{\partial x}+\mu_\mathrm{t}\frac{\partial u_x}{\partial y} & \mu_\mathrm{t}\frac{\partial u_z}{\partial x}+\mu_\mathrm{t}\frac{\partial u_x}{\partial z}\\ \mu_\mathrm{t}\frac{\partial u_x}{\partial y}+\mu_\mathrm{t}\frac{\partial u_y}{\partial x} & \mu_\mathrm{t}\frac{\partial u_y}{\partial y}+\mu_\mathrm{t}\frac{\partial u_y}{\partial y} & \mu_\mathrm{t}\frac{\partial u_z}{\partial y}+\mu_\mathrm{t}\frac{\partial u_y}{\partial z}\\ \mu_\mathrm{t}\frac{\partial u_x}{\partial z}+\mu_\mathrm{t}\frac{\partial u_z}{\partial x} & \mu_\mathrm{t}\frac{\partial u_y}{\partial z}+\mu_\mathrm{t}\frac{\partial u_z}{\partial y} & \mu_\mathrm{t}\frac{\partial u_z}{\partial z}+\mu_\mathrm{t}\frac{\partial u_z}{\partial z}\end{bmatrix}.$$

Due to the fact that we are only interested in the main diagonal elements (trace), we just consider these terms for now. The matrices of term 1, term 2 and term 3 have to be summed up and the trace operator has to be applied. It follows:

$$\underline{\mathrm{tr}\left(\bar{\boldsymbol{\tau}}_\mathrm{t} - \frac{2}{3}\rho\mathbf{I}k\right)} = \underbrace{\underbrace{2\mu_\mathrm{t}\left[\frac{\partial \bar{u}_x}{\partial x} + \frac{\partial \bar{u}_y}{\partial y} + \frac{\partial \bar{u}_z}{\partial z}\right]}_{\text{Term 1}} - \underbrace{3\frac{2}{3}\mu_\mathrm{t}\left[\frac{\partial \bar{u}_x}{\partial x} + \frac{\partial \bar{u}_y}{\partial y} + \frac{\partial \bar{u}_z}{\partial z}\right]}_{\text{Term 2}}}_{=0}$$

$$- \underbrace{3\frac{2}{3}\rho k}_{\text{Term 3}} = -2\rho k\ . \quad (8.74)$$

The result of the trace operator to the Boussinesq hypothesis is $-2\rho k$. Hence, the trace of the RHS and LHS of equation (8.64) is equal. If we would remove the term $-\frac{2}{3}\rho\delta_{ij}k$ on the RHS of equation (8.64), the trace of the RHS would not be equal to the trace of the Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_\mathrm{t}$ and hence, the Boussinesq eddy viscosity assumption would be wrong because $\bar{\boldsymbol{\tau}}_\mathrm{t}$ is traceless, cf. chapter 6.

Forums Discussion

It is worth to mention that there were a lot of people asking about the term $-\frac{2}{3}\rho\delta_{ij}k$ in public forums. Even I made wrong statements at the beginning in a way that within the OpenFOAM® toolbox, this term is neglected. Finally, we can not find this term in OpenFOAM® which is related to a very simple correlation that is given below. For those who are interested in the discussion on *cfd-online.com*, you can go to: www.cfd-online.com/Forums/openfoam-solving/58214-calculating-divdevreff.html.

Keep in mind that this thread can cause confusion because only the last posts are correct and as *Gerhard Holzinger* mentioned, the term is put into a modified pressure and is not neglected in OpenFOAM®. How this is working, is given on the next page.

Analogy to the Cauchy Stress Tensor, Shear-Rate Tensor and Pressure

Comparing the last derived equations with those of chapter 6, it is obvious that there are similarities. Analyzing equation (6.7) and (8.66), we can evaluate the same kind of behavior:

$$\underbrace{\boldsymbol{\sigma}}_{\text{(Cauchy)−Stress tensor}} = \underbrace{\boldsymbol{\tau}}_{\text{shear−rate tensor (traceless)}} + \underbrace{-p\mathbf{I}}_{\text{pressure (=trace)}} , \tag{8.75}$$

$$\underbrace{\bar{\boldsymbol{\sigma}}_{\mathrm{t}}}_{\text{(Reynolds)−Stress tensor}} = \underbrace{\bar{\boldsymbol{\tau}}_{\mathrm{t}}}_{\text{(RA)−shear−rate tensor (traceless)}} + \underbrace{-\frac{2}{3}\rho\mathbf{I}k}_{\text{add. term (=trace)}} , \tag{8.76}$$

$$\underbrace{\mathbf{A}}_{\text{complete matrix}} = \underbrace{\mathbf{A}^{\text{dev}}}_{\text{deviatoric part (traceless)}} + \underbrace{\mathbf{A}^{\text{hyd}}}_{\text{hydro. part (=trace)}} . \tag{8.77}$$

If we compare the terms, we can observe that the term $-\frac{2}{3}\rho k$ seems to behave like a pressure. Using equation (8.42) and replacing the Reynolds-Averaged Cauchy stress tensor $\bar{\boldsymbol{\sigma}}$ and the Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_{\mathrm{t}}$ by their definitions (6.7) and (8.66), we can highlight the similarities better:

$$\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla\bullet(\bar{\mathbf{U}}\otimes\bar{\mathbf{U}}) = \underbrace{\nabla\bullet\bar{\boldsymbol{\tau}} + \nabla\bullet(-p\mathbf{I})}_{\nabla\bullet\bar{\boldsymbol{\sigma}}} + \rho\mathbf{g} + \underbrace{\nabla\bullet\bar{\boldsymbol{\tau}}_{\mathrm{t}} + \nabla\bullet\left(-\frac{2}{3}\rho k\mathbf{I}\right)}_{\nabla\bullet\bar{\boldsymbol{\sigma}}_{\mathrm{t}}}, \tag{8.78}$$

$$\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla\bullet(\bar{\mathbf{U}}\otimes\bar{\mathbf{U}}) = \nabla\bullet\bar{\boldsymbol{\tau}} + \nabla\bullet\bar{\boldsymbol{\tau}}_{\mathrm{t}} + \rho\mathbf{g} + \nabla\bullet(-p\mathbf{I}) + \nabla\bullet\left(-\frac{2}{3}\rho k\mathbf{I}\right), \tag{8.79}$$

$$\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla\bullet(\bar{\mathbf{U}}\otimes\bar{\mathbf{U}}) = \nabla\bullet(\bar{\boldsymbol{\tau}} + \bar{\boldsymbol{\tau}}_{\mathrm{t}}) + \rho\mathbf{g} - \nabla\bullet\Big(\underbrace{p\mathbf{I} + \frac{2}{3}\rho k\mathbf{I}}_{=\,p^*\mathbf{I}}\Big). \tag{8.80}$$

Introducing a modified pressure $p^* = p + \frac{2}{3}\rho k$ and replacing the shear-rate tensors by their definitions (for the shear-rate tensor $\bar{\boldsymbol{\tau}}$, we mark the molecular viscosity μ by the subscript l), we get the following equation:

$$\begin{aligned}\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla\bullet(\bar{\mathbf{U}}\otimes\bar{\mathbf{U}}) = \nabla\bullet\bigg(&\left[2\mu_{\mathrm{l}}\bar{\mathbf{D}} - \frac{2}{3}\mu_{\mathrm{l}}\left(\nabla\bullet\bar{\mathbf{U}}\right)\mathbf{I}\right] \\ &+\left[2\mu_{\mathrm{t}}\bar{\mathbf{D}} - \frac{2}{3}\mu_{\mathrm{t}}\left(\nabla\bullet\bar{\mathbf{U}}\right)\mathbf{I}\right]\bigg) + \rho\mathbf{g} - \nabla\bullet(p^*\mathbf{I}) ,\end{aligned} \tag{8.81}$$

$$\rho \frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho \nabla \bullet (\bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left(\left[\mu_{\mathrm{l}} \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} (\nabla \bullet \bar{\mathbf{U}}) \mathbf{I} \right\} \right] \right.$$
$$\left. + \left[\mu_{\mathrm{t}} \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} (\nabla \bullet \bar{\mathbf{U}}) \mathbf{I} \right\} \right] \right) + \rho \mathbf{g} - \nabla \bullet (p^* \mathbf{I}) \ , \quad (8.82)$$

$$\frac{\partial}{\partial t}\rho\bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left([\mu_{\mathrm{l}} + \mu_{\mathrm{t}}] \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} (\nabla \bullet \bar{\mathbf{U}}) \mathbf{I} \right\} \right) + \rho \mathbf{g} - \nabla \bullet (p' \mathbf{I}) \ . \quad (8.83)$$

Introducing an effective viscosity μ_{eff} that is simply the sum of the molecular and turbulent (eddy) viscosity:

$$\mu_{\mathrm{eff}} = \mu_{\mathrm{l}} + \mu_{\mathrm{t}} \ , \quad (8.84)$$

we can rewrite the Reynolds-Averaged-Navier-Stokes equations, that include the effective viscosity and a modified pressure field p^* as:

$$\frac{\partial}{\partial t}\rho\bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left(\mu_{\mathrm{eff}} \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} (\nabla \bullet \bar{\mathbf{U}}) \mathbf{I} \right\} \right) + \rho \mathbf{g} - \nabla \bullet (p^* \mathbf{I}) \ , \quad (8.85)$$

$$\frac{\partial}{\partial t}\rho\bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left(\underbrace{2\mu_{\mathrm{eff}}\bar{\mathbf{D}} - \frac{2}{3}\mu_{\mathrm{eff}} (\nabla \bullet \bar{\mathbf{U}}) \mathbf{I}}_{\bar{\boldsymbol{\tau}}_{\mathrm{eff}}} \right) + \rho \mathbf{g} - \nabla \bullet (p^* \mathbf{I}) \ . \quad (8.86)$$

After introducing the effective shear-rate tensor $\bar{\boldsymbol{\tau}}_{\mathrm{eff}}$, we can simplify the equation to:

$$\boxed{\frac{\partial}{\partial t}\rho\bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \bar{\boldsymbol{\tau}}_{\mathrm{eff}} - \nabla \bullet (p^* \mathbf{I}) + \rho \mathbf{g}} \ . \quad (8.87)$$

It is clear that this equation is similar to equation (2.26). The differences within the equations are, that we use a modified pressure p^* and a new viscosity μ_{eff} field; it should be obvious that we have mean quantities here.

After that, the only unknown in that equation is the eddy viscosity μ_{t}. If we introduce an effective *Cauchy-Stress tensor* $\bar{\boldsymbol{\sigma}}_{\mathrm{eff}}$, we are able to build the general form of the momentum equation. It follows:

$$\bar{\boldsymbol{\sigma}}_{\mathrm{eff}} = \bar{\boldsymbol{\tau}}_{\mathrm{eff}} - p^* \mathbf{I} \ , \quad (8.88)$$

$$\boxed{\frac{\partial}{\partial t}\rho\bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \bar{\boldsymbol{\sigma}}_{\mathrm{eff}} + \rho \mathbf{g}} \ . \quad (8.89)$$

Note: If we solve the incompressible Reynolds-Averaged Navier-Stokes equations, we are not calculating the real pressure field p. Instead we have the modified pressure p^*. For most of the problems this is not a big deal and we do not have to consider this. Only if we are using some modified equations in OpenFOAM® where we need the *real pressure*, we have to recalculate the real pressure field by subtracting the kinetic part.

The reason for introducing the Boussinesq eddy hypothesis and the advantages are given in the next section.

8.5 Eddy Viscosity Approximation

The Boussinesq theory allows us to eliminate the Reynolds-Stresses with known quantities. However, we get new unknown quantities like the eddy viscosity μ_t and the kinetic energy of the turbulence k.

Wilcox [1994] listed plenty of theories and models that relates the eddy viscosity to known quantities. Commonly the turbulent (eddy) viscosity is characterized with the kinetic energy of the turbulence k and a characteristic length L. Furthermore, the kinetic energy of the turbulence can be related to a velocity $q = \sqrt{k}$. This two values enable us to derive a correlation between the velocity q (kinetic energy of the turbulence k), the characteristic length L and the eddy viscosity. The assumption that was invented is:

$$\boxed{\mu_\mathrm{t} \approx C_\mu \rho q L} \ . \tag{8.90}$$

The parameter C_μ is a dimensionless constant. The challenge now is to relate the characteristic length L and the velocity q to known quantities. This is done by using turbulence models.

8.6 Algebraic Models

At the beginning of computational fluid dynamics the power of personal and super computers were restricted and therefore it was necessary to have simple models that approximate the Reynolds-Stresses $-\rho\overline{u_i' u_j'}$. These models commonly use the introduced Boussinesq eddy viscosity theory. The estimation of the eddy viscosity μ_t is done by using algebraic expressions. A few models are described in Wilcox [1994] chapter 3. Algebraic models can be used for simple flow patterns but hence the flow is getting complex (imagine geometries in combustion, or even flow separation), these models will fail and produces non-physical values for the eddy viscosity.

8.7 Turbulence Energy Equation Models

The most common approximations for the Reynolds-Stresses (finally to calculate the characteristic length scale L and the kinetic energy of the turbulence k) are called *turbulence energy equation models*. There are one-equation and tow-equation models. Due to the fact that we need the values of the velocity q $(=\sqrt{k})$ and the characteristic length L, it is logical to use two-equation models, where each equation models one parameter. Therefore, we focus only on this kind of approximations for now.

In general the velocity q is calculated using the kinetic energy of the turbulence k. To evaluate k we can make use of the already know relation between the trace of the Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_{\mathrm{t}}$ and k, cf. (8.71). To get the equation of the kinetic energy of the turbulence k, we *simply* have to take the trace of the Reynolds-Stress equation. How we get this equations are discussed in the following sections.

8.8 Incompressible Reynolds-Stress Equation

To derive the Reynolds-Stress equation, we will use the Navier-Stokes equation (5.10) with bulk viscosity equals to zero, no source terms and incompressibility (dilatation term is zero). The start point for the derivation is:

$$\rho \frac{\partial u_i}{\partial t} + \rho \frac{\partial}{\partial x_j}(u_j u_i) = \frac{\partial}{\partial x_j}\left[2\mu\left\{\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right\}\right] - \frac{\partial p}{\partial x_i} \ . \tag{8.91}$$

To make life easier, we will split the convective term by using the product rule. Hence, we can remove one term due to the continuity equation (non-conserved equation). We get:

$$\rho \frac{\partial}{\partial x_j}(u_j u_i) = \rho u_j \frac{\partial u_i}{\partial x_j} + \underbrace{\cancel{\rho u_i \frac{\partial u_j}{\partial x_j}}}_{\text{continuity}} \ . \tag{8.92}$$

Replacing the convective term with the new form, put everything to the LHS and introduce the Navier-Stokes operator $\mathcal{N}$, we get:

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left[2\mu\left\{\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right\}\right] + \frac{\partial p}{\partial x_i} = \mathcal{N}(u_i) \ . \tag{8.93}$$

It is clear that the Navier-Stokes operator $\mathcal{N}$ has to be equal to zero and thus we can write:

$$\mathcal{N}(u_i) = 0 \ . \tag{8.94}$$

With the new information, we are able to derive the Reynolds-Stress equation. In order to form this equation we multiply the Navier-Stokes operator by the fluctuation with respect to the different space directions:

$$u_i'\mathcal{N}(u_j) + u_j'\mathcal{N}(u_i) = 0 \ . \tag{8.95}$$

The next step is to apply the expression (8.1) to the Navier-Stokes operator $\mathcal{N}(u_i)$ and average the whole equation by using the Reynolds time-averaging method (8.9). This leads to the following equation:

$$\overline{u_i'\mathcal{N}(\bar{u}_j + u_j') + u_j'\mathcal{N}(\bar{u}_i + u_i')} = 0 \ . \tag{8.96}$$

This equation has to be evaluated to get the Reynolds-Stress equation. The derivation itself is not a big deal but we have to have the feeling for different behaviors of the terms and hence, we need to be familiar with the mathematics. In the following, we will give a brief summary of the operations and relations and present the Reynolds-Stress equation without any derivation. The full derivation of this tensor equation is given in the appendix in section 12.1.

Operations and relations

For the derivation of the Reynolds-Stress equation we need to build the following tensor equation with formula (8.96):

$$\begin{aligned}
&\overline{u_x'\mathcal{N}(\bar{u}_x + u_x') + u_y'\mathcal{N}(\bar{u}_z + u_z')} + \overline{u_x'\mathcal{N}(\bar{u}_y + u_y') + u_y'\mathcal{N}(\bar{u}_x + u_x')} \\
+&\overline{u_x'\mathcal{N}(\bar{u}_z + u_z') + u_y'\mathcal{N}(\bar{u}_y + u_y')} + \overline{u_y'\mathcal{N}(\bar{u}_x + u_x') + u_z'\mathcal{N}(\bar{u}_z + u_z')} \\
+&\overline{u_y'\mathcal{N}(\bar{u}_y + u_y') + u_z'\mathcal{N}(\bar{u}_x + u_x')} + \overline{u_y'\mathcal{N}(\bar{u}_z + u_z') + u_z'\mathcal{N}(\bar{u}_y + u_y')} \\
+&\overline{u_z'\mathcal{N}(\bar{u}_x + u_x') + u_x'\mathcal{N}(\bar{u}_z + u_z')} + \overline{u_z'\mathcal{N}(\bar{u}_y + u_y') + u_x'\mathcal{N}(\bar{u}_x + u_x')} \\
+&\overline{u_z'\mathcal{N}(\bar{u}_z + u_z') + u_x'\mathcal{N}(\bar{u}_y + u_y')} = 0 \ .
\end{aligned}$$

For the derivation we further use the following relations, rules and tricks:

- Reynolds time-averaged terms that are linear in the fluctuation are zero ,
- The derivative $\frac{\partial u_i'}{\partial x_i} = 0$,

- Product rule (1.2) ,
- Adding and subtracting terms to be able to use the product rule; $g(x) = g(x) + f(x) - f(x)$.

If we use these assumptions, we can derive the Reynolds-Stress equation. The result of the derivation procedure is a more or less *complex* equation. Hence, the Reynolds-Stress equation is given as:

$$\boxed{\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial u_k} = -\bar{\sigma}_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \bar{\sigma}_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k} + C_{ijk}\right) + \epsilon_{ij} - \Pi_{ij}} \ . \tag{8.97}$$

After knowing the Reynolds-Stress equation, we are able to derive the equation for the kinetic energy of the turbulence k. The Reynolds-Stress equation also gives insight into the nature of the turbulent stresses and can be used to understand the turbulence in more detail or it can be used for further investigations in deriving more accurate turbulence models.

8.9 The Incompressible Kinetic Energy Equation

The derivation of the kinetic energy equation of the turbulence (per unit mass) for incompressible flows is simple after knowing the Reynolds-Stress equation due to the fact of the relation given by equation (8.67). In order to get the equation, we have to take the trace of equation (8.97). It follows:

$$\begin{aligned}&\mathrm{tr}\left\{\frac{\partial \sigma_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \sigma_{\mathrm{t}_{ij}}}{\partial u_k}\right\} \\ &\qquad = \mathrm{tr}\left\{-\sigma_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \sigma_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \sigma_{\mathrm{t}_{ij}}}{\partial x_k} + C_{ijk}\right) + \epsilon_{ij} - \Pi_{ij}\right\} .\end{aligned} \tag{8.98}$$

After applying the trace operator to each term we get:

For the time derivation we get:

$$\begin{aligned}\mathrm{tr}\left\{\frac{\partial \sigma_{\mathrm{t}_{ji}}}{\partial t}\right\} &= \frac{\partial \sigma_{\mathrm{t}_{xx}}}{\partial t} + \frac{\partial \sigma_{\mathrm{t}_{yy}}}{\partial t} + \frac{\partial \sigma_{\mathrm{t}_{zz}}}{\partial t} = -\rho \frac{\partial u'_x u'_x}{\partial t} - \rho \frac{\partial u'_y u'_y}{\partial t} - \rho \frac{\partial u'_z u'_z}{\partial t} \\ &= -\rho \frac{\partial}{\partial t} \underbrace{\left(u'_x u'_x + u'_y u'_y + u'_z u'_z\right)}_{(8.67) \to 2k} = \boxed{-2\rho \frac{\partial k}{\partial t}} \ .\end{aligned} \tag{8.99}$$

If we apply the trace operator to the convective term, we get:

$$\begin{aligned}
\mathrm{tr}\left\{\bar{u}_k \frac{\partial \sigma_{\mathrm{t}_{ij}}}{\partial u_k}\right\} &= \bar{u}_k \frac{\partial \sigma_{\mathrm{t}_{xx}}}{\partial u_k} + \bar{u}_k \frac{\partial \sigma_{\mathrm{t}_{yy}}}{\partial u_k} + \bar{u}_k \frac{\partial \sigma_{\mathrm{t}_{zz}}}{\partial u_k} \\
&= -\rho \bar{u}_k \frac{\partial \overline{u'_x u'_x}}{\partial u_k} - \rho \bar{u}_k \frac{\partial \overline{u'_y u'_y}}{\partial u_k} - \rho \bar{u}_k \frac{\partial \overline{u'_z u'_z}}{\partial u_k} \\
&= -\rho \bar{u}_k \frac{\partial}{\partial u_k}(\overline{u'_x u'_x} + \overline{u'_y u'_y} + \overline{u'_z u'_z}) = \boxed{-2\rho \bar{u}_k \frac{\partial k}{\partial u_k}} \, .
\end{aligned} \tag{8.100}$$

The first and second term of equation (8.97) lead to:

$$\mathrm{tr}\left\{-\sigma_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \sigma_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k}\right\} = -\sigma_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_i}{\partial x_k} - \sigma_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_i}{\partial x_k} = \boxed{2\rho \overline{u'_i u'_k} \frac{\partial \bar{u}_i}{\partial x_k}} \, . \tag{8.101}$$

The first part of the third term results in:

$$\begin{aligned}
\mathrm{tr}\left\{\frac{\partial}{\partial x_k}\left(\nu \frac{\partial \sigma_{\mathrm{t}_{ij}}}{\partial x_k}\right)\right\} &= \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \sigma_{\mathrm{t}_{xx}}}{\partial x_k}\right) + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \sigma_{\mathrm{t}_{yy}}}{\partial x_k}\right) + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \sigma_{\mathrm{t}_{zz}}}{\partial x_k}\right) \\
&= -\frac{\partial}{\partial x_k}\left(\rho\nu \frac{\partial \overline{u'_x u'_x}}{\partial x_k}\right) - \frac{\partial}{\partial x_k}\left(\rho\nu \frac{\partial \overline{u'_x u'_x}}{\partial x_k}\right) - \frac{\partial}{\partial x_k}\left(\rho\nu \frac{\partial \overline{u'_x u'_x}}{\partial x_k}\right) \\
&= -\frac{\partial}{\partial x_k}\left(\mu \frac{\partial}{\partial x_k}(\overline{u'_x u'_x} + \overline{u'_y u'_y} + \overline{u'_z u'_z})\right) \\
&= \boxed{-2\frac{\partial}{\partial x_k}\left(\mu \frac{\partial k}{\partial x_k}\right)} \, .
\end{aligned} \tag{8.102}$$

The second part of the third term, C_{ijk}, results in:

$$\mathrm{tr}\left\{\frac{\partial}{\partial x_k}\rho \overline{u'_i u'_j u'_k} + \frac{\partial}{\partial x_k}\left[\overline{p' u'_j}\delta_{ik} + \overline{p' u'_i}\delta_{jk}\right]\right\} = \boxed{\underline{\frac{\partial}{\partial x_j}\rho \overline{u'_j u'_i u'_i}} + 2\frac{\partial}{\partial x_j}\overline{p' u'_j}} \, . \tag{8.103}$$

The evaluation of the second term that includes the pressure can be done in an easy way. It is simply twice the trace of one of the terms. The first term is a third rank tensor $\mathbf{T}^3$ and the trace results in the underlined term on the RHS. This can be demonstrated by analyzing the first entries of the third rank tensor:

$$\mathrm{tr}\left(\rho \overline{u'_x u'_j u'_k}\right) = \mathrm{tr}\begin{bmatrix} \rho \overline{u'_x u'_x u'_x} & \rho \overline{u'_x u'_x u'_y} & \rho \overline{u'_x u'_x u'_z} \\ \rho \overline{u'_x u'_y u'_x} & \rho \overline{u'_x u'_y u'_y} & \rho \overline{u'_x u'_y u'_z} \\ \rho \overline{u'_x u'_z u'_x} & \rho \overline{u'_x u'_z u'_y} & \rho \overline{u'_x u'_z u'_z} \end{bmatrix} = \rho \overline{u'_x u'_i u'_i} \, . \tag{8.104}$$

In a similar way to C_{ijk}, the term ϵ_{ij} can be manipulated. Thus, we get:

$$\mathrm{tr}\left\{2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}\right\} = \boxed{2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}} \,. \tag{8.105}$$

The last term of equation (8.97), Π_{ij}, is zero due to the fact that $\frac{\partial u_i'}{\partial x_i} = 0$:

$$\mathrm{tr}\left\{\overline{p'\left[\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right]}\right\} = \overline{p'\left[\cancel{\frac{\partial u_x'}{\partial x}} + \cancel{\frac{\partial u_x'}{\partial x}}\right]} + \overline{p'\left[\cancel{\frac{\partial u_z'}{\partial y}} + \cancel{\frac{\partial u_y'}{\partial y}}\right]} + \overline{p'\left[\cancel{\frac{\partial u_z'}{\partial z}} + \cancel{\frac{\partial u_z'}{\partial z}}\right]} = 0 \,. \tag{8.106}$$

If we sum up all terms, we get the kinetic energy equation of the turbulence, k, for incompressible fluids:

$$-2\rho\frac{\partial k}{\partial t} - 2\rho\bar{u}_k\frac{\partial k}{\partial u_k} = 2\rho\overline{u_i'u_k'}\frac{\partial \bar{u}_i}{\partial x_k} - 2\frac{\partial}{\partial x_k}\left(\mu\frac{\partial k}{\partial x_k}\right) + \frac{\partial}{\partial x_k}\rho\overline{u_j'u_i'u_i'} + 2\frac{\partial}{\partial x_k}\overline{p'u_i'} + 2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}} \,. \tag{8.107}$$

Finally, we divide the whole equation by -2 to get the final form of the incompressible kinetic energy equation:

$$\rho\frac{\partial k}{\partial t} + \rho\bar{u}_k\frac{\partial k}{\partial u_k} = \underbrace{-\rho\overline{u_i'u_k'}\frac{\partial \bar{u}_i}{\partial x_k}}_{P_k} + \frac{\partial}{\partial x_k}\left(\mu\frac{\partial k}{\partial x_k}\right) \underbrace{-\frac{\partial}{\partial x_j}\frac{\rho}{2}\overline{u_j'u_i'u_i'} - \frac{\partial}{\partial x_j}\overline{p'u_j'}}_{\text{turbulent diffusion}} - \underbrace{\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}}_{\text{dissipation } \epsilon} \,. \tag{8.108}$$

If we merge the terms that include the turbulent diffusion, use the term P_k, that denotes the production rate of the kinetic energy and the acronym ϵ, we end up with the common kinetic energy equation as:

$$\boxed{\rho\frac{\partial k}{\partial t} + \rho\bar{u}_k\frac{\partial k}{\partial u_k} = \frac{\partial}{\partial x_k}\left(\mu\frac{\partial k}{\partial x_k}\right) + P_k - \frac{\partial}{\partial x_j}\left[\frac{\rho}{2}\overline{u_j'u_i'u_i'} + \overline{p'u_j'}\right] - \epsilon} \,. \tag{8.109}$$

The production rate and turbulent diffusion term has to be modeled. For the turbulent diffusion we use the assumption that the diffusion is based on the gradients:

$$-\left[\frac{\rho}{2}\overline{u_j'u_i'u_i'} + \overline{p'u_j'}\right] \approx \frac{\mu_t}{\mathrm{Pr}_t}\frac{\partial k}{\partial x_j} \ . \tag{8.110}$$

Here, Pr_t denotes the turbulent Prandtl number and is assumed to be one. In the literature we it is also common to denote the turbulent Prandtl number by σ_k. Due to the fact that we use sigma to describe any kind of stress tensor, we avoid the usage of another sigma quantity here.

The production rate is modeled with the assumption given by equation (8.64) but with the difference, that we do not need the term $-2\rho k$; **Recall**: This term was just added to equilibrate both sides. Hence, the production rate term is given by:

$$P_k = -\rho\overline{u_i'u_j'}\frac{\partial \bar{u}_i}{\partial x_j} \approx \mu_t\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_i}{\partial x_j}\right)\frac{\partial \bar{u}_i}{\partial x_j} \ . \tag{8.111}$$

The dissipation ϵ, that describe the transfer of the turbulence into internal energy (a better description given in the next section), is coupled to a characteristic length scale L.

Recall: After we derived the RANS equations, we figured out that we need to calculate the Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_t$. To get this value we introduced the Boussinesq eddy viscosity hypothesis and related the eddy viscosity μ_t to a characteristic length scale L and a velocity q. Up to now, we eliminated one unknown ($q = \sqrt{k}$) by using the kinetic energy k but we also introduced a new unknown quantity, the dissipation ϵ. Thus, we still have two unknown, the length scale L and the dissipation ϵ. The good thing is, both quantities can be related.

8.10 The Relation between ϵ and L

The most common equation that is used to estimate the length scale L is based on the observation that the dissipation phenomena can also be observed in the energy transport and thus in its equation. In fluid flows which are in a so called turbulent equilibrium, it is possible to derive a relation between the kinetic energy k, the length scale L and the dissipation ϵ:

$$\epsilon \approx \frac{k^{\frac{3}{2}}}{L} \ . \tag{8.112}$$

The idea behind this relation is the so called **energy cascade** for high turbulent flow fields (high Reynolds numbers). The concept can be described as follows: The kinetic energy of the turbulence is transformed from big scale eddies to small scale eddies. If we reach the smallest scale (this vortexes are named Kolmogorov vortexes), the viscose effect will transfer the energy of motion into internal energy. This phenomena is called dissipation.

8.11 The Equation for the Dissipation Rate ϵ

To calculate the length scale L and close the equation for the turbulent energy k, we need the equation for the dissipation ϵ. This equation can be derived by using the Navier-Stokes equation (like we did for the Reynolds-Stress equation) but due to the fact that most terms on the RHS have to be modeled, we should describe this equation more like a model than an exact equation. Hence, the complete derivation is not shown. In general we are using the following equation for the dissipation ϵ:

$$\rho \frac{\partial \epsilon}{\partial t} + \rho \bar{u}_j \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon 1} P_k \frac{\epsilon}{k} - \rho C_{\epsilon 2} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left(\frac{\mu_{\mathrm{t}}}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right) \tag{8.113}$$

As we can see, the whole right side is more like a playground of parameters and assumptions than a real fundamental equation. But the equation allows us to estimate the dissipation ϵ. The quantity can than be used for the kinetic energy equation and allows us to estimate the length scale L and hence, we are able to approximate the the eddy viscosity μ_{t}.

Now we can rewrite the Boussinesq eddy hypothesis (8.90) with the new quantities:

$$\mu_{\mathrm{t}} = \rho C_\mu \sqrt{k} L = \rho C_\mu \sqrt{k} \frac{\sqrt{k^3}}{\epsilon} = \rho C_\mu \frac{k^2}{\epsilon} \ . \tag{8.114}$$

The model parameters of the equations above are:

$$C_\mu = 0.09 \ , \quad C_{\epsilon_1} = 1.44 \ , \quad C_{\epsilon_2} = 1.92 \ , \quad \sigma_\epsilon = 1.3 \ .$$

8.12 Coupling of the Parameters

As we could see in the last sections, the turbulence modeling is a complex topic. The easiest equations for the turbulence modeling were derived. Furthermore, we observed that all parameters are coupled. The kinetic energy of the turbulence k, the length scale L, the dissipation ϵ and the eddy viscosity μ_{t}.

There are a lot of more considerations that have to be taken into account if turbulence modeling is used. Just think about the turbulence behavior close to the walls compared to the far field. Another example would be the turbulence modeling of flow separation. The section about the turbulence model gave us a feeling that the topic about turbulent flows are extreme complex. A lot of research was done and till today the turbulence has still to be modeled and can only be applied and resolved with all details for a couple of problems.

In the literature we will find different equations that give reasonable results for a special kind of problem(s). Good references for further investigations into the turbulence modeling are the books of Ferziger and Perić [2008], Bird et al. [1960] and Wilcox [1994].

8.13 Turbulence Modeling for Compressible Fluids

As already discussed during the Reynolds averaging procedure for the incompressible mass conservation equation, the varying density has to be taken into account during for compressible fluids. Therefore, we get:

$$\rho = \bar{\rho} + \rho' \ . \tag{8.115}$$

This lead to more unknown terms that will make the problem even more complex; compare the already derived Reynolds time-averaged compressible mass conservation equation (8.24) which is given again:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i + \overline{\rho' u_i'}) = 0 \ . \tag{8.116}$$

Here we need approximations for the correlation between ρ' and u_i', that are vanishing for incompressible fluids. If we go further and think about the momentum equations, we can imagine, that things get even worse.

To get rid of the additional correlation between ρ' and u_i', we introduce a mathematical method suggested by Favre. This concept is based on mathematics and therefore not physical correct. What we do is simple. We introduce a mass-averaged velocity field $\tilde{u}_i$, that is defined as:

$$\tilde{u}_i = \frac{1}{\bar{\rho}} \lim_{T\to\infty} \int_t^{t+T} \rho(t,x) u_i(t,x) \mathrm{d}\tau \ . \tag{8.117}$$

Here, $\bar{\rho}$ denotes the Reynolds time-averaged density and the tilde above the velocity u_i marks the quantity to be Favre averaged instead of Reynolds averaged. In terms of the Reynolds time-averaging procedure we are allowed to say:

$$\bar{\rho}\tilde{u}_i = \overline{\rho u_i} \ . \tag{8.118}$$

To show what happens here, we will expand the RHS:

$$\bar{\rho}\tilde{u}_i = \overline{(\bar{\rho}+\rho')(\bar{u}_i+u_i')} = \overline{\bar{\rho}\bar{u}_i} + \cancel{\overline{\bar{\rho}u_i'}} + \cancel{\overline{\rho'\bar{u}_i}} + \overline{\rho' u_i'} = \bar{\rho}\bar{u}_i + \overline{\rho' u_i'} \ . \tag{8.119}$$

If we use this expression for equation (8.116), we end up with:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i) = 0 \ . \tag{8.120}$$

This equation looks just similar to the laminar mass conservation or the Reynolds time-averaged equation. Wilcox [1994] explained this kind of averaging as follows:

≫*What we have done is treat the momentum per unit volume, ρu_i, as the depended variable rather than the velocity. This is a sensible thing to do from a physical point of view,..*≪.

If you are interested into that kind of averaging, a lot of information can be found in Wilcox [1994] and Bird et al. [1960].

Note: The key argument to use the Favre averaging procedure is to simplify the averaging procedure and get rid of additional correlations that have to be modeled. Hence, we end up with the same set of equations for incompressible turbulent flow fields but now we use the Favre-weighted quantities.

Chapter 9

Calculation of the Shear-Rate Tensor in OpenFOAM®

In this chapter we will discuss the implementation of the calculation of the shear-rate tensor $\boldsymbol{\tau}$, $\bar{\boldsymbol{\tau}}_{\mathrm{t}}$ or $\tilde{\boldsymbol{\tau}}_{\mathrm{t}}$; real, Reynolds-averaged or Favre-averaged quantities. In OpenFOAM® we calculate the shear-rate tensor by calling the functions `divDevReff` or `divDevRhoReff`.

The following discussion is based on the OpenFOAM® version 2.3.1. Be prepared that the code can look different for other versions. If you are asking yourself for that reason, you have to understand the concept of *hacking*. For those who are interested you can read the book of Erickson [2014].

9.1 The Inco. Shear-Rate Tensor, divDevReff

For incompressible fluids, the momentum equation that is going to be constructed in the *UEqn.H* file looks equal to the following code (snippet from pimpleFoam):

```
tmp<fvVectorMatrix> UEqn
(
      fvm::ddt(U)                   (I)
    + fvm::div(phi, U)              (II)
    + MRF.DDt(U)                    (III)
    + turbulence->divDevReff(U)     (IV)
    ==
      fvOptions(U)                  (V)
);
```

Listing 9.1: $FOAM_SOLVERS/incompressible/pimpleFoam/UEqn.H

Lets analyze the code. First of all we observe different terms. The first one is the time derivation (I). The second term is the convective term (II). After that, some additional correction term due to MRF (III) is added. The next one is the the shear-rate tensor (IV) and finally we have a term (V) that handles additional sources within the *fvOptions* dictionary.

For now we will focus on the term (IV) `turbulence->divDevReff(U)`. First of all, we will discuss the meaning of the name `divDevReff`:

$$\nabla \bullet \boldsymbol{\tau} = \nabla \bullet \boldsymbol{\sigma}^{\mathrm{dev}} \tag{9.1}$$

The divergence of the shear-rate tensor is equal to the divergence of the deviatoric part of the stress tensor $\boldsymbol{\sigma}$. The R comes from the Reynolds-Average approach. An additional Rho defines if we are using a density based or non density based solver. Finally we are interested in the effective transport which includes laminar and turbulent transport phenomena. Therefore, we get the name `divDevReff` for incompressible and `divDevRhoReff` for compressible fluids.

The analyze of the function is very simple and can be checked with the code source guide named **Doxygen**.

The object named `turbulence`, which is based on the general *turbulenceModel* class and further derived from the *incompressibleTurbulenceModel* class, will call the function `divDevReff(U)`. The corresponding function that is called and implemented is:

```
tmp<fvVectorMatrix> laminar::divDevReff(volVectorField& U) const
{
    return
    (
      - fvm::laplacian(nuEff(), U)
      - fvc::div(nuEff()*dev(T(fvc::grad(U))))
    );
}
```

Listing 9.2: .../turbulenceModel/incompressible/RAS/laminar/laminar.C

First, we can see that we have the kinematic viscosity included, which indicates incompressible equations. The second thing that can be observed is the fact, that we calculate one part implicit (`fvm`) and another part explicit (`fvc`). Furthermore, a new function named `dev()` is called.

The new function `dev()` is implemented as:

```
template<class Cmpt>
inline Tensor<Cmpt> dev(const Tensor<Cmpt>& t)
{
    return t - SphericalTensor<Cmpt>::oneThirdsI*tr(t);
}
```

Listing 9.3: $FOAM_SRC/OpenFOAM/primitives/Tensor/TensorI.H

Analyzing the C++ Functions

Starting with the function `dev()`, we can see that the function simply calculates the deviatoric part of the matrix, cf. (1.31). Therefore, we can write:

$$\mathbf{A}^{\text{dev}} = \mathbf{A} - \mathbf{A}^{\text{hyd}} = \mathbf{A} - \frac{1}{3}\,\text{tr}(\mathbf{A})\mathbf{I}\ . \tag{9.2}$$

In addition, the function `dev()` needs an argument. The argument is the transposed matrix that we get, if we build the dyadic product of the two vectors, Nabla ∇ and the velocity vector $\mathbf{U}$. Thus, we can write:

$$\mathbf{A} = \left[\text{grad}(\bar{\mathbf{U}})\right]^T = \left[\nabla \otimes \bar{\mathbf{U}}\right]^T\ . \tag{9.3}$$

If we express the C++ code with the expressions above, we can rewrite the code into a mathematic form. Hence, the first term of the `divDevReff` function can be written as:

$$-\,\text{fvm} :: \text{laplacian}(\nu_{\text{eff}}, \bar{\mathbf{U}}) = -\nabla \bullet \left(\nu_{\text{eff}}(\nabla \otimes \bar{\mathbf{U}})\right)\ , \tag{9.4}$$

the second term is equal to:

$$-\,\text{fvc} :: \text{div}(\nu_{\text{eff}} * \text{dev}(\text{T}(\text{fvc} :: \text{grad}(\bar{\mathbf{U}})))) = -\nabla \bullet \left(\nu_{\text{eff}} * \text{dev}((\nabla \otimes \bar{\mathbf{U}})^T)\right)\ , \tag{9.5}$$

and the `dev`-function is similar to:

$$\text{dev}((\nabla \otimes \bar{\mathbf{U}})^T) = (\nabla \otimes \bar{\mathbf{U}})^T - \frac{1}{3}\,\text{tr}((\nabla \otimes \bar{\mathbf{U}})^T)\mathbf{I}\ . \tag{9.6}$$

Finally, we are able to put all terms together and end up with:

$$-\nabla \bullet \bar{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \left(\nu_{\text{eff}}(\nabla \otimes \bar{\mathbf{U}})\right) - \nabla \bullet \left(\nu_{\text{eff}}\left[(\nabla \otimes \bar{\mathbf{U}})^T - \frac{1}{3}\,\text{tr}((\nabla \otimes \bar{\mathbf{U}})^T)\mathbf{I}\right]\right)\ . \tag{9.7}$$

After we push the first term into the second one:

$$-\nabla \bullet \bar{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \left(\nu_{\text{eff}} (\nabla \otimes \bar{\mathbf{U}}) + \nu_{\text{eff}} (\nabla \otimes \bar{\mathbf{U}})^T - \frac{1}{3} \nu_{\text{eff}} \operatorname{tr}((\nabla \otimes \bar{\mathbf{U}})^T) \mathbf{I} \right) \quad , \tag{9.8}$$

and rewrite the last term by using the relation (7.9), we end up with:

$$-\nabla \bullet \bar{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \left(\nu_{\text{eff}} (\nabla \otimes \bar{\mathbf{U}}) + \nu_{\text{eff}} (\nabla \otimes \bar{\mathbf{U}})^T - \frac{1}{3} \nu_{\text{eff}} \underbrace{\cancel{(\nabla \bullet \bar{\mathbf{U}})}}_{\text{continuity}} \mathbf{I} \right) \quad . \tag{9.9}$$

The last term is zero due to the continuity equation. Therefore, the effective shear-rate tensor $\bar{\boldsymbol{\tau}}_{\text{eff}}$ for incompressible fluids is calculated as:

$$\begin{aligned} -\nabla \bullet \bar{\boldsymbol{\tau}}_{\text{eff}} &= -\nabla \bullet \underbrace{\left(\nu_{\text{eff}} (\nabla \otimes \bar{\mathbf{U}}) + \nu_{\text{eff}} (\nabla \otimes \bar{\mathbf{U}})^T \right)}_{\bar{\boldsymbol{\tau}}_{\text{eff}}} \\ &= -\nabla \bullet \left(2\nu_{\text{eff}} \underbrace{\left[\frac{1}{2} \left\{ (\nabla \otimes \bar{\mathbf{U}}) + (\nabla \otimes \bar{\mathbf{U}})^T \right\} \right]}_{\text{deformation rate tensor } \bar{\mathbf{D}}} \right) \quad . \end{aligned} \tag{9.10}$$

As we demonstrated now, the calculation of the incompressible shear-rate tensor is correct implemented into the version 2.3.1 because the derived equation is similar to equation (5.36). The sign difference of the term corresponds to the position at the LHS in OpenFOAM® whereas in equation (5.36) the shear-rate tensor stands on the RHS.

Stability

During the analyze of the function, we figured out that the term $\frac{1}{3}\nu_{\text{eff}} \operatorname{tr}(\nabla \otimes \mathbf{U})$ is kept. The reason for that is based on numerics. The term simply stabilizes the calculation because the continuity equation is never 100% zero. This is based on the discretization, interpolation and accuracy of the machine.

In newer OpenFOAM® versions like 4.x, the incompressible solvers will call `dev2()` that is normally used for compressible flows. The difference of `dev2` and `dev` will be shown later and is simple a difference of the factor two at some position of the code. However, due to the continuity equation, we can cancel the additional term again and hence, the equation is also valid. If we are using `dev2()` instead of `dev()` for incompressible solvers will lead to an even better stabilization and convergence rate. This is the reason why it was introduced in OpenFOAM® 3.0.0.

9.2 The Compr. Shear-Rate Tensor, divDevRhoReff

If we focus on compressible fluids, the shear-rate tensor has a different formulation. The constructed momentum equation looks similar to the one we had for incompressible fluids but now we have the density included and we call a new function named `divDevRhoReff`. The code snippet is based on rhoPimpleFoam.

```
tmp<fvVectorMatrix> UEqn
(
    fvm::ddt(rho, U)                (I)
      + fvm::div(phi, U)                (II)
      + MRF.DDt(rho, U)                 (III)
      + turbulence->divDevRhoReff(U)    (IV)
      ==
      fvOptions(rho, U)                 (V)
);
```

Listing 9.4: $FOAM_SOLVERS/compressible/rhoPimpleFoam/UEqn.H

As before, we have the time derivation (I), the convective (II), some additional correction due to MRF (III), the shear-rate tensor (IV) and the term (V) that handles additional sources within the *fvOptions* dictionary.

For the analyze of the function, we proceed like before. First we investigate into the call of the function `turbulence->divDevRhoReff(U)`.

Note: The keyword `Rho` is now included in the name of the function. This indicates that we calculate the shear-rate tensor based on the theory for compressible fluids. Thus, the dilatation term is included due to expansion and compression phenomena which can be related to the non-constant density.

The shear-rate tensor that is calculated for a compressible fluid is given below.

```
tmp<fvVectorMatrix> laminar::divDevRhoReff(volVectorField& U) const
{
    return
    (
      - fvm::laplacian(muEff(), U)
      - fvc::div(muEff()*dev2(T(fvc::grad(U))))
    );
}
```

Listing 9.5: .../turbulenceModel/compressible/RAS/laminar/laminar.C

The function is similar to `dev()` but now we have the molecular instead of the kinematic viscosity and call a new function named `dev2`. The code of the new function is presented below. It is *somehow* calculating the deviatoric part of a tensor but subtraction twice the hydrostatic part instead of once. The reason for that is obvious after we analyze the code snippet.

```
template<class Cmpt>
inline Tensor<Cmpt> dev2(const Tensor<Cmpt>& t)
{
    return t - SphericalTensor<Cmpt>::twoThirdsI*tr(t);
}
```

Listing 9.6: OpenFOAM/primitives/Tensor/TensorI.H

Analyzing the C++ Functions

The argument that is return by the function `dev2()` represents equation (1.31) with the already mentioned difference that we subtract the hydrostatic part twice; `twoThirdsI`:

$$\mathbf{A}^{\text{dev}} = \mathbf{A} - 2\mathbf{A}^{\text{hyd}} = \mathbf{A} - \frac{2}{3}\,\text{tr}(\mathbf{A})\mathbf{I} \tag{9.11}$$

The argument of the function `dev2()` is equal to the one we had in the incompressible case. Hence, it can be evaluated by (9.3). Rewriting the C++ code into the different equations, we are able to rewrite the first term as:

$$-\nabla \bullet \tilde{\boldsymbol{\tau}}_{\text{eff}} = -\text{fvm} :: \text{laplacian}(\mu_{\text{eff}}, \tilde{\mathbf{U}}) = -\nabla \bullet \left(\mu_{\text{eff}}(\nabla \otimes \tilde{\mathbf{U}})\right) \ , \tag{9.12}$$

the second term to:

$$-\,\text{fvc} :: \text{div}(\mu_{\text{eff}} * \text{dev2}(\text{T}(\text{fvc} :: \text{grad}(\tilde{\mathbf{U}})))) = -\nabla \bullet \left(\mu_{\text{eff}} * \text{dev2}((\nabla \otimes \tilde{\mathbf{U}})^T)\right) \ , \tag{9.13}$$

and the third term like:

$$\text{dev2}((\nabla \otimes \tilde{\mathbf{U}})^T) = (\nabla \otimes \tilde{\mathbf{U}})^T - \frac{2}{3}\,\text{tr}((\nabla \otimes \tilde{\mathbf{U}})^T)\mathbf{I} \tag{9.14}$$

After combining the three terms, it follows:

$$-\nabla \bullet \tilde{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \left(\mu_{\text{eff}}(\nabla \otimes \tilde{\mathbf{U}})\right) - \nabla \bullet \left(\mu_{\text{eff}}\left[(\nabla \otimes \tilde{\mathbf{U}})^T - \frac{2}{3}\,\text{tr}((\nabla \otimes \tilde{\mathbf{U}})^T)\mathbf{I}\right]\right) \ . \tag{9.15}$$

After we pushed the divergence operator out, we get:

$$-\nabla \bullet \tilde{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \left(\mu_{\text{eff}}(\nabla \otimes \tilde{\mathbf{U}}) + \mu_{\text{eff}} \left[(\nabla \otimes \tilde{\mathbf{U}})^T - \frac{2}{3}\,\text{tr}((\nabla \otimes \tilde{\mathbf{U}})^T)\mathbf{I} \right] \right) \ . \quad (9.16)$$

By eliminating the brackets inside, it follows:

$$-\nabla \bullet \tilde{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \left(\mu_{\text{eff}} \nabla \otimes \tilde{\mathbf{U}} + \mu_{\text{eff}}(\nabla \otimes \tilde{\mathbf{U}})^T - \frac{2}{3}\mu_{\text{eff}}\,\text{tr}((\nabla \otimes \tilde{\mathbf{U}})^T)\mathbf{I} \right) \ , \quad (9.17)$$

and finally, we get the known shear-rate tensor by using equation (7.9) as:

$$-\nabla \bullet \tilde{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \underbrace{\left(\mu_{\text{eff}} \nabla \otimes \tilde{\mathbf{U}} + \mu_{\text{eff}}(\nabla \otimes \tilde{\mathbf{U}})^T - \frac{2}{3}\mu_{\text{eff}}(\nabla \bullet \tilde{\mathbf{U}})\mathbf{I} \right)}_{\text{effective shear-rate tensor } \bar{\boldsymbol{\tau}}_{\text{eff}}} \ . \quad (9.18)$$

To get a more familiar equation, we do some simple mathematics and end up with:

$$-\nabla \bullet \tilde{\boldsymbol{\tau}}_{\text{eff}} = -\nabla \bullet \left(2\mu_{\text{eff}} \underbrace{\left[\frac{1}{2} \left\{ (\nabla \otimes \tilde{\mathbf{U}}) + (\nabla \otimes \tilde{\mathbf{U}})^T \right\} \right]}_{\text{deformation rate tensor } \tilde{\mathbf{D}}} - \frac{2}{3}\mu_{\text{eff}}(\nabla \bullet \tilde{\mathbf{U}})\mathbf{I} \right) \ . \quad (9.19)$$

As we demonstrated, the calculation of the compressible shear-rate tensor is implemented in OpenFOAM® correctly. The equation above is equal to the averaged shear-rate tensor $\bar{\boldsymbol{\tau}}$ in equation (8.86) with the difference that we use Favre averaged quantities here. As before, the difference in the sign is based on to the fact that the term stands on the LHS in OpenFOAM®.

9.3 Influence of Turbulence Models

If we use a compressible based solver in OpenFOAM® and simulate a laminar flow pattern, the momentum equation will not change based on the fact that it is hard coded. The question now is, what happens if we do so (not use a turbulence model)?

As we saw in the chapters above, the equations for full resolved eddies, Reynolds-Averaged or Favre-Averaged flow fields are identical. The only difference is related to the viscosity. Hence, if we do not use a turbulence model, the contribution of the eddy viscosity μ_{t} is zero. It follows:

$$\mu_{\text{eff}} = \mu_{\text{l}} + \cancel{\mu_{\text{t}}} \ . \quad (9.20)$$

Chapter 10

SIMPLE, PISO and PIMPLE algorithm

Solving the Navier-Stokes equations requires numerical techniques for coupling the pressure and momentum quantities. This is done by the common `SIMPLE`, `PISO` and `PIMPLE` algorithms. Why we need these numerical methods can be understood after we introduce the difficulties that come into handy when we solve the equations. Further information about these algorithms can be found in Ferziger and Perić [2008] and Moukalled et al. [2015].

Let us consider the general momentum equation (2.26) and apply the incompressibility character – the density is constant and can be taken out of the derivatives –, we get:

$$\rho \frac{\partial \mathbf{U}}{\partial t} = -\rho \nabla \bullet (\mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau} - \nabla p + \rho \mathbf{g} \ . \tag{10.1}$$

Note: In the above equation we did not introduce the shear-rate tensor. Thats why the sign is negative.

Now we divide the whole equation by the density ρ. Hence, $\boldsymbol{\tau}$ has to be expressed by equation (5.36) and it follows:

$$\frac{\partial \mathbf{U}}{\partial t} = -\nabla \bullet (\mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau}_{\text{inco}} - \nabla \frac{p}{\rho} + \mathbf{g} \ . \tag{10.2}$$

Based on the fact that the density is constant, there is no need to solve any energy equation and we only need to solve the momentum equation. As we can see, there are four unknown quantities, the pressure p and the three velocity components denoted by $\mathbf{U}$. The problem is, that we have four unknown and three equations (momentum in x, y and z). The remaining equation that we can use it the mass conservation equation (2.13) but this equation even does not have the pressure included and therefore we need some special techniques to solve the momentum equation. This is also known as the *pressure-momentum coupling* problem.

The idea, to get rid of the problem, is to use the mass conservation equation somehow. What we finally do, is to apply the divergence operator onto the momentum equation. After doing a semi-discretization, that means, we only discretized the time derivative while the space derivatives are kept in partial differential form, we can use the mass conservation equation to eliminate terms and end up with the well known Poisson equation for the pressure p.

Now we have an equation for the momentum and the pressure. In general these equations are solved sequential. That means, that we solve for U_x while we keep all other variables constant. In other words, we first solve the equation for U_x, then for U_y, then for U_z and then for p.

The strategy now is to find a pressure and momentum field that fulfill the mass conservation and of course the case conditions at some defined time. This is achieved within the pressure-momentum coupling algorithms `PISO`, `SIMPLE` and `PIMPLE`. As a simple rule (not valid all the time), we can say:

- `SIMPLE`:= Semi-Implicit-Method-Of-Pressure-Linked-Equations.
  In OpenFOAM® we are using this algorithm for steady-state analyzes.

- `PISO`:= Pressure-Implicit-Split-Operator.
  In OpenFOAM® we are using this algorithm for transient calculation. The calculation is limited in the time step based on the Courant number.

- `PIMPLE`:= Merged `PISO`–`SIMPLE`.
  This algorithm combines both algorithms and allows us to use bigger time-steps (Co >> 1).

Note: There is a family of different algorithms available. For example, the `SIMPLE` algorithm is not consistent. That means, that during the derivation of the pressure equation, we neglect one term. Therefore, different investigations were done to calculate the missing term and are known under the terms of `SIMPLER`, `SIMPLEM`, `SIMPLEC` and so on. A very good overview is given in Moukalled et al. [2015].

10.1 The `SIMPLE` algorithm in OpenFOAM®

If we use any kind of `SIMPLE` based solver in OpenFOAM®, we do not have a time derivation. A time derivation is normally a natural limiter for the solution. That means, for a special time interval Δt, the solution can only go on by this time step and not further. Based on the fact that we do not have the time derivation within that algorithm, we are only interested in the steady-state behavior and based on the missing *natural limiter* Δt and the fact that the `SIMPLE` algorithm is not consistent (missing term), we need to under-relax the equations to achieve stability. Otherwise, the solver just blow up and gives a *floating point exception* (dividing by zero).

Furthermore, the time step Δt should be always set to 1. Doing that, the time will indicate the number of iterations that we did within the `SIMPLE` loop. Changing the time step to other values will *not influence* the solution. It simply let us reach the *pseudo end time* faster or not. In other word, we do more or less iterations. Of course, changing Δt can affect the results but only if we will do not reach the steady state solution.

For the `SIMPLE` algorithm it is very important to estimate the relaxation factors for the fields and equations for good stability and fast convergence rate.

10.1.1 `SIMPLEC` in OpenFOAM®

In the release version 3.0.0, the `SIMPLEC` algorithm can be used in all `SIMPLE` and `PIMPLE` operating algorithms. For that purpose, we have to add some special keyword to the `SIMPLE` or `PIMPLE` control dictionary in the `fvSolutions` file. Activating the `SIMPLEC` method can be done by adding the following keyword:

```
SIMPLE
{
    consistent   true;
}

PIMPLE
{
    consistent   true;
}
```

Listing 10.1: `SIMPLE` operating in `SIMPLEC` mode

As already mentioned in the previous section, the `SIMPLEC` algorithm include the missing pressure term. The added character »`C`« stands for consistency.

Using the `SIMPLEC` method will require more iterations for each single segregated calculation step but the convergence rate will increased. The release notes report a speed-up of three times. Furthermore, larger values for the under-relaxation factors can be choosen.

Note: The `consistency` keyword can be added to the `PIMPLE` dictionary too, but will only affect the algorithm, if we operate in the `PIMPLE` mode. Otherwise, this keyword will not affect the numerical procedure. How to use the `PIMPLE` algorithm correct, will be discussed later.

10.2 The `PISO` algorithm in OpenFOAM®

The two main differences to the `SIMPLE` algorithm are the included time derivation term and the consistency of the pressure-velocity coupling equation. Based on this two additional criteria, we do not need to under-relax the fields and equations but need to fulfill a stability criterion. Based on the simulation type, we have to make sure that the so called Courant number is not larger than one.

The Courant number can be visualized as follows: If the dimensionless number is smaller than one, the information from one cell can only reach the next neighbor cell within one time step. Otherwise, the information can reach a second or third neighbor cell which is not allowed based on some explicit aspects. Therefore, the Courant number has to be smaller than one. In general, a small value has to be considered at the beginning of a simulation, which can then be increased to some – case depended – value.

$$\mathrm{Co} = \frac{\mathbf{U}\Delta t}{\Delta x} \ . \tag{10.3}$$

The Courant number depends on the local cell velocity $\mathbf{U}$, the time step Δt and the distant between the cells Δx. In OpenFOAM®, the calculation is based on the cell volume and not on the distance Δx. Based on formula (10.3), we can derive the following aspects:

- The higher the local cell velocity $\mathbf{U}$, the larger the Courant number,
- The larger the time step Δt, the larger the Courant number,
- The smaller the distance Δx, the larger the Courant number.

The main aspect here is, that if we refine the mesh, increase the velocity or the time step, the Courant number will increase. To fulfill the criteria in equation (10.3), the time step has to be adjusted based on the mesh size and the velocity.

Note: The criteria has to be fulfilled for each cell. That means, that one bad cell can limit the whole simulation.

10.3 The `PIMPLE` algorithm in OpenFOAM®

The `PIMPLE` algorithm is one of the most used one if we have transient problems because it combines the `PISO` and `SIMPLE` (`SIMPLEC`) one. The advantage is, that we can use larger Courant numbers (Co >> 1) and therefore, the time step can be increased drastically.

The principal of the algorithm is as follows: Within one time step, we search a steady-state solution with under-relaxation. After we found the solution, we go on in time. For this, we need the so called outer correction loops, to ensure that *explicit* parts of the equations are converged. After we reach a defined tolerance criterion within the steady-state calculation, we leave the outer correction loop and move on in time. This is done till we reach the end time of the simulation.

Note: The `PIMPLE` algorithm in OpenFOAM® can also work in `PISO` mode, if we set the **`nOuterCorrectors`** to zero. This can be checked, if we start any `PIMPLE` solver. The output should be as follow:

```
Create mesh for time = 0

PIMPLE: Operating solver in PISO mode
```

Listing 10.2: The output of the pimple algorithm

10.4 The correct usage of the PIMPLE algorithm

The usage of the `PIMPLE` algorithm is explained and discussed within this section. First of all, the settings that can be set for controlling the algorithm has to be written into the *fvSolution* dictionary. Here, we need to define the algorithm control dictionary named `PIMPLE`.

```
PIMPLE
{
    //- Settings that we can made
}
```

Listing 10.3: The control dictionary within the fvSolution file

The keyword has to be added to the *fvSolution* file, otherwise the solver will through out an error. Nevertheless, it is sufficient just to create an empty dictionary. If we do so, the code will use default values based on the constructor of the class.

```
// * * * * * * * * * * * * * * Constructors  * * * * * * * * * * * * //

Foam::pimpleControl::pimpleControl
(
  fvMesh& mesh,
  const word& dictName
)
:
    solutionControl(mesh, dictName),
    nCorrPIMPLE_(0),
    nCorrPISO_(0),
    corrPISO_(0),
    turbOnFinalIterOnly_(true),
    converged_(false)
{
    read();
```

Listing 10.4: The constructor of the pimpleControl class

As we can see, the constructor will initialize all values with zero first, and set two booleans. One to `true` and the other one to `false`. After that, we go into the read function. Here, we will read the `PIMPLE` dictionary in the *fvSolution* file. If there is no entry to read, the default values are set. For the `nOuterCorrectors` a value of one is used. The same is valid for the `nCorrectors`. Finally the `turbOnFinalIterOnly` is set to false. If this switch is turned on, we solve the turbulence equation within each outer loop, otherwise we only solve it at the last iteration, after we leave the outer loop to go on in time.

```
// * * * * * * * * * * Protected Member Functions  * * * * * * * * * //

void Foam::pimpleControl::read()
{
    solutionControl::read(false);

    // Read solution controls
    const dictionary& pimpleDict = dict();
    nCorrPIMPLE_ = pimpleDict.lookupOrDefault<label>
    (
        "nOuterCorrectors",
        1
    );
    nCorrPISO_ = pimpleDict.lookupOrDefault<label>("nCorrectors", 1);
    turbOnFinalIterOnly_ =
        pimpleDict.lookupOrDefault<Switch>
        (
            "turbOnFinalIterOnly",
            true
        );
}
```

Listing 10.5: The read function of the pimpleControl class

In addition, we see that the `nOuterCorrectors` are related to the `PIMPLE` and the `nCorrectors` (inner loops) to the `PISO` algorithm.

The `read()` function will also call another `read(argument)` function from the *solutionControl* class. Here, we initialize other essential algorithm control parameters like the `nNonOrthogonalCorrectors`, `momentumPredictor`, `transonic`, `consistent` and `residualControls` (not shown in the code).

```
// * * * * * * * * * * Protected Member Functions  * * * * * * * * * //

void Foam::solutionControl::read(const bool absTolOnly)
{
    const dictionary& solutionDict = this->dict();

    // Read solution controls
    nNonOrthCorr_ =
        solutionDict.lookupOrDefault<label>
        (
```

```
            "nNonOrthogonalCorrectors",
            0
        );
    momentumPredictor_ =
        solutionDict.lookupOrDefault("momentumPredictor", true);
    transonic_ = solutionDict.lookupOrDefault("transonic", false);
    consistent_ = solutionDict.lookupOrDefault("consistent", false);

    // Read residual information
    const dictionary residualDict
    (
        solutionDict.subOrEmptyDict("residualControl")
    );

    // Residual controls not shown
    ...
```

Listing 10.6: The read function of the solutionControl class

To sum up. If we use the `PIMPLE` algorithm without any specific keyword, we will have the following set-up:

- `nOuterCorrectors` (nCorrPimple) is set to 1 ,
- `nCorrectors` (nCorrPiso) is set to 1 ,
- `nNonOrthogonalCorrectors` (corrPiso) is set to 0 ,
- `turbOnFinalIterOnly` is set to false ,
- `momentumPredictor` is set to true ,
- `transonic` is set to false ,
- `consistent` is set to false ,
  false means using `SIMPLE`; true means using `SIMPLEC`
- No residual control information is set .

For the further analyze, a simple non-steady test case is provided and the key-ideas of the `PIMPLE` algorithm are demonstrated.

10.4.1 The test case

To demonstrate the behavior of different settings within the *fvSolution* file, a simple 2D transient pipe flow will be considered; this is not the best case because the big advantage of the `PIMPLE` method comes with complex geometries.

The pipe is contracted in the middle in order to accelerate the fluid and to create some vortex after that; compare figure (10.1).

The kinematic viscosity ν is set to $1e^{-5}$ and the extrusion of the 2D mesh in z-direction is 0.01m. The OpenFOAM® version that is used is 4.x and the case is available on www.holzmann-cfd.de/pimpleCase/pimpleCase.tar.gz.

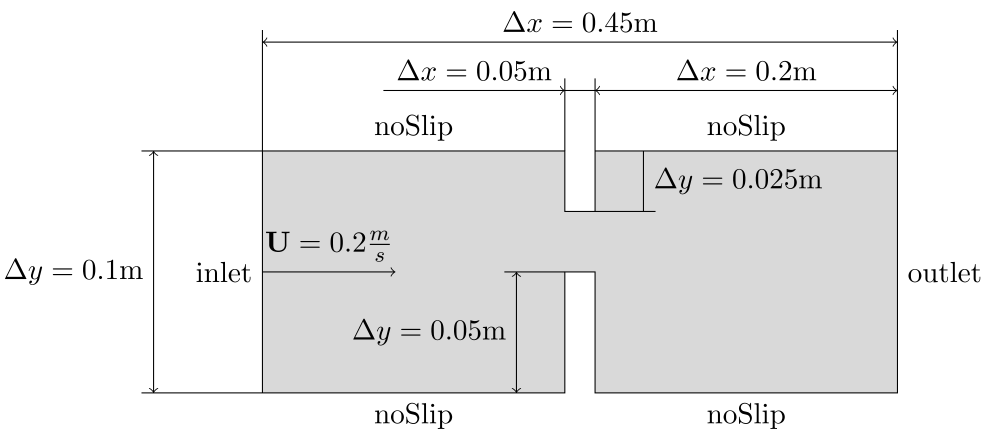


Figure 10.1: The 2D pipe flow domain for the analyze of the PIMPLE algorithm.

Another example and further explanations about the equations that are solved can be found in Holzmann [2014] and an even more detailed introduction into the method and how the pressure-momentum coupling is done in OpenFOAM® is given in Moukalled et al. [2015].

10.4.2 First considerations

In the following, we are using the above domain with the mentioned boundary conditions to demonstrate the usage of the `PIMPLE` algorithm. First of all, we investigate into some basic behavior of the problem.

With the usage of the Bernoulli equation, we can estimate the maximum time step for the simulation. The area at the inlet is $A = 0.1\text{m} \cdot 0.01\text{m} = 0.001\text{m}^2$.

Therefore, we get a volumetric flux $\phi = UA = 0.2\frac{\text{m}}{\text{s}}0.001\text{m}^2 = 0.0002\frac{\text{m}^3}{\text{s}}$. This flux has to cross the small section in the middle of the domain and thus, the velocity has to increase, while the pressure will drop. The cross section has an area of $A_{\text{cross}} = 0.025\text{m} \cdot 0.01\text{m} = 0.00025\text{m}^2$. Hence, the velocity in the cross section became around $U_{\text{cross}} = 0.8\frac{\text{m}}{\text{s}}$. Based on the fact that the flow will be contracted in the cross section, the velocity will further rise. So let us assume that we will get the maximum velocity of $1.2\frac{\text{m}}{\text{s}}$ somewhere in the mesh for the first guess. The resulting time step, with a cell distance of $\Delta x = 0.002\text{m}$, can then be evaluated with equation (10.3):

$$\Delta t = \frac{1 \cdot 0.002}{1.2}\text{s} = 0.0016\text{s} \ .$$

The generated mesh is a pure hexaeder mesh and thus we do not need any orthogonal corrections.

First, we will use the *pisoFoam* solver and the evaluated time step as a reference for the residuals and velocity contour plot. After that, we will use the *pimpleFoam* solver and apply different keywords and settings.

To make the simple problem more complex, we use the `Gauss linear` discretization scheme, that tends to produce non physical results, if the stability criterion is not strictly fulfilled.

10.4.3 Run the case with the `PISO` algorithm

The first step is to generate a reference case. This is done using the *pisoFoam* solver.

Due to the fact, that we solve the flow without a turbulence model, we will naturally get some vortexes which result in high transient behavior. This will make the system more stiff and harder to solve. Furthermore, we can expect, that the residual plots for the time steps look similar for each case, based on the transient character. At last, based on the high transient behavior, we will see some very interesting numerical phenomenon at the end of the discussion.

After the solver finished its work, we get the simulation results shown in figure 10.2 and 10.3. Here, we used a fixed time step (not adjustable). That means, based on the fact that the velocity will change during the simulation, the Courant number will change too, cf. (10.3).

During the simulation a maximum Courant number of 1.4 and a maximum magnitude of the velocity of around $1.3\frac{\text{m}}{\text{s}}$ are achieved. This is the first indication, that our time step approximation works fine for this case. Although we reach higher Courant number than one, the simulation is still stable. It should be clear that the time step approximation based on equation (10.3) can only be used for very simple geometries; moreover it is common to adjust the time step based on the Courant number than using a fixed Δt.

Another thing that we can observe in front of the contraction area are velocity stripes. This is based on the *Gauss linear* scheme and indicate that we are close to the instability limit and is a common habit of that scheme.

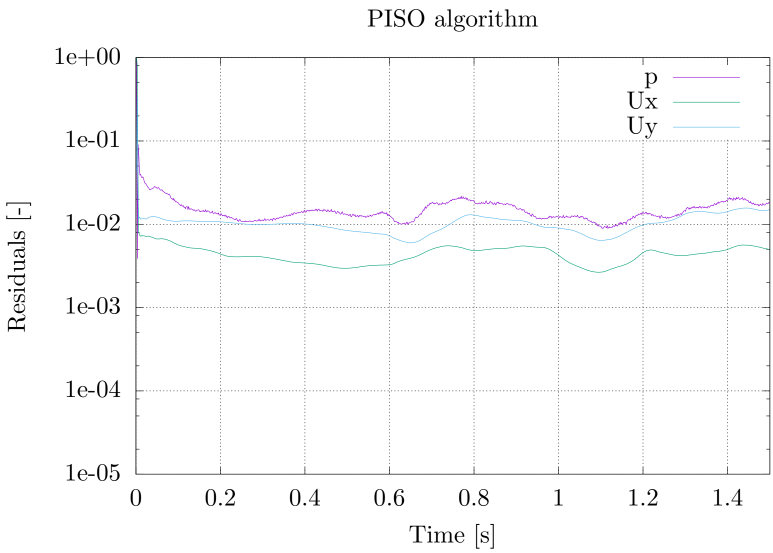


Figure 10.2: Residual plot for the *pisoFoam* solver; fixed $\Delta t = 0.0016$s.

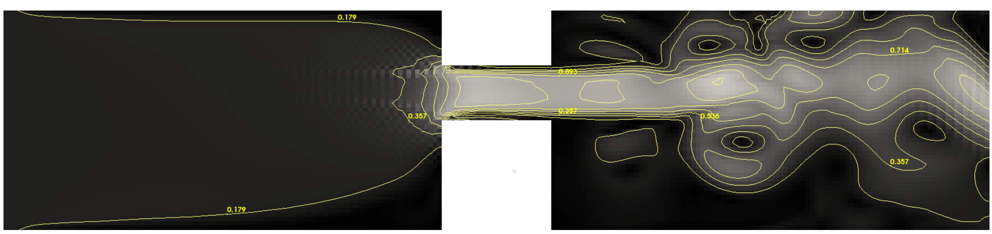


Figure 10.3: Velocity contours generated with *pisoFoam* and a fixed $\Delta t = 0.0016$s.

10.4.4 `PIMPLE` working as `PISO`

Now we are using the same case without any changes and run the **`pimpleFoam`** solver on it. Based on the fact that the `PIMPLE` entry within the **`fvSolution`** is empty, OpenFOAM® will use default values and hence, the *pimpleFoam* solver is equal to *pisoFOAM*. That can be proofed by checking the residuals and contour plots of this calculation and the last one. We see that both solutions are equal.

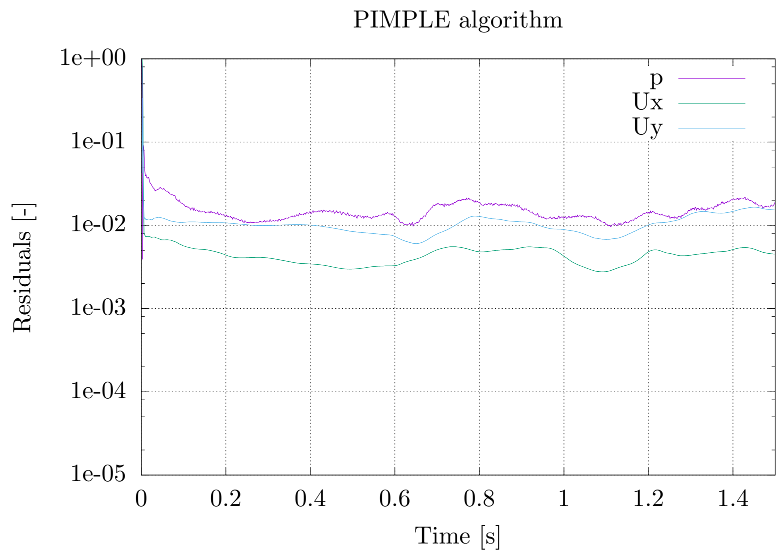


Figure 10.4: Residuals of the calculation with the `PIMPLE` algorithm that is working in `PISO` mode.

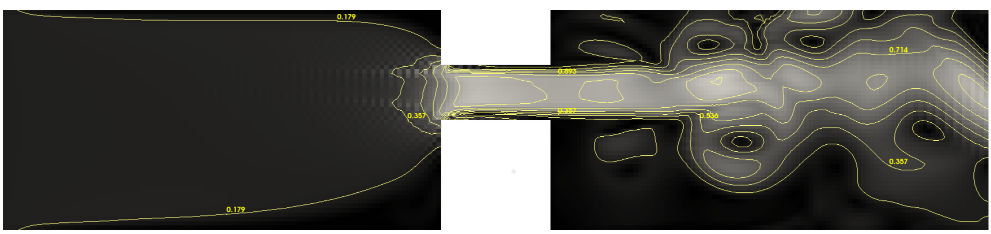


Figure 10.5: Velocity contours of the `PIMPLE` algorithm that is working in `PISO` mode.

10.4.5 PIMPLE working as PISO with large Δt

Now we want to increase the time step to $\Delta t = 0.025$s, to reach the end time of the simulation much faster. This will increase the Courant number based on equation (10.3) and hence, the simulation should crash. Finally, we observe what we expect and after a few time steps the solver crashes with a *Floating Point Exception* (division by zero). The residual plot demonstrates that after the evaluation of the flow, critical velocities are reached and the algorithm will break.

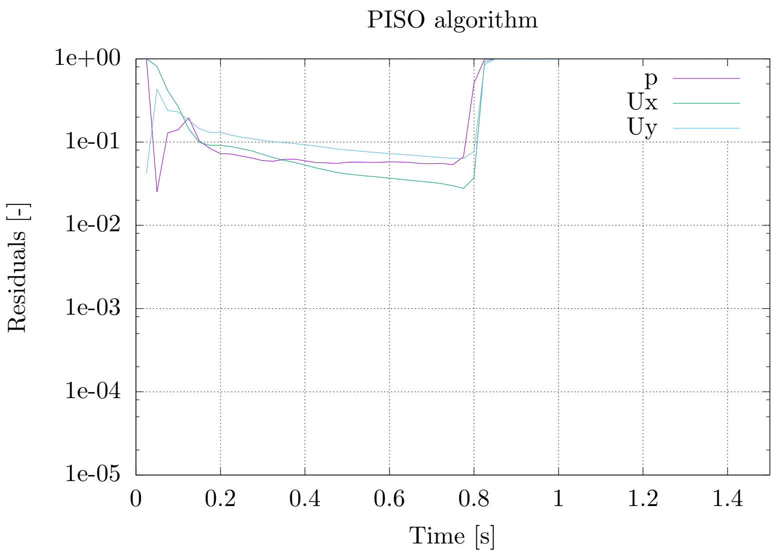


Figure 10.6: Residuals of the calculation with the PIMPLE algorithm that is working in PISO mode using a large time step

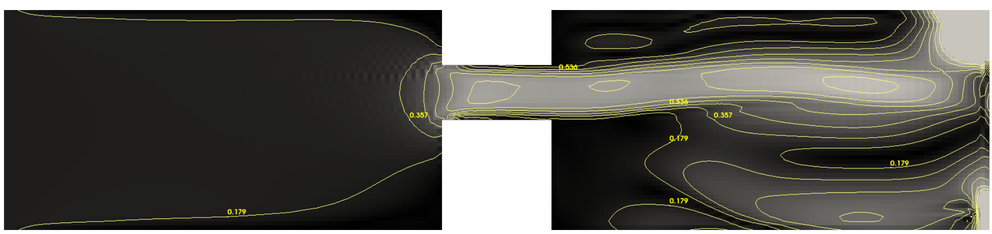


Figure 10.7: Velocity contours of the PIMPLE algorithm that is working in PISO mode with a large time step.

In figure 10.7 the time step is given, when the instability is initiated. On the right top and bottom we can see areas where the velocity is already larger than $60\frac{\text{m}}{\text{s}}$ (total gray areas). Within the next two time steps, the instability moves further to the left side and the velocities increases to values larger than $50.000\frac{\text{m}}{\text{s}}$. Respectively the pressure will blow up too. This happens until the accuracy and the delineation of the computer results into a zero value.

10.4.6 PIMPLE algorithm modified (add outer corrections)

Up to know, we run the PIMPLE algorithm in PISO mode. Now we will use the merged PISO-SIMPLE method by manipulating the algorithm. We can do this by adding the following keywords to the PIMPLE directory.

```
PIMPLE
{
    // Outer Loops (Pressure-Momentum Correction)
    nOuterCorrectors     5;
}
```

Listing 10.7: The control dictionary within the fvSolution file

The nOuterCorrectors will set the nCorrPIMPLE_ variable to five and hence, we make five outer corrections (pressure-momentum correction loop). That include, re-building the velocity matrix with the new flux field, correct the pressure with the new velocity matrix and correct the fluxes based on the new pressure. Finally, we correct the velocities and go back to the re-guessing step till we reached five times.

First of all, we would think that we will improve our calculation and make the algorithm more robust and stable but in fact the solver crashes. This can be seen in the residual and contour plot. In figure 10.9, the whole right part has already incredible large velocities which will move on to the left, till, as before, the solver crashes. Furthermore, we see, that the crash happens already earlier as before; compare residual plot 10.8. The reason for that is the usage of the outer corrector loop. As we already said, the PIMPLE algorithm is a combination of PISO and SIMPLE. Moreover, we know that the SIMPLE algorithm is not stable without relaxation. The outer corrector loops can be considered as a SIMPLE loop and thus without under-relaxation, the procedure can be unstable. Finally, it is not like the real SIMPLE algorithm because we have the limiting time step, that stabilizes the whole solution procedure.

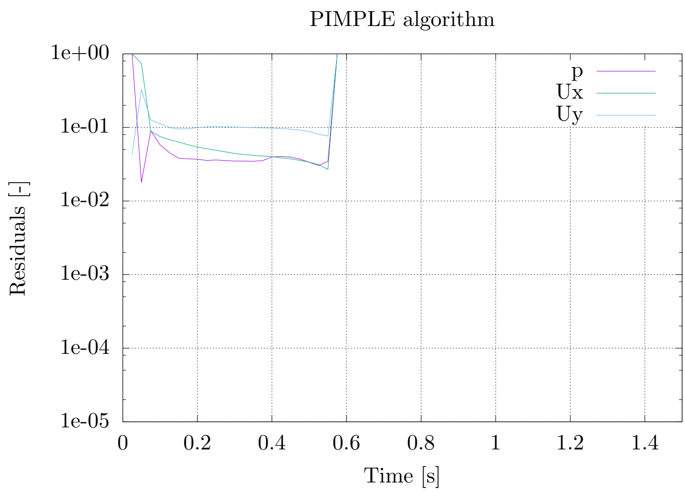


Figure 10.8: Residuals of the calculation with the `PIMPLE` algorithm and `nOuterCorrectors = 5`.

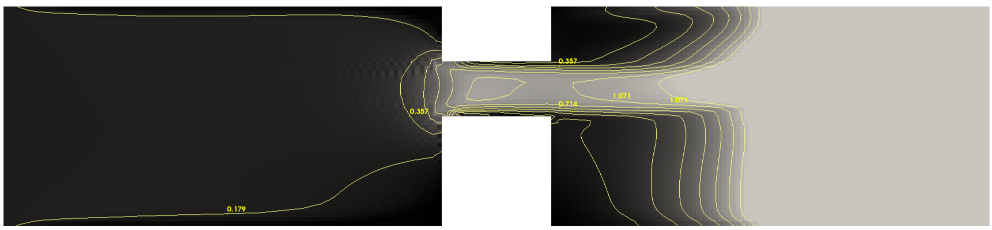


Figure 10.9: Velocity contours of the `PIMPLE` algorithm with the usage of five `nOuterCorrectors`.

The difference with `nOuterCorrectors`

As we already discussed, the difference with the usage of the outer loop correction is, that we recalculate the fluxes, pressure and momentum more often within one time step. All in all, we do this five times here. Doing a more detailed analyze of the residuals, we get the plot shown in figure 10.10.

As we can see, within one time step, we have five more iteration steps (`SIMPLE`). If we would put a line through the highest peaks of each quantity, we would get figure 10.8.

The reason for the crash can be explained as follow: If we go on in time, the flow field will further develop and within the small gap, we will get higher velocities.

After some critical velocity is reached, the solution will diverge. The fact that we are looping fife times more over one time step will speed up the divergence after it is initiated and hence, the solver fails faster than in the case before.

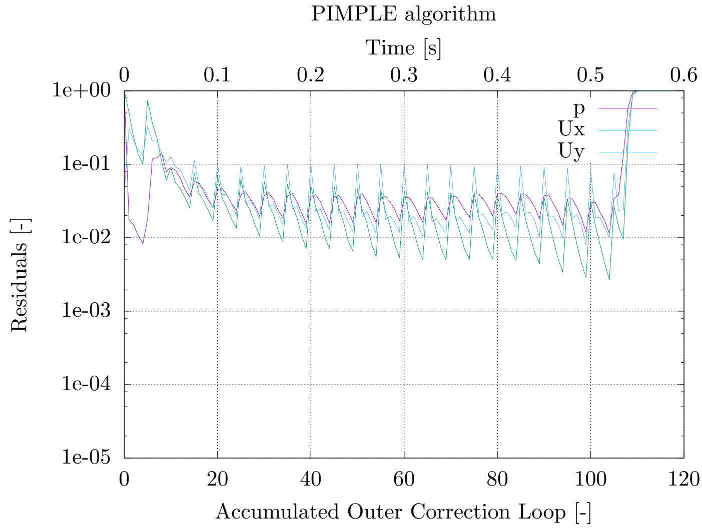


Figure 10.10: Residuals of the outer loop iterations.

10.4.7 `PIMPLE` algorithm further modified (add inner corrections)

Commonly it is helpful and suggested, that we recalculate the pressure with the new updated fluxes but with the old matrix of the momentum (`PISO` corrections - pressure correction loop). For that purpose we have to add a new keyword to the `PIMPLE` dictionary as shown in the code snipped below.

```
PIMPLE
{
    // Outer Loops (Pressure-Momentum Correction)
    nOuterCorrectors     5;

    // Inner Loops (Pressure Correction)
    nCorrectors          2;
}
```

Listing 10.8: The control dictionary within the fvSolution file

As before, instead of getting a more stable algorithm, the solver already crashes in the second time step. Therefore, we can not analyze the general residual plot but we can evaluate the curvatures of the outer and inner iterations.

Recall: For one time step, we calculate five outer loops and within one outer loop, we calculate twice the pressure.

Figure 10.11 shows the inner and outer loops of the first two time steps. What we observe is, that within the first time step, the solution tends to diverge already. This trend is continued within the second time step till the solver crashes. The result of the first time step calculation is given in figure 10.12. Increasing the

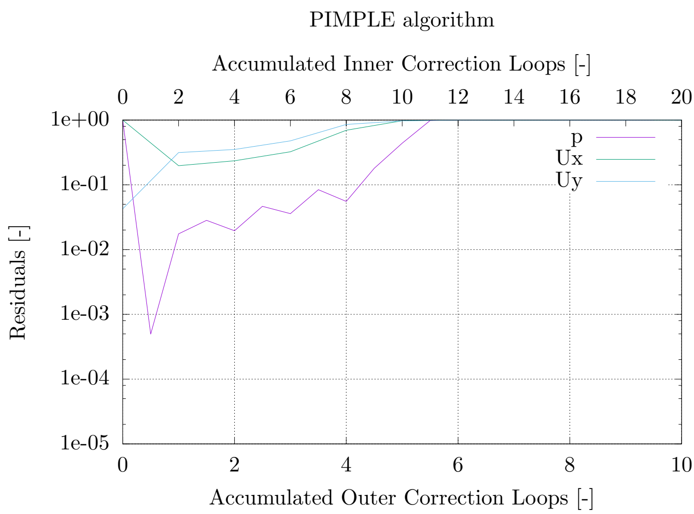


Figure 10.11: Residuals of the iterations of the inner and outer correction loops; `nOuterCorrectors = 5` and `nCorrectors = 2`.

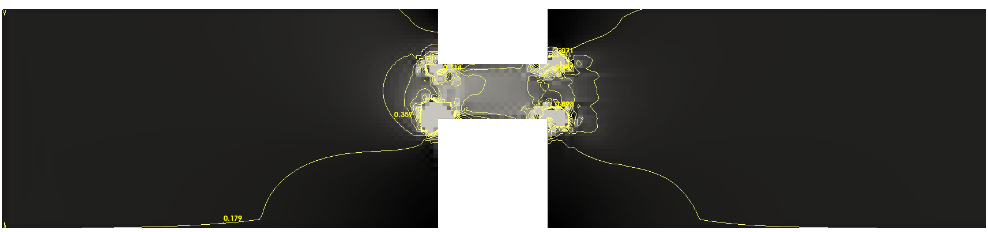


Figure 10.12: Velocity contours; `nOuterCorrectors = 5` and `nCorrectors = 2`.

outer loops would lead to an even faster abort. This is because we can already observe, that within the first time step, the solution tends to diverge. Using more outer iterations will help to establish the wrong solution and lead to a failure of the algorithm already in the first time step.

Up to now, it seems that the `PIMPLE` algorithm only offers disadvantages. The reason for that is based on the wrong usage of the method. The first step for the correct usage of the algorithm is discussed in the next section.

10.4.8 `PIMPLE` algorithm with under-relaxation

To make the `PIMPLE` algorithm work fine, stable and more robust, we have to think about the `SIMPLE` method (outer correction loop). As we already mentioned in section 10.1, the method is not consistent and hence, we are forced to use the under-relaxation technique. Therefore, it is essential to tell OpenFOAM® the specific under-relaxation factors that should be used for the fields and/or equations. The relaxation information is put into another dictionary within the *fvSolution* file.

```
PIMPLE
{
    // Outer Loops (Pressure-Momentum Correction)
    nOuterCorrectors     100;

    // Inner Loops (Pressure Correction)
    nCorrectors          2;
}
relaxationFactors
{
    fields
    {
        p          0.4;
        pFinal     0.4;  // Last outer loop
    }

    equations
    {
        U          0.6;
        UFinal     0.6;  // Last outer loop
    }
}
```

Listing 10.9: The relaxation dictionary within the fvSolution file

Note: The usage of the `SIMPLEC` algorithm can be activated by using the consistency keyword.

As we can see, we have two relaxation factors. One for all outer iterations except the last one and one that is used just for the last one. There is a big discussion about the value of the *Final* one. The question is, are we allowed to under-relax the final iteration like we did it for the previous outer loops? In general, if we do not set it to one, the solution should somehow be not time consistent. However, if we have a lot of outer iterations already done, it should be fine to use a value smaller than one for the *Final* iteration. This will stabilize the whole simulation because the value of one can produce diverging results sometimes.

If we do not specify any relaxation factor, the default value of one is used for all outer iterations. If we specify only the the relaxation factor for p and $\mathbf{U}$ without the *Final* one, the final relaxation factors are set to one by default.

Starting the simulation with the above mentioned relaxation factors and the increase of the outer correction loops (to see what happens), lead to the results shown in figure 10.13 and 10.14. First of all, for each time step we are doing 100 outer corrections and within one outer loop two inner corrections. That means, that we calculate for one time step, 100 momentum-pressure and 200 pressure correction calculations. Checking the time depended residuals, we get similar plots than using

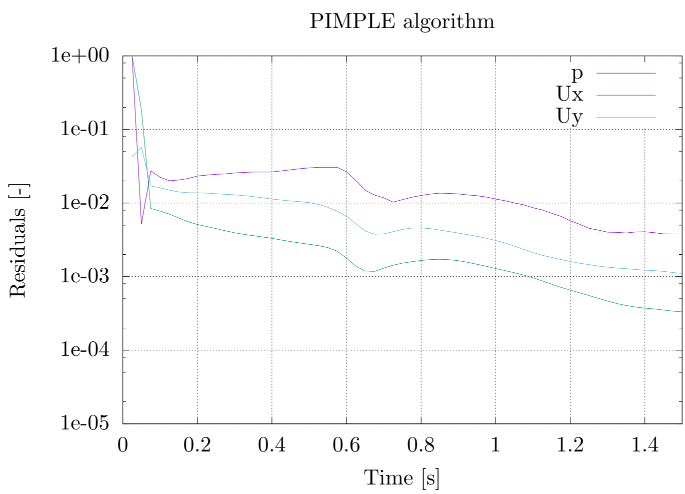


Figure 10.13: Residuals of the iterations of the inner and outer correction loops; `nOuterCorrectors = 100` and `nCorrectors = 2`.

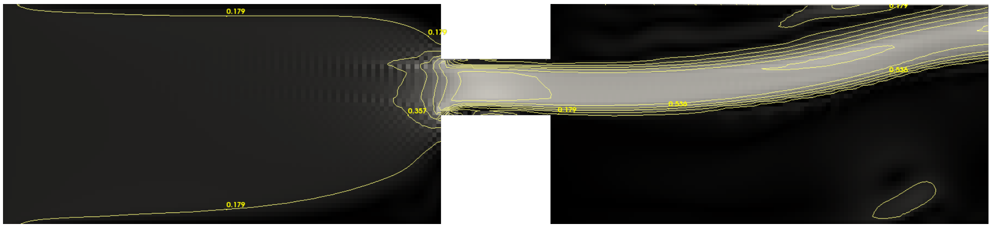


Figure 10.14: Velocity contours; `nOuterCorrectors = 100` and `nCorrectors = 2`.

the `PISO` mode but now we have one essential difference. Within one time step we have much more iterations to find the correct solution; cf. figure 10.15. And thats why we are allowed to increase the time step without taking care that Co < 1. In the following case the Courant number is larger than 20 and the simulation is still stable.

Comparing the contour plots of figure 10.3 and 10.14, we observe big differences. It seems that the `PIMPLE` algorithm smooths the whole solution. The reasons for that could be related to the *too* large time step that we were using within the `PISO` mode (Co ≈ 1.3), the fact, that the *Final* under-relaxation factor was not set to one or that the time step within the `PIMPLE` mode was way too large (Co ≈ 20)

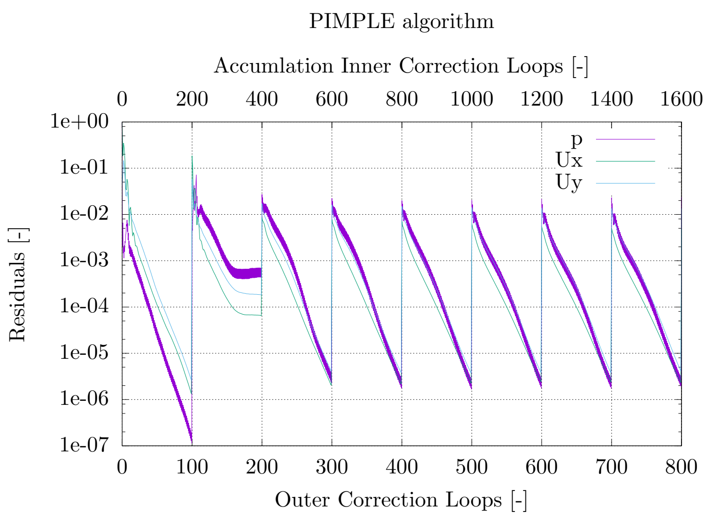


Figure 10.15: Residuals of the iterations of the inner and outer correction loops; `nOuterCorrectors = 100` and `nCorrectors = 2`.

and hence, we over jump some important and essential transient information which will influence the flow significantly. In our case, it is related to the last mentioned hypothesis. Based on the large time step, we do not recognize the establishment of a back flow vortex.

Note: For high transient calculations, you should keep in mind, that it is important to keep the time step in a range where all important phenomena that influence the flow field can be resolved.

The current investigated case can be changed in a way that the time step is adjusted by the highest Courant number. By using Co = 4 and re-run the simulation without changing any other setting, we get the result given in figure 10.16. The new result is very close to the `PISO` calculation compared to the result observed with a fixed time step.

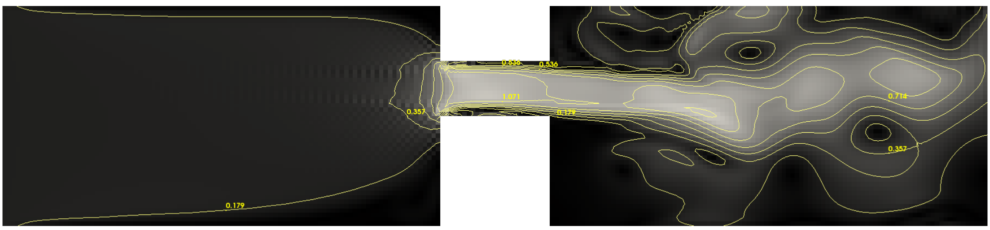


Figure 10.16: Velocity contours; `nOuterCorrectors = 100` and `nCorrectors = 2`; additional residual control added and Courant number controlled

10.4.9 `PIMPLE` algorithm speed up

Instead of looping over the `nOuterCorrectors` till we reach the set value for each time step, it would be much better to leave the loop after we a defined residual limit is fulfilled for each quantity. For that purpose, we *should* also add the residual control sub dictionary to the `PIMPLE` dictionary.

Doing that, OpenFOAM® will run the outer corrector loop until the residual criterion for each quantity is fulfilled. This will reduce the calculation time extremely and ensure good accuracy within each time step.

The next listing shows the correct usage of the `PIMPLE` algorithm. Of course, you can also turn on or off the different switches we already know.

```
PIMPLE
{
    // Outer Loops (Pressure-Momentum Correction)
    nOuterCorrectors     100;

    // Inner Loops (Pressure Correction)
    nCorrectors          2;

    residualControls
    {
        p
        {
            relTol 0;

            // If this initial tolerance is reached, leave
            tolerance 5e-5;
        }

        U
        {
            relTol 0;

            // If this initial tolerance is reached, leave
            tolerance 1e-4;
        }
    }
}

relaxationFactors
{
    fields
    {
        p           0.4;
        pFinal      0.4;  // Last outer loop
    }
    equations
    {
        U           0.6;
        UFinal      0.6;  // Last outer loop
    }
}
```

Listing 10.10: The residualControl dictionary within the fvSolution file

The added residual control will speed up the whole `PIMPLE` procedure. We can now set-up 1000 outer correctors and the algorithm will automatically leave the loop, after each residual criterion is fulfilled. The corresponding residual and contour plots are given below.

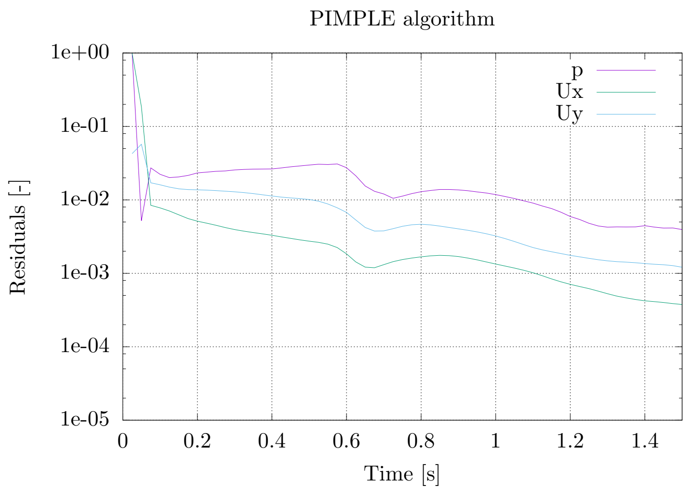


Figure 10.17: Residuals of the iterations of the inner and outer correction loops; `nOuterCorrectors = 100` and `nCorrectors = 2`; additional residual control added .

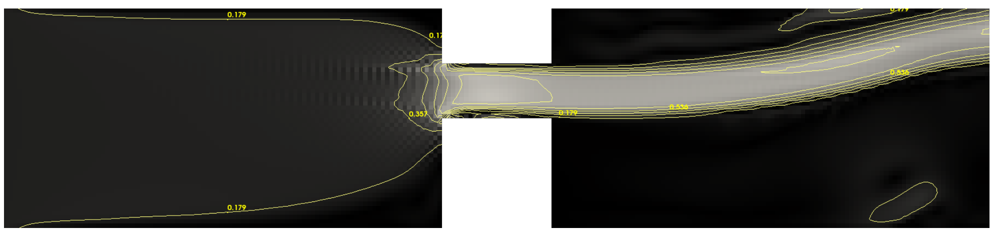


Figure 10.18: Velocity contours; `nOuterCorrectors = 100` and `nCorrectors = 2`; additional residual control added

The decrease of the calculation effort can also be seen in figure 10.19 because within the same amount of outer loops, the solution is already further with respect to the simulation time than in the case before – here we have eleven time steps

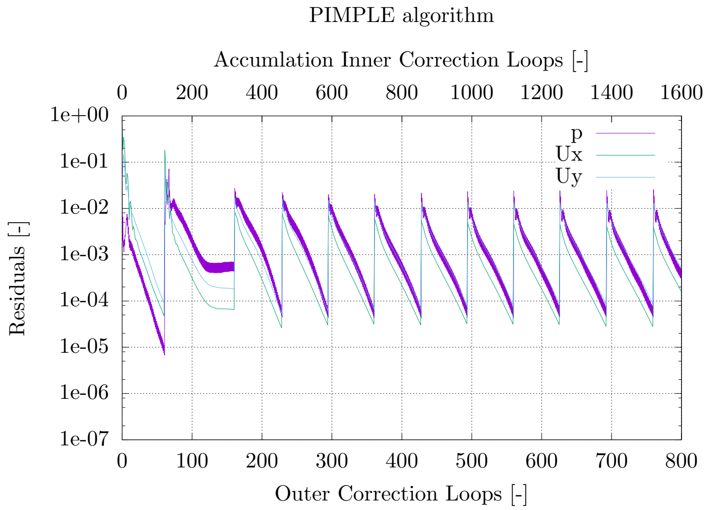


Figure 10.19: Residuals of the iterations of the inner and outer correction loops; `nOuterCorrectors = 100` and `nCorrectors = 2`; additional residual control added.

whereas before we had only seven within the same amount of outer loop iterations.

10.4.10 `PIMPLE` conclusion

As we saw in the last sections, the `PIMPLE` algorithm can be used to enlarge the time step. It was presented and discussed how the algorithm should be used and which advantages it offers.

For simple cases and flow pattern the `PIMPLE` method does not provide to much advantages. For more complex geometries, skewed, non-orthogonal meshes that include different kinds of cells and complex flow patterns or if we have to solve stiff systems, the `PIMPLE` algorithm will provide much more advantages and can stabilize the simulation whereas the case would fail with `PISO` all the time or at least require extreme small time steps.

In advance, the `PIMPLE` algorithm has to be applied correctly and the time step can not be chosen as large as we want. We should always know which time scale can be achieved or which phenomena we are interested in. Different settings will lead to different solutions, if we do not take care about the numerics.

Chapter 11

OpenFOAM® tutorials

For those who want to deal with OpenFOAM® and search for special tutorials, you can checkout my website, www.Holzmann-cfd.de, that offers a lot of additional cases related to the following topics:

- Meshing with `snappyHexMesh`,
- Solving and meshing (different scenarios),
- Using the dynamic mesh library,
- Setting up boundary conditions for `AMI` and `ACMI`,
- Generating own boundary conditions using the `codedFixedValue`,
- Coupling DAKOTA® with OpenFOAM®,
- Coupling OpenFOAM® with Blender®.

Furthermore, you can find different libraries and publications an my website.

For OpenFOAM® beginners

If you are not familiar with OpenFOAM® I recommend you to check out the following website, wiki.openfoam.com. Here you find a new wiki that offers a lot of information; you can thank *Jószef Nagy* for the good work and all contributers mentioned on the site. In addition you will find some *three weeks series* in which you will learn a lot of stuff. Furthermore, the User-Guide of OpenFOAM® should be read.

Chapter 12

Appendix

12.1 The Incompressible Reynolds-Stress-Equation

The derivation of the Reynolds-Stress tensor is structured as follows:

- The derivation of the time derivative is shown completely for all terms ,
- The derivation of the convective derivative is shown completely for term a) ,
- The derivation of the shear-rate derivative is shown completely for term a) ,
- The derivation of the pressure term is shown completely for all terms .

The derivation is given in all details to demonstrate how we get to the equation. Furthermore, we will be able to understand the terms and the reason why we have to add terms in order to apply the product rule.

Recall: In section 8.8 we introduced the way how we will use the momentum equation in order to build the Reynolds-Stress equation. Therefore, we multiplied the momentum equation with respect to the different fluctuations and set the sum of all terms to zero. Here, we introduced the Navier-Stokes operator $\mathcal{N}$. Finally, we build the equation that has to be evaluated which is given for completeness again:

$$
\begin{aligned}
&\underbrace{\overline{u'_x\mathcal{N}(\bar{u}_x+u'_x)+u'_y\mathcal{N}(\bar{u}_z+u'_z)}}_{\text{a)}}+\underbrace{\overline{u'_x\mathcal{N}(\bar{u}_y+u'_y)+u'_y\mathcal{N}(\bar{u}_x+u'_x)}}_{\text{b)}}\\
+&\underbrace{\overline{u'_x\mathcal{N}(\bar{u}_z+u'_z)+u'_y\mathcal{N}(\bar{u}_y+u'_y)}}_{\text{c)}}+\underbrace{\overline{u'_y\mathcal{N}(\bar{u}_x+u'_x)+u'_z\mathcal{N}(\bar{u}_z+u'_z)}}_{\text{d)}}\\
+&\underbrace{\overline{u'_y\mathcal{N}(\bar{u}_y+u'_y)+u'_z\mathcal{N}(\bar{u}_x+u'_x)}}_{\text{e)}}+\underbrace{\overline{u'_y\mathcal{N}(\bar{u}_z+u'_z)+u'_z\mathcal{N}(\bar{u}_y+u'_y)}}_{\text{f)}}\\
+&\underbrace{\overline{u'_z\mathcal{N}(\bar{u}_x+u'_x)+u'_x\mathcal{N}(\bar{u}_z+u'_z)}}_{\text{g)}}+\underbrace{\overline{u'_z\mathcal{N}(\bar{u}_y+u'_y)+u'_x\mathcal{N}(\bar{u}_x+u'_x)}}_{\text{h)}}\\
+&\underbrace{\overline{u'_z\mathcal{N}(\bar{u}_z+u'_z)+u'_x\mathcal{N}(\bar{u}_y+u'_y)}}_{\text{i)}}=0\ .
\end{aligned}
$$

Furthermore, we introduced the rules and tricks we are using during the derivation procedure:

- Reynolds time-averaged terms that are linear in the fluctuation are zero ,
- The derivative $\frac{\partial u'_i}{\partial x_i}=0$,
- Product rule (1.2) ,
- Adding and subtracting terms to be able to use the product rule; $g(x) = g(x)+f(x)-f(x)$.

With that information, we will now demonstrate the derivation of the Reynolds-Stress equation in the order given above.

The Time Derivative

a)

$$
\begin{aligned}
&\overline{u'_x\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}+u'_y\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}}\\
&\qquad=\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}+\cancel{\overline{u'_y\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_y\rho\frac{\partial u'_z}{\partial t}}=\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_z}{\partial t}}\ .
\end{aligned}
\tag{12.1}
$$

b)

$$\overline{u'_x\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}+u'_y\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}}$$
$$=\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}+\cancel{\overline{u'_y\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_y\rho\frac{\partial u'_x}{\partial t}}=\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_x}{\partial t}}\ . \tag{12.2}$$

c)

$$\overline{u'_x\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}+u'_y\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}}$$
$$=\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}+\cancel{\overline{u'_y\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_y\rho\frac{\partial u'_y}{\partial t}}=\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_y}{\partial t}}\ . \tag{12.3}$$

d)

$$\overline{u'_y\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}+u'_z\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}}$$
$$=\cancel{\overline{u'_y\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_y\rho\frac{\partial u'_x}{\partial t}}+\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}=\overline{u'_y\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}\ . \tag{12.4}$$

e)

$$\overline{u'_y\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}+u'_z\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}}$$
$$=\cancel{\overline{u'_y\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_y\rho\frac{\partial u'_y}{\partial t}}+\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}=\overline{u'_y\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}\ . \tag{12.5}$$

f)

$$\overline{u'_y\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}+u'_z\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}}$$
$$=\cancel{\overline{u'_y\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_y\rho\frac{\partial u'_z}{\partial t}}+\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}=\overline{u'_y\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}\ . \tag{12.6}$$

g)

$$\overline{u'_z\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}+u'_x\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}}$$
$$=\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}+\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}=\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}\ . \tag{12.7}$$

h)

$$\overline{u'_z\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}+u'_x\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}}$$
$$=\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}+\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}=\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}\ . \quad (12.8)$$

i)

$$\overline{u'_z\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}+u'_x\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}}$$
$$=\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}+\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}=\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}\ . \quad (12.9)$$

Sorting the terms,

$$\begin{aligned}
&\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}\\
&+\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}\\
&+\overline{u'_y\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_y\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}\ .
\end{aligned}$$

and using the product rule, we end up with:

$$\rho\frac{\partial\overline{u'_xu'_x}}{\partial t}+\rho\frac{\partial\overline{u'_yu'_y}}{\partial t}+\rho\frac{\partial\overline{u'_zu'_z}}{\partial t}+\rho\frac{\partial\overline{u'_xu'_y}}{\partial t}+\rho\frac{\partial\overline{u'_xu'_z}}{\partial t}$$
$$+\rho\frac{\partial\overline{u'_yu'_z}}{\partial t}+\rho\frac{\partial\overline{u'_yu'_x}}{\partial t}+\rho\frac{\partial\overline{u'_zu'_y}}{\partial t}+\rho\frac{\partial\overline{u'_zu'_x}}{\partial t}\ .$$

The above expression can be written in one single term by using the Einsteins summation convention:

$$\boxed{\rho\frac{\partial\overline{u'_ju'_i}}{\partial t}=\frac{\partial\rho\overline{u'_ju'_i}}{\partial t}}\ . \quad (12.10)$$

The Convective Term

First we will focus on the convective term of part a)

$$
\begin{aligned}
&\overline{u'_x\left[\rho\left(\bar{u}_x+u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_x+u'_x\right)+\rho\left(\bar{u}_y+u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_x+u'_x\right)+\rho\left(\bar{u}_z+u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_x+u'_x\right)\right]}\\
+&\overline{u'_y\left[\rho\left(\bar{u}_x+u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_z+u'_z\right)+\rho\left(\bar{u}_y+u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_z+u'_z\right)+\rho\left(\bar{u}_z+u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_z+u'_z\right)\right]}
\end{aligned}
$$

$$
\begin{aligned}
=&\overline{\left(u'_x\rho\bar{u}_x+u'_x\rho u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_x+u'_x\right)+\left(u'_x\rho\bar{u}_y+u'_x\rho u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_x+u'_x\right)}\\
&\qquad\qquad\qquad+\overline{\left(u'_x\rho\bar{u}_z+u'_x\rho u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_x+u'_x\right)}\\
+&\overline{\left(u'_y\rho\bar{u}_x+u'_y\rho u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_z+u'_z\right)+\left(u'_y\rho\bar{u}_y+u'_y\rho u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_z+u'_z\right)}\\
&\qquad\qquad\qquad+\overline{\left(u'_y\rho\bar{u}_z+u'_y\rho u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_z+u'_z\right)}
\end{aligned}
$$

$$
\begin{aligned}
=&\cancel{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}\bar{u}_x}}+\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}+\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}+\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}+\cancel{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}\bar{u}_x}}+\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}\\
+&\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}+\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}+\cancel{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}\bar{u}_x}}+\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}+\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}+\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}\\
+&\cancel{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}\bar{u}_z}}+\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}+\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}+\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}+\cancel{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}\bar{u}_z}}+\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}\\
+&\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}+\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}+\cancel{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}\bar{u}_z}}+\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}+\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}+\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}
\end{aligned}
$$

$$
\begin{aligned}
=\ &\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{1}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{2}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}}_{3}+\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{4}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{5}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}}_{6}\\
+\ &\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{7}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{8}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}}_{9}+\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{10}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{11}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}}_{12}\\
+\ &\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{13}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{14}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}}_{15}+\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{16}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{17}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}}_{18}\ .
\end{aligned}
\tag{12.11}
$$

The same procedure can be done with the terms marked as b) to i). Hence, we will end up always with the last line of equation (12.11) result with respect to the used quantities. Thus, we end up with:

b)

$$
\begin{aligned}
&\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{19}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{20}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_y}}_{21}+\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{22}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{23}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_y}}_{24}\\
+&\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{25}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{26}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_y}}_{27}+\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{28}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{29}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_x}}_{30}\\
+&\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{31}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{32}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_x}}_{33}+\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{34}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{35}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_x}}_{36}\;,
\end{aligned}
$$

c)

$$
\begin{aligned}
&\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{37}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{38}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_z}}_{39}+\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{40}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{41}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_z}}_{42}\\
+&\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{43}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{44}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_z}}_{45}+\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{46}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{47}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_y}}_{48}\\
+&\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{49}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{50}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_y}}_{51}+\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{52}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{53}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_y}}_{54}\;,
\end{aligned}
$$

d)

$$
\begin{aligned}
=&\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{55}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{56}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_x}}_{57}+\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{58}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{59}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_x}}_{60}\\
+&\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{61}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{62}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_x}}_{63}+\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{64}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{65}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_z}}_{66}\\
+&\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{67}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{68}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_z}}_{69}+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{70}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{71}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_z}}_{72}\;,
\end{aligned}
$$

e)

$$\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{73}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{74}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_y}}_{75}+\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{76}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{77}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_y}}_{78}$$

$$+\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{79}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{80}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_y}}_{81}+\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{82}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{83}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_x}}_{84}$$

$$+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{85}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{86}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_x}}_{87}+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{88}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{89}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_x}}_{90},$$

f)

$$\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{91}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{92}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}}_{93}+\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{94}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{95}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}}_{96}$$

$$+\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{97}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{98}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}}_{99}+\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{100}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{101}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_y}}_{102}$$

$$+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{103}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{104}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_y}}_{105}+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{106}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{107}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_y}}_{108},$$

g)

$$=\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{109}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{110}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_x}}_{111}+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{112}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{113}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_x}}_{114}$$

$$+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{115}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{116}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_x}}_{117}+\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{118}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{119}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_z}}_{120}$$

$$+\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{121}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{122}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_z}}_{123}+\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{124}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{125}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_z}}_{126},$$

h)

$$\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{127}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{128}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_y}}_{129}+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{130}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{131}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_y}}_{132}$$
$$+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{133}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{134}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_y}}_{135}+\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{136}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{137}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}}_{138}$$
$$+\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{139}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{140}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}}_{141}+\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{142}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{143}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}}_{144},$$

i)

$$\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{145}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{146}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_z}}_{147}+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{148}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{149}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_z}}_{150}$$
$$+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{151}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{152}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_z}}_{153}+\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{154}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{155}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_y}}_{156}$$
$$+\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{157}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{158}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_y}}_{159}+\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{160}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{161}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_y}}_{162}.$$

Analyzing the sum of terms, we figure out that there are different kind of terms:

- Terms that only include the fluctuation quantities ,
- Terms that include the mean quantity inside the derivation ,
- Terms that include the mean quantity outside the derivation .

Lets consider the terms that contains the fluctuation quantities for now:

$$
\begin{aligned}
&\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}}_{3}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}}_{6}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}}_{9}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}}_{12}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}}_{15}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}}_{18}\\
+&\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_y}}_{21}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_y}}_{24}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_y}}_{27}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_x}}_{30}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_x}}_{33}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_x}}_{36}\\
+&\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_z}}_{39}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_z}}_{42}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_z}}_{45}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_y}}_{48}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_y}}_{51}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_y}}_{54}\\
+&\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_x}}_{57}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_x}}_{60}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_x}}_{63}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_z}}_{66}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_z}}_{69}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_z}}_{72}\\
+&\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_y}}_{75}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_y}}_{78}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_y}}_{81}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_x}}_{84}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_x}}_{87}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_x}}_{90}\\
+&\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}}_{93}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}}_{96}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}}_{99}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_y}}_{102}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_y}}_{105}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_y}}_{108}\\
+&\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_x}}_{111}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_x}}_{114}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_x}}_{117}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_z}}_{120}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_z}}_{123}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_z}}_{126}\\
+&\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_y}}_{129}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_y}}_{132}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_y}}_{135}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}}_{138}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}}_{141}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}}_{144}\\
+&\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_z}}_{147}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_z}}_{150}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_z}}_{153}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_y}}_{156}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_y}}_{159}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_y}}_{162}\ .
\end{aligned}
$$

We get 54 terms that can be combined using the product rule. One example would be:

$$
\overline{\rho\frac{\partial}{\partial x}u'_y u'_z u'_x}=\overline{\rho u'_z u'_x\frac{\partial}{\partial x}u'_y}+\overline{\rho u'_y u'_x\frac{\partial}{\partial x}u'_z}+\overline{\rho u'_y u'_z\frac{\partial}{\partial x}u'_x}\ . \tag{12.12}
$$

In other words, three terms can be combined to one term. Applying the product rule to the terms, we will realize that not all terms can be combined. Therefore we have to add 27 terms of the following kind:

$$\overline{\rho u'_i u'_j \cancel{\frac{\partial}{\partial x_k} u'_k}} = 0 \ . \tag{12.13}$$

After adding these terms we end up with 81 terms that can be reduced to 27. Finally we get:

$$\begin{aligned}
&\overline{\rho\frac{\partial}{\partial x}u'_x u'_x u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_x u'_x u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_x u'_x u'_z} + \overline{\rho\frac{\partial}{\partial x}u'_x u'_y u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_x u'_y u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_x u'_y u'_z} \\
&+ \overline{\rho\frac{\partial}{\partial x}u'_x u'_z u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_x u'_z u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_x u'_z u'_z} + \overline{\rho\frac{\partial}{\partial x}u'_y u'_x u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_y u'_x u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_y u'_x u'_z} \\
&+ \overline{\rho\frac{\partial}{\partial x}u'_y u'_y u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_y u'_y u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_y u'_y u'_z} + \overline{\rho\frac{\partial}{\partial x}u'_y u'_z u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_y u'_z u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_y u'_z u'_z} \\
&+ \overline{\rho\frac{\partial}{\partial x}u'_z u'_x u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_z u'_x u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_z u'_x u'_z} + \overline{\rho\frac{\partial}{\partial x}u'_z u'_y u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_z u'_y u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_z u'_y u'_z} \\
&+ \overline{\rho\frac{\partial}{\partial x}u'_z u'_z u'_x} + \overline{\rho\frac{\partial}{\partial y}u'_z u'_z u'_y} + \overline{\rho\frac{\partial}{\partial z}u'_z u'_z u'_z} \ .
\end{aligned}$$

Now it is obvious that we can rewrite this equation using the Einsteins summation convention. In addition, we will put the density inside the derivative due to the fact that it is constant. After applying the Reynolds time-averaging, we end up with the convective term as:

$$\boxed{\overline{\rho\frac{\partial}{\partial x_k}u'_i u'_j u'_k} = \frac{\partial}{\partial x_k}\rho\overline{u'_i u'_j u'_k}} \ . \tag{12.14}$$

Now, we will consider all terms that contain the mean quantity inside the derivative:

$$
\begin{aligned}
&\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{2}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{5}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{8}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{11}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{14}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{17}\\
+\ &\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{20}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{23}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{26}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{29}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{32}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{35}\\
+\ &\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{38}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{41}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{44}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{47}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{50}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{53}\\
+\ &\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{56}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{59}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{62}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{65}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{68}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{71}\\
+\ &\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{74}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{77}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{80}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{83}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{86}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{89}\\
+\ &\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{92}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{95}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{98}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{101}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{104}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{107}\\
+\ &\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{110}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{113}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{116}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{119}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{122}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{125}\\
+\ &\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{128}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{131}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{134}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{137}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{140}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{143}\\
+\ &\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{146}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{149}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{152}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{155}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{158}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{161}\ .
\end{aligned}
$$

Again, we end up with 54 terms. This terms can be sorted and rearranged into twice 27 terms. Doing so, we will see that we can simplify the first 27 terms using the Einsteins summation convention to:

$$\boxed{\overline{\rho u'_i u'_k}\frac{\partial}{\partial x_k}\bar{u}_j=\rho\overline{u'_i u'_k}\frac{\partial}{\partial x_k}\bar{u}_j}\ . \tag{12.15}$$

and the second 27 terms could be written as:

$$\boxed{\overline{\rho u'_j u'_k \frac{\partial}{\partial x_k} \bar{u}_i} = \rho \overline{u'_j u'_k} \frac{\partial}{\partial x_k} \bar{u}_i} \,. \tag{12.16}$$

Note: If *you* want to check if everything is fine with the above equation, just build the sum of the two last equations and you will see that you get the 52 terms.

Finally we have to consider all terms that contain the mean of the quantities outside of the derivative:

$$\begin{aligned}
&\underbrace{\overline{u'_x \rho \bar{u}_x \frac{\partial}{\partial x} u'_x}}_{1} + \underbrace{\overline{u'_x \rho \bar{u}_y \frac{\partial}{\partial y} u'_x}}_{4} + \underbrace{\overline{u'_x \rho \bar{u}_z \frac{\partial}{\partial z} u'_x}}_{7} + \underbrace{\overline{u'_y \rho \bar{u}_x \frac{\partial}{\partial x} u'_z}}_{10} + \underbrace{\overline{u'_y \rho \bar{u}_y \frac{\partial}{\partial y} u'_z}}_{13} + \underbrace{\overline{u'_y \rho \bar{u}_z \frac{\partial}{\partial z} u'_z}}_{16} \\
+ &\underbrace{\overline{u'_x \rho \bar{u}_x \frac{\partial}{\partial x} u'_y}}_{19} + \underbrace{\overline{u'_x \rho \bar{u}_y \frac{\partial}{\partial y} u'_y}}_{22} + \underbrace{\overline{u'_x \rho \bar{u}_z \frac{\partial}{\partial z} u'_y}}_{25} + \underbrace{\overline{u'_y \rho \bar{u}_x \frac{\partial}{\partial x} u'_x}}_{28} + \underbrace{\overline{u'_y \rho \bar{u}_y \frac{\partial}{\partial y} u'_x}}_{31} + \underbrace{\overline{u'_y \rho \bar{u}_z \frac{\partial}{\partial z} u'_x}}_{34} \\
+ &\underbrace{\overline{u'_x \rho \bar{u}_x \frac{\partial}{\partial x} u'_z}}_{37} + \underbrace{\overline{u'_x \rho \bar{u}_y \frac{\partial}{\partial y} u'_z}}_{40} + \underbrace{\overline{u'_x \rho \bar{u}_z \frac{\partial}{\partial z} u'_z}}_{43} + \underbrace{\overline{u'_y \rho \bar{u}_x \frac{\partial}{\partial x} u'_y}}_{46} + \underbrace{\overline{u'_y \rho \bar{u}_y \frac{\partial}{\partial y} u'_y}}_{49} + \underbrace{\overline{u'_y \rho \bar{u}_z \frac{\partial}{\partial z} u'_y}}_{52} \\
+ &\underbrace{\overline{u'_y \rho \bar{u}_x \frac{\partial}{\partial x} u'_x}}_{55} + \underbrace{\overline{u'_y \rho \bar{u}_y \frac{\partial}{\partial y} u'_x}}_{58} + \underbrace{\overline{u'_y \rho \bar{u}_z \frac{\partial}{\partial z} u'_x}}_{61} + \underbrace{\overline{u'_z \rho \bar{u}_x \frac{\partial}{\partial x} u'_z}}_{64} + \underbrace{\overline{u'_z \rho \bar{u}_y \frac{\partial}{\partial y} u'_z}}_{67} + \underbrace{\overline{u'_z \rho \bar{u}_z \frac{\partial}{\partial z} u'_z}}_{70} \\
+ &\underbrace{\overline{u'_y \rho \bar{u}_x \frac{\partial}{\partial x} u'_y}}_{73} + \underbrace{\overline{u'_y \rho \bar{u}_y \frac{\partial}{\partial y} u'_y}}_{76} + \underbrace{\overline{u'_y \rho \bar{u}_z \frac{\partial}{\partial z} u'_y}}_{79} + \underbrace{\overline{u'_z \rho \bar{u}_x \frac{\partial}{\partial x} u'_x}}_{82} + \underbrace{\overline{u'_z \rho \bar{u}_y \frac{\partial}{\partial y} u'_x}}_{85} + \underbrace{\overline{u'_z \rho \bar{u}_z \frac{\partial}{\partial z} u'_x}}_{88} \\
+ &\underbrace{\overline{u'_y \rho \bar{u}_x \frac{\partial}{\partial x} u'_z}}_{91} + \underbrace{\overline{u'_y \rho \bar{u}_y \frac{\partial}{\partial y} u'_z}}_{94} + \underbrace{\overline{u'_y \rho \bar{u}_z \frac{\partial}{\partial z} u'_z}}_{97} + \underbrace{\overline{u'_z \rho \bar{u}_x \frac{\partial}{\partial x} u'_y}}_{100} + \underbrace{\overline{u'_z \rho \bar{u}_y \frac{\partial}{\partial y} u'_y}}_{103} + \underbrace{\overline{u'_z \rho \bar{u}_z \frac{\partial}{\partial z} u'_y}}_{106} \\
+ &\underbrace{\overline{u'_z \rho \bar{u}_x \frac{\partial}{\partial x} u'_x}}_{109} + \underbrace{\overline{u'_z \rho \bar{u}_y \frac{\partial}{\partial y} u'_x}}_{112} + \underbrace{\overline{u'_z \rho \bar{u}_z \frac{\partial}{\partial z} u'_x}}_{115} + \underbrace{\overline{u'_x \rho \bar{u}_x \frac{\partial}{\partial x} u'_z}}_{118} + \underbrace{\overline{u'_x \rho \bar{u}_y \frac{\partial}{\partial y} u'_z}}_{121} + \underbrace{\overline{u'_x \rho \bar{u}_z \frac{\partial}{\partial z} u'_z}}_{124} \\
+ &\underbrace{\overline{u'_z \rho \bar{u}_x \frac{\partial}{\partial x} u'_y}}_{127} + \underbrace{\overline{u'_z \rho \bar{u}_y \frac{\partial}{\partial y} u'_y}}_{130} + \underbrace{\overline{u'_z \rho \bar{u}_z \frac{\partial}{\partial z} u'_y}}_{133} + \underbrace{\overline{u'_x \rho \bar{u}_x \frac{\partial}{\partial x} u'_x}}_{136} + \underbrace{\overline{u'_x \rho \bar{u}_y \frac{\partial}{\partial y} u'_x}}_{139} + \underbrace{\overline{u'_x \rho \bar{u}_z \frac{\partial}{\partial z} u'_x}}_{142} \\
+ &\underbrace{\overline{u'_z \rho \bar{u}_x \frac{\partial}{\partial x} u'_z}}_{145} + \underbrace{\overline{u'_z \rho \bar{u}_y \frac{\partial}{\partial y} u'_z}}_{148} + \underbrace{\overline{u'_z \rho \bar{u}_z \frac{\partial}{\partial z} u'_z}}_{151} + \underbrace{\overline{u'_x \rho \bar{u}_x \frac{\partial}{\partial x} u'_y}}_{154} + \underbrace{\overline{u'_x \rho \bar{u}_y \frac{\partial}{\partial y} u'_y}}_{157} + \underbrace{\overline{u'_x \rho \bar{u}_z \frac{\partial}{\partial z} u'_y}}_{160} \,.
\end{aligned}$$

To simplify these terms, we use the product rule (1.2) to combine two terms to one. An example would be:

$$\overline{\rho \bar{u}_z \frac{\partial}{\partial z} u'_x u'_y} = \overline{u'_y \rho \bar{u}_z \frac{\partial}{\partial z} u'_x} + \overline{u'_x \rho \bar{u}_z \frac{\partial}{\partial z} u'_y} \ . \tag{12.17}$$

After combining the terms, we can rewrite the sum by using the Einsteins summation convention because the derivatives are always with respect to the mean quantities. Hence, we end up with 27 terms that can be expressed as:

$$\boxed{\overline{\rho \bar{u}_k \frac{\partial}{\partial u_k} u'_i u'_j} = \bar{u}_k \frac{\partial}{\partial u_k} \rho \overline{u'_i u'_j}} \ . \tag{12.18}$$

Now, the convective term is manipulated and derived. Combining all terms, we end up with:

$$\boxed{\bar{u}_k \frac{\partial \rho \overline{u'_i u'_j}}{\partial u_k} + \rho \overline{u'_j u'_k} \frac{\partial \bar{u}_i}{\partial x_k} + \rho \overline{u'_i u'_k} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k} \rho \overline{u'_i u'_j u'_k}} \ . \tag{12.19}$$

The Shear-Rate Term

a)

$$\begin{aligned}
&\overline{-u'_x \left\{ \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial(\bar{u}_x + u'_x)}{\partial x} + \frac{\partial(\bar{u}_x + u'_x)}{\partial x} \right) \right] - \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial(\bar{u}_x + u'_x)}{\partial y} + \frac{\partial(\bar{u}_y + u'_y)}{\partial x} \right) \right] \right.} \\
&\overline{\left. - \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial(\bar{u}_x + u'_x)}{\partial z} + \frac{\partial(\bar{u}_z + u'_z)}{\partial x} \right) \right] \right\} - u'_y \left\{ \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial(\bar{u}_z + u'_z)}{\partial x} + \frac{\partial(\bar{u}_x + u'_x)}{\partial z} \right) \right] \right.} \\
&\overline{\left. - - \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial(\bar{u}_z + u'_z)}{\partial y} + \frac{\partial(\bar{u}_y + u'_y)}{\partial z} \right) \right] - \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial(\bar{u}_z + u'_z)}{\partial z} + \frac{\partial(\bar{u}_y + u'_y)}{\partial z} \right) \right] \right\}}
\end{aligned}$$

$$\begin{aligned}
= &- \cancel{\overline{u'_x \frac{\partial}{\partial x} \left(\mu \frac{\partial \bar{u}_x}{\partial x} \right)}} - \overline{u'_x \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_x}{\partial x} \right)} - \cancel{\overline{u'_x \frac{\partial}{\partial x} \left(\mu \frac{\partial \bar{u}_x}{\partial x} \right)}} - \overline{u'_x \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_x}{\partial x} \right)} - \cancel{\overline{u'_x \frac{\partial}{\partial y} \left(\mu \frac{\partial \bar{u}_x}{\partial y} \right)}} - \overline{u'_x \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_x}{\partial y} \right)} \\
&- \cancel{\overline{u'_x \frac{\partial}{\partial y} \left(\mu \frac{\partial \bar{u}_y}{\partial x} \right)}} - \overline{u'_x \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_y}{\partial x} \right)} - \cancel{\overline{u'_x \frac{\partial}{\partial z} \left(\mu \frac{\partial \bar{u}_x}{\partial z} \right)}} - \overline{u'_x \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_x}{\partial z} \right)} - \cancel{\overline{u'_x \frac{\partial}{\partial z} \left(\mu \frac{\partial \bar{u}_z}{\partial x} \right)}} - \overline{u'_x \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_z}{\partial x} \right)} \\
&- \cancel{\overline{u'_y \frac{\partial}{\partial x} \left(\mu \frac{\partial \bar{u}_z}{\partial x} \right)}} - \overline{u'_y \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_z}{\partial x} \right)} - \cancel{\overline{u'_y \frac{\partial}{\partial x} \left(\mu \frac{\partial \bar{u}_x}{\partial z} \right)}} - \overline{u'_y \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_x}{\partial z} \right)} - \cancel{\overline{u'_y \frac{\partial}{\partial y} \left(\mu \frac{\partial \bar{u}_z}{\partial y} \right)}} - \overline{u'_y \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_z}{\partial y} \right)} \\
&- \cancel{\overline{u'_y \frac{\partial}{\partial y} \left(\mu \frac{\partial \bar{u}_y}{\partial z} \right)}} - \overline{u'_y \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_y}{\partial z} \right)} - \cancel{\overline{u'_y \frac{\partial}{\partial z} \left(\mu \frac{\partial \bar{u}_z}{\partial z} \right)}} - \overline{u'_y \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_z}{\partial z} \right)} - \cancel{\overline{u'_y \frac{\partial}{\partial z} \left(\mu \frac{\partial \bar{u}_z}{\partial z} \right)}} - \overline{u'_y \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_z}{\partial z} \right)}
\end{aligned}$$

$$\begin{aligned}
= &- \overline{u'_x \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_x}{\partial x} \right)} - \overline{u'_x \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_x}{\partial x} \right)} - \overline{u'_x \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_x}{\partial y} \right)} - \overline{u'_x \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_y}{\partial x} \right)} - \overline{u'_x \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_x}{\partial z} \right)} - \overline{u'_x \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_z}{\partial x} \right)} \\
&- \overline{u'_y \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_z}{\partial x} \right)} - \overline{u'_y \frac{\partial}{\partial x} \left(\mu \frac{\partial u'_x}{\partial z} \right)} - \overline{u'_y \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_z}{\partial y} \right)} - \overline{u'_y \frac{\partial}{\partial y} \left(\mu \frac{\partial u'_y}{\partial z} \right)} - \overline{u'_y \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_z}{\partial z} \right)} - \overline{u'_y \frac{\partial}{\partial z} \left(\mu \frac{\partial u'_z}{\partial z} \right)}
\end{aligned}$$

For the parts b) to i) we will just write the final terms:

b)

$$
\begin{aligned}
&-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial y}\right)}\\
&-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial x}\right)}
\end{aligned}
$$

c)

$$
\begin{aligned}
&-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_z}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}\\
&-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial y}\right)}
\end{aligned}
$$

d)

$$
\begin{aligned}
&-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial x}\right)}\\
&-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_z}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}
\end{aligned}
$$

e)

$$
\begin{aligned}
&-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial y}\right)}\\
&-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial x}\right)}
\end{aligned}
$$

f)

$$
\begin{aligned}
&-\underbrace{\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}}_{*}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_z}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}\\
&-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial y}\right)}
\end{aligned}
$$

g)

$$
\begin{aligned}
&-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial x}\right)}\\
&-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_z}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}
\end{aligned}
$$

h)

$$-\underbrace{\overline{u_z'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_y'}{\partial x}\right)}}_{**}-\overline{u_z'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_x'}{\partial y}\right)}-\overline{u_z'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_y'}{\partial y}\right)}-\overline{u_z'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_y'}{\partial y}\right)}-\overline{u_z'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_y'}{\partial z}\right)}-\overline{u_z'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_z'}{\partial y}\right)}$$
$$-\overline{u_x'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_x'}{\partial x}\right)}-\overline{u_x'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_x'}{\partial x}\right)}-\overline{u_x'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_x'}{\partial y}\right)}-\overline{u_x'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_y'}{\partial x}\right)}-\overline{u_x'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_x'}{\partial z}\right)}-\overline{u_x'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_z'}{\partial x}\right)}$$

i)

$$-\overline{u_z'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_z'}{\partial x}\right)}-\overline{u_z'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_x'}{\partial z}\right)}-\overline{u_z'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_z'}{\partial y}\right)}-\overline{u_z'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_y'}{\partial z}\right)}-\overline{u_z'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_z'}{\partial z}\right)}-\overline{u_z'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_z'}{\partial z}\right)}$$
$$-\overline{u_x'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_y'}{\partial x}\right)}-\overline{u_x'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_x'}{\partial y}\right)}-\overline{u_x'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_y'}{\partial y}\right)}-\overline{u_x'\frac{\partial}{\partial y}\left(\mu\frac{\partial u_y'}{\partial y}\right)}-\overline{u_x'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_y'}{\partial z}\right)}-\overline{u_x'\frac{\partial}{\partial z}\left(\mu\frac{\partial u_z'}{\partial y}\right)}$$

After the manipulation we find 102 terms. Again we want to put the fluctuation terms together, hence we need the product rule. Analyzing the sum, we can figure out that there is no way to apply the product rule. The trick is simply to add the missing 204 terms. One example is given now. Taking the term (*) of f) and (**) of h), we get:

$$-\overline{u_y'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_z'}{\partial x}\right)}-\overline{u_z'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_y'}{\partial x}\right)}\,. \tag{12.20}$$

This two terms can not be merged, hence we need two terms in addition:

$$-\overbrace{\overline{u_y'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_z'}{\partial x}\right)}}^{1}\underbrace{-\overbrace{\overline{\mu\frac{\partial u_y'}{\partial x}\frac{\partial u_z'}{\partial x}}}^{2}+\overbrace{\overline{\mu\frac{\partial u_y'}{\partial x}\frac{\partial u_z'}{\partial x}}}^{3}}_{\text{added}}-\overbrace{\overline{u_z'\frac{\partial}{\partial x}\left(\mu\frac{\partial u_y'}{\partial x}\right)}}^{4}$$
$$\underbrace{-\overbrace{\overline{\mu\frac{\partial u_z'}{\partial x}\frac{\partial u_y'}{\partial x}}}^{5}+\overbrace{\overline{\mu\frac{\partial u_z'}{\partial x}\frac{\partial u_y'}{\partial x}}}^{6}}_{\text{added}}\,. \tag{12.21}$$

Now we are able to combine term 1 – 2 and 4 – 5 using the product rule. Furthermore term 3 and 6 are similar and can be combined too:

$$-\underbrace{\overline{\frac{\partial}{\partial x}u_y'\left(\mu\frac{\partial u_z'}{\partial x}\right)}}_{7}-\underbrace{\overline{\frac{\partial}{\partial x}u_z'\left(\mu\frac{\partial u_y'}{\partial x}\right)}}_{8}+2\mu\overline{\frac{\partial u_z'}{\partial x}\frac{\partial u_y'}{\partial x}}\,. \tag{12.22}$$

Now we see that the term 7 and 8 can be combined using the product rule again. Finally we end up with:

$$-\overline{\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y u'_z}{\partial x}\right)} + \overline{2\mu\frac{\partial u'_z}{\partial x}\frac{\partial u'_y}{\partial x}} \ . \tag{12.23}$$

Repeating this procedure for all terms, we will reduce the already existing 102 terms of a) to i) to 54. At the end we would realize that we can rewrite the sum of the 54 terms as:

$$\boxed{-\overline{\frac{\partial}{\partial x_k}\left(\mu\frac{\partial u'_i u'_j}{\partial x_k}\right)} = -\frac{\partial}{\partial x_k}\left(\mu\frac{\partial \overline{u'_i u'_j}}{\partial x_k}\right)} \ . \tag{12.24}$$

The new introduced terms (due to the trick), can be expressed as:

$$\boxed{\overline{2\mu\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}} = 2\mu\overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}}} \ . \tag{12.25}$$

Summing up, the shear-rate terms can be written as:

$$\boxed{-\frac{\partial}{\partial x_k}\left(\mu\frac{\partial \overline{u'_i u'_j}}{\partial x_k}\right) + 2\mu\overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}}} \ . \tag{12.26}$$

The pressure derivative

a)

$$\overline{u'_x\frac{\partial(\bar{p}+p')}{\partial x}} + \overline{u'_y\frac{\partial(\bar{p}+p')}{\partial z}} = \cancel{\overline{u'_x\frac{\partial\bar{p}}{\partial x}}} + \overline{u'_x\frac{\partial p'}{\partial x}} + \cancel{\overline{u'_y\frac{\partial\bar{p}}{\partial z}}} + \overline{u'_y\frac{\partial p'}{\partial z}} = \overline{u'_x\frac{\partial p'}{\partial x}} + \overline{u'_y\frac{\partial p'}{\partial z}} \ , \tag{12.27}$$

b)

$$\overline{u'_x\frac{\partial(\bar{p}+p')}{\partial y}} + \overline{u'_y\frac{\partial(\bar{p}+p')}{\partial x}} = \cancel{\overline{u'_x\frac{\partial\bar{p}}{\partial y}}} + \overline{u'_x\frac{\partial p'}{\partial y}} + \cancel{\overline{u'_y\frac{\partial\bar{p}}{\partial x}}} + \overline{u'_y\frac{\partial p'}{\partial x}} = \overline{u'_x\frac{\partial p'}{\partial y}} + \overline{u'_y\frac{\partial p'}{\partial x}} \ , \tag{12.28}$$

c)

$$\overline{u'_x \frac{\partial(\bar{p}+p')}{\partial z}} + \overline{u'_y \frac{\partial(\bar{p}+p')}{\partial y}} = \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_x \frac{\partial p'}{\partial z}} + \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_y \frac{\partial p'}{\partial y}} = \overline{u'_x \frac{\partial p'}{\partial z}} + \overline{u'_y \frac{\partial p'}{\partial y}} \ , \tag{12.29}$$

d)

$$\overline{u'_y \frac{\partial(\bar{p}+p')}{\partial x}} + \overline{u'_z \frac{\partial(\bar{p}+p')}{\partial z}} = \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_y \frac{\partial p'}{\partial x}} + \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_z \frac{\partial p'}{\partial z}} = \overline{u'_y \frac{\partial p'}{\partial x}} + \overline{u'_z \frac{\partial p'}{\partial z}} \ , \tag{12.30}$$

e)

$$\overline{u'_y \frac{\partial(\bar{p}+p')}{\partial y}} + \overline{u'_z \frac{\partial(\bar{p}+p')}{\partial x}} = \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_y \frac{\partial p'}{\partial y}} + \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_z \frac{\partial p'}{\partial x}} = \overline{u'_y \frac{\partial p'}{\partial y}} + \overline{u'_z \frac{\partial p'}{\partial x}} \ , \tag{12.31}$$

f)

$$\overline{u'_y \frac{\partial(\bar{p}+p')}{\partial z}} + \overline{u'_z \frac{\partial(\bar{p}+p')}{\partial y}} = \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_y \frac{\partial p'}{\partial z}} + \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_z \frac{\partial p'}{\partial y}} = -\overline{u'_y \frac{\partial p'}{\partial z}} + \overline{u'_z \frac{\partial p'}{\partial y}} \ , \tag{12.32}$$

g)

$$\overline{u'_z \frac{\partial(\bar{p}+p')}{\partial x}} + \overline{u'_x \frac{\partial(\bar{p}+p')}{\partial z}} = \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_z \frac{\partial p'}{\partial x}} + \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_x \frac{\partial p'}{\partial z}} = \overline{u'_z \frac{\partial p'}{\partial x}} + \overline{u'_x \frac{\partial p'}{\partial z}} \ , \tag{12.33}$$

h)

$$\overline{u'_z \frac{\partial(\bar{p}+p')}{\partial y}} + \overline{u'_x \frac{\partial(\bar{p}+p')}{\partial x}} = \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_z \frac{\partial p'}{\partial y}} + \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_x \frac{\partial p'}{\partial x}} = \overline{u'_z \frac{\partial p'}{\partial y}} + \overline{u'_x \frac{\partial p'}{\partial x}} \ , \tag{12.34}$$

i)

$$\overline{u'_z \frac{\partial(\bar{p}+p')}{\partial z}} + \overline{u'_x \frac{\partial(\bar{p}+p')}{\partial y}} = \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_z \frac{\partial p'}{\partial z}} + \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_x \frac{\partial p'}{\partial y}} = \overline{u'_z \frac{\partial p'}{\partial z}} + \overline{u'_x \frac{\partial p'}{\partial y}} \ . \tag{12.35}$$

Summing up and sorting:

$$\overline{u'_x\frac{\partial p'}{\partial x}}+\overline{u'_x\frac{\partial p'}{\partial y}}+\overline{u'_x\frac{\partial p'}{\partial z}}+\overline{u'_y\frac{\partial p'}{\partial x}}+\overline{u'_y\frac{\partial p'}{\partial y}}+\overline{u'_y\frac{\partial p'}{\partial z}}+\overline{u'_z\frac{\partial p'}{\partial x}}+\overline{u'_z\frac{\partial p'}{\partial y}}+\overline{u'_z\frac{\partial p'}{\partial z}}$$
$$+\overline{u'_x\frac{\partial p'}{\partial x}}+\overline{u'_y\frac{\partial p'}{\partial x}}+\overline{u'_z\frac{\partial p'}{\partial x}}+\overline{u'_x\frac{\partial p'}{\partial y}}+\overline{u'_y\frac{\partial p'}{\partial y}}+\overline{u'_z\frac{\partial p'}{\partial y}}+\overline{u'_x\frac{\partial p'}{\partial z}}+\overline{u'_y\frac{\partial p'}{\partial z}}+\overline{u'_z\frac{\partial p'}{\partial z}}\;. \tag{12.36}$$

leads to the following expression:

$$\overline{u'_i\frac{\partial p'}{\partial x_j}}+\overline{u'_j\frac{\partial p'}{\partial x_i}}\;. \tag{12.37}$$

Finally we use the product rule,

$$\overline{u'_i\frac{\partial p'}{\partial x_j}}=-\overline{p'\frac{\partial u'_i}{\partial x_j}}+\overline{\frac{\partial p'u'_i}{\partial x_j}}\;, \tag{12.38}$$

$$\overline{u'_j\frac{\partial p'}{\partial x_i}}=-\overline{p'\frac{\partial u'_j}{\partial x_i}}+\overline{\frac{\partial p'u'_j}{\partial x_i}}\;, \tag{12.39}$$

$$-\overline{p'\frac{\partial u'_i}{\partial x_j}}+\overline{\frac{\partial p'u'_i}{\partial x_j}}-\overline{p'\frac{\partial u'_j}{\partial x_i}}+\overline{\frac{\partial p'u'_j}{\partial x_i}}\;. \tag{12.40}$$

to get the final form. By using the Kronecker delta function (due to the fact that the pressure is only in the main diagonal of a matrix), we get:

$$\boxed{-\overline{p'\left[\frac{\partial u'_i}{\partial x_j}+\frac{\partial u'_j}{\partial x_i}\right]}+\frac{\partial}{\partial x_k}\left[\overline{p'u'_j}\delta_{ik}+\overline{p'u'_i}\delta_{jk}\right]}\;. \tag{12.41}$$

Now the derivation of the Reynolds-Stress equation is done. Putting all terms together, we can write the Reynolds-stress equation in the following form:

$$\frac{\partial\rho\overline{u'_ju'_i}}{\partial t}+\bar{u}_k\frac{\partial\rho\overline{u'_iu'_j}}{\partial u_k}+\rho\overline{u'_ju'_k}\frac{\partial\bar{u}_i}{\partial x_k}+\rho\overline{u'_iu'_k}\frac{\partial\bar{u}_j}{\partial x_k}+\frac{\partial}{\partial x_k}\rho\overline{u'_iu'_ju'_k}-\frac{\partial}{\partial x_k}\left(\mu\frac{\partial\overline{u'_iu'_j}}{\partial x_k}\right)$$
$$+2\mu\overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}}-\overline{p'\left[\frac{\partial u'_i}{\partial x_j}+\frac{\partial u'_j}{\partial x_i}\right]}+\frac{\partial}{\partial x_k}\left[\overline{p'u'_j}\delta_{ik}+\overline{p'u'_i}\delta_{jk}\right]=0\;. \tag{12.42}$$

Applying the definition of the Reynolds-Stress tensor (8.40), re-order the terms and multiply the whole equation by -1, we end up with the following form; **recall**: In almost all literatures we find the definition of the Reynolds-Stress tensor denoted by $\boldsymbol{\tau}$. In addition we use the relation between the kinematic and dynamic viscosity: $\mu = \nu\rho$. Hence, we get:

$$\begin{aligned}\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial u_k} &= -\bar{\sigma}_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \bar{\sigma}_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k}\right) + \underbrace{2\mu \overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}}_{\epsilon_{ij}} \\ &- \underbrace{\overline{p'\left[\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right]}}_{\Pi_{ij}} + \underbrace{\frac{\partial}{\partial x_k}\rho\overline{u_i' u_j' u_k'} + \frac{\partial}{\partial x_k}\left[\overline{p' u_j'}\delta_{ik} + \overline{p' u_i'}\delta_{jk}\right]}_{\frac{\partial}{\partial x_k}\underbrace{\left(\rho\overline{u_i' u_j' u_k'} + \overline{p' u_j'}\delta_{ik} + \overline{p' u_i'}\delta_{jk}\right)}_{C_{ijk}}} \quad . \end{aligned} \tag{12.43}$$

Finally, we can write the common Reynolds-Stress equation:

$$\boxed{\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial u_k} = -\bar{\sigma}_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \bar{\sigma}_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k} + C_{ijk}\right) + \epsilon_{ij} - \Pi_{ij}} \, . \tag{12.44}$$

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