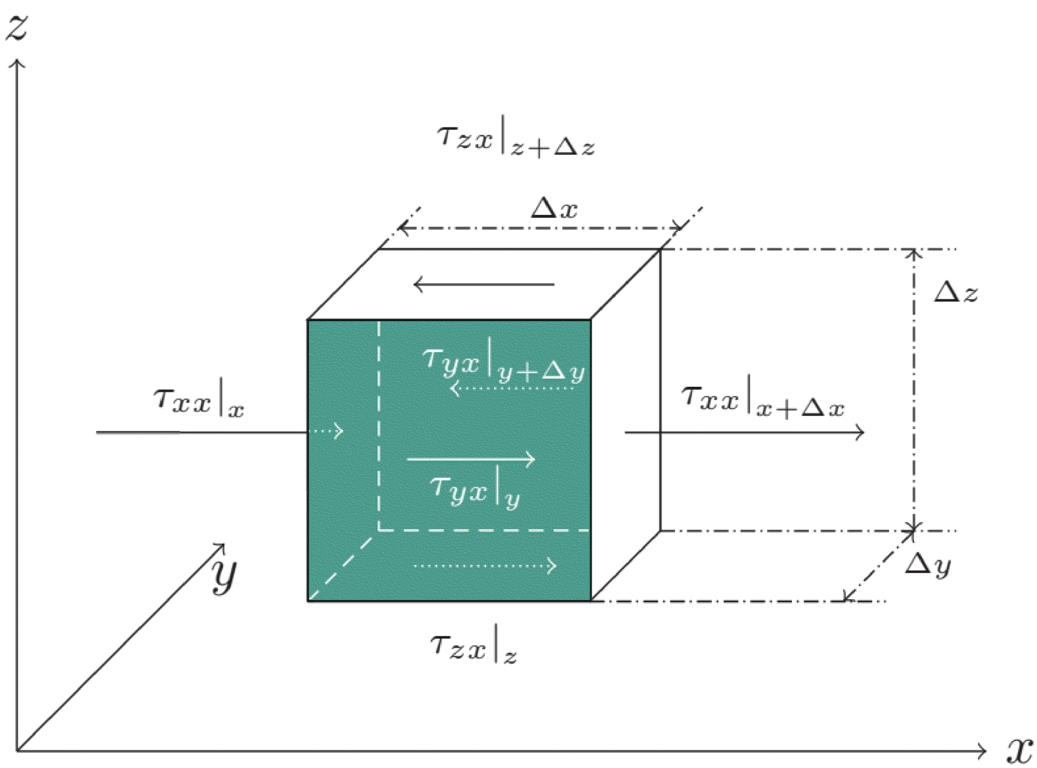
MATHEMATICS, NUMERICS, DERIVATIONS AND OPENFOAM®

The Basics for Numerical Simulations.



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***D**edidcated to the OpenFOAM® community and to all colleagues and people who support my work on Holzmann CFD. The ambition to write the book was based on my personal love to the open source thought. Thus, my objective is to give any interested CFD lover an introduction to computational fluid dynamics while showing interesting equations and some relations which are not given — or at least I did not realize them — in most of the famous books and papers in that particular area. In addition, the book should prepare you for the tasks that you may work on during your personal career, hopefully with OpenFOAM®.*

***T**he book can be ordered as a soft-cover version if enough interest exists. Please feel free to write an email to me (Dr. mont. Tobias Holzmann) via the email address Tobias.Holzmann@Holzmann-cfd.de.*

***T**o get further information about projects, developments and the latest news of my work, feel free to follow Holzmann CFD on `Twitter, LinkedIn, XING or Youtube`.*

***E**ach feedback is warmly welcomed and will be considered in new releases. If there are mistakes, typos or chapters that should be re-organized, do not hesitate to write me an email.*

***C**ooperations are welcomed. If one wants to contribute to the book, please feel free to contact me. The book is hosted on a private repository and you will get access to work with me on that project.*

***S**upport my work with a voluntary donation. Writing the book was a lot of work and as a free book, it offers a lot of information, tips and tricks as well as some interesting not-always-obvious correlations. https://holzmann-cfd.de/openfoam/community/support-holzmann-cfd.*

What is this book about

This book collects aspects of mathematics, numerics and derivations used in the field of computational fluid dynamics (CFD) and OpenFOAM®. The author of the book tries to keep the book up-to-date.

Differences in the release versions

The release notes of the book are available at https://holzmann-cfd.de. Check the download section of the website for the release notes. All changes made during a revision are listed here.

Acknowledgment

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How to cite?

The citation format depends on the journal one is using or to your personal style. The following citation is just an example based on the format that is used in this document:

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Outline

This book gives an introduction to the underlying mathematics used in the field of computational fluid dynamics. After presenting the mathematic aspects, all conservation equations are derived using a finite volume element, $\mathrm{d}V$. In the beginning, the derivation of the mass and momentum equation is described. Subsequently, all kinds of the energy equation are discussed and presented, namely the kinetic energy, internal energy, total energy, and the enthalpy equation. Based on the nature of the equations, the general governing equation is introduced afterward, and it is demonstrated how to use the general conservation equation in order to derive other ones.

The subsequent chapters discuss the definition of the shear-rate tensor $\boldsymbol{\tau}$ for Newtonian fluids. After that, a discussion between the analogy of the Cauchy stress tensor $\boldsymbol{\sigma}$, the shear-rate tensor $\boldsymbol{\tau}$ and the pressure p is given. All equations are summed up with a *one page summary* at the end.

Based on the fact that engineering applications are mostly turbulent, the Reynolds-Averaging methods are presented and explained. Subsequently, the incompressible equations are derived, and finally, the closure problem is discussed in detail. Here, the Reynolds-Stress equation — which is fully derived in the appendix — and the analogy to the Cauchy stress tensor is shown. To close the subject of turbulent flows, the eddy-viscosity theory is introduced, and the equation for the turbulent kinetic energy k and dissipation ϵ are deducted. The topic ends with a brief description of the derivation for the compressible Navier-Stokes-Equations equations and its difficulties and validity.

The last chapters of the book are related to the detailed explanation of the implementation of the shear-rate tensor calculation in OpenFOAM®. During the investigation into the C++ code, the mathematical equations are given, and a few words about the numerical stabilization is said.

Finally, a more general discussion of the different pressure-momentum coupling algorithms is given. Subsequently, the `PIMPLE`-algorithm is explained while considering an OpenFOAM® case.

The last chapter is related to OpenFOAM® beginners who are seeking for tutorials and some other useful information and websites.

Contents

Chapter 1

Basic Mathematics

In the field of computational fluid dynamics, the essential point is to understand the equations and mathematics. This knowledge is required if one is going to implement, reorder or manipulate equations within a defined software or toolbox. There are many ways to represent equations, and thus a brief collection of essential mathematics are given in this chapter. The beauty of mathematics is also described in Jasak [1996], Dantzig and Rappaz [2009], Greenshields [2015] and Moukalled et al. [2015] and other well-known literature.

In the field of numerical simulations, we are dealing with `tensors` $\mathbf{T}^n$ of rank n. A `tensor` stands for any field. A field can represent a scalar, a vector or the well known tensor that represents a matrix (normally a 3 by 3 matrix in the field of computational fluid dynamics while using the finite volume method). This tensor is of rank two. To keep things clear, we use the following definition which is similar to Greenshields [2015]:

Zero rank `tensor` $\mathbf{T}^0 :=$ scalar a
First rank `tensor` $\mathbf{T}^1 :=$ vector $\mathbf{a}$
Second rank `tensor` $\mathbf{T}^2 :=$ tensor $\mathbf{T}$ (commonly a 3x3 matrix)
Third rank `tensor` $\mathbf{T}^3 :=$ tensor T_{ijk}

If the rank of a tensor is larger than zero, the tensor is `always` written in bold symbols/letters. Tensors which have a rank larger than two are not needed in most of the equations presented in this book. The only exception is the derivation of the Reynolds-Stress equation.

1.1 Basic Rules of Derivatives

The governing conservation equations in fluid dynamics are partial differential equations. Due to that aspect, a summary of the rules that are needed to manipulate and analyze the equations is presented now.

Considering the sum of two quantities ϕ and χ that are derived according to τ, the derivative can be split as follows:

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

If we have the derivative of the product of the two quantities, it is possible to use the `product` `rule` to split the term. In other words, we have to keep one quantity constant while deriving the other one:

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

The product rule still holds, if more than two quantities are multiplied such as:

$$\frac{\partial \phi\chi\zeta}{\partial \tau} = \chi\frac{\partial \phi\zeta}{\partial \tau} + \phi\frac{\partial \chi\zeta}{\partial \tau} + \zeta\frac{\partial \phi\chi}{\partial \tau} \tag{1.3}$$

A constant quantity C can be taken inside or outside of a derivative without any constrain:

$$\frac{\partial\, C\, \phi\chi}{\partial \tau} = C\,\frac{\partial \phi\chi}{\partial \tau} \ . \tag{1.4}$$

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 — if the equation contains several similar terms which are summed up — by applying the Einsteins summation convention. Assuming the sum of the following derivatives of the arbitrary variable ϕ_i (such as the mass conservation) in x, y and z direction, the Cartesian form is written as:

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

To simplify this equation, the Einsteins summation convention can be applied. Commonly, the summation sign $\sum$ is neglected to keep things clear:

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

A more complex example that demonstrates the advantage of the Einsteins summation convention is the convective term of the momentum equation (it is not necessary to know the meaning of this terms right now). Due to the fact that the momentum is a vector quantity, the three single terms of each direction are given as:

$$\begin{aligned} &\frac{\partial u_x u_x}{\partial x} + \frac{\partial u_y u_x}{\partial y} + \frac{\partial u_z u_x}{\partial z} \ , \\ &\frac{\partial u_x u_y}{\partial x} + \frac{\partial u_y u_y}{\partial y} + \frac{\partial u_z u_y}{\partial z} \ , \\ &\frac{\partial u_x u_z}{\partial x} + \frac{\partial u_y u_z}{\partial y} + \frac{\partial u_z u_z}{\partial z} \ . \end{aligned}$$

Applying the Einsteins convention, the nine terms can be represented as follow:

$$\sum_i \frac{\partial u_i u_j}{\partial x_i} = \frac{\partial u_i u_j}{\partial x_i} \qquad i = x, y, z; \;\; j = x, y, z \ . \tag{1.6}$$

The Einsteins summation convention is widely used in literature. Hence, it is essential to know the meaning and how it is applied.

1.3 General Tensor Mathematics

A common and easy way to deal with equations is to use the vector notation instead of the Einsteins summation convention. The vector notation requires knowledge about special mathematics. Therefore, a brief description of different operations which are applied to scalars, vectors and tensors are given now. For that purpose arbitrary quantities are defined now: 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 of interest, one uses either the numeric indices $(1, 2, 3)$ or the space components (x, y, z). Furthermore, the unit vectors $\mathbf{e}_i$ and the identity matrix $\mathbf{I}$ are defined as usual:

$$\mathbf{e}_1 = \mathbf{e}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \quad \mathbf{e}_2 = \mathbf{e}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} , \quad \mathbf{e}_3 = \mathbf{e}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} , \quad \mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} .$$

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 $\mathbf{T}$:

$$\phi\mathbf{b} = \begin{pmatrix} \phi b_x \\ \phi b_y \\ \phi b_z \end{pmatrix} , \qquad \phi\mathbf{T} = \begin{bmatrix} \phi T_{xx} & \phi T_{xy} & \phi T_{xz} \\ \phi T_{yx} & \phi T_{yy} & \phi T_{yz} \\ \phi T_{zx} & \phi T_{zy} & \phi T_{zz} \end{bmatrix} . \tag{1.7}$$

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 $\bullet$:

$$\phi = \mathbf{a} \bullet \mathbf{b} = \mathbf{a}^T \mathbf{b} = \sum_{i=1}^{3} a_i b_i \ . \tag{1.8}$$

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

$$\mathbf{b} = \mathbf{T} \bullet \mathbf{a} = \sum_{i=1}^{3} \sum_{j=1}^{3} T_{ij} a_j \mathbf{e}_i = \begin{pmatrix} T_{11}a_1 & + & T_{12}a_2 & + & T_{13}a_3 \\ T_{21}a_1 & + & T_{22}a_2 & + & T_{23}a_3 \\ T_{31}a_1 & + & T_{32}a_2 & + & T_{33}a_3 \end{pmatrix} . \tag{1.9}$$

$$\mathbf{b} = \mathbf{a} \bullet \mathbf{T} = \mathbf{T}^T \bullet \mathbf{a} = \sum_{i=1}^{3} \sum_{j=1}^{3} a_j T_{ji} \mathbf{e}_i = \begin{pmatrix} a_1T_{11} & + & a_2T_{21} & + & a_3T_{31} \\ a_1T_{12} & + & a_2T_{22} & + & a_3T_{32} \\ a_1T_{13} & + & a_2T_{23} & + & a_3T_{33} \end{pmatrix} , \tag{1.10}$$

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 $\mathbf{:}$ sign:

$$\phi = \mathbf{T} \mathbf{:} \mathbf{S} = \sum_{i=1}^{3}\sum_{j=1}^{3} T_{ij}S_{ij} = T_{11}S_{11} + T_{12}S_{12} + T_{13}S_{13} + T_{21}S_{21} \\ + T_{22}S_{22} + T_{23}S_{23} + T_{31}S_{31} + T_{32}S_{32} + T_{33}S_{33}\ . \tag{1.11}$$

The Outer Product

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

$$\mathbf{T} = \mathbf{a} \otimes \mathbf{b} = \mathbf{a}\mathbf{b}^T = \begin{bmatrix} a_x b_x & a_x b_y & a_x b_z \\ a_y b_x & a_y b_y & a_y b_z \\ a_z b_x & a_z b_y & a_z b_z \end{bmatrix} . \tag{1.12}$$

In most of the literature we will find that the dyadic sign $\otimes$ is neglected for brevity as shown below:

$$\mathbf{ab}\ . \tag{1.13}$$

Keep in mind, that both variants are used in literature whereas the last one is more common, but the first one is mathematically correct. In this book we use the definition of equation (1.12), to be consistent with the mathematics.

Differential Operators

In vector notation, the spatial derivative 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 $\mathbf{a}$:

$$\operatorname{grad}\phi = \nabla\phi = \begin{pmatrix} \frac{\partial\phi}{\partial x} \\ \frac{\partial\phi}{\partial y} \\ \frac{\partial\phi}{\partial z} \end{pmatrix} . \tag{1.14}$$

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

$$\operatorname{grad} \mathbf{b} = \nabla \otimes \mathbf{b} = \begin{bmatrix} \frac{\partial}{\partial x} b_x & \frac{\partial}{\partial x} b_y & \frac{\partial}{\partial x} b_z \\ \frac{\partial}{\partial y} b_x & \frac{\partial}{\partial y} b_y & \frac{\partial}{\partial y} b_z \\ \frac{\partial}{\partial z} b_x & \frac{\partial}{\partial z} b_y & \frac{\partial}{\partial z} b_z \end{bmatrix} . \tag{1.15}$$

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

$$\nabla \mathbf{b} . \tag{1.16}$$

In this book, we use the first notation (with the dyadic sign) to be consistent within the mathematics. The gradient operation *increases* 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, $\nabla\bullet$:

$$\operatorname{div} \mathbf{b} = \nabla \bullet \mathbf{b} = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} b_i = \frac{\partial b_1}{\partial x_1} + \frac{\partial b_2}{\partial x_2} + \frac{\partial b_3}{\partial x_3} . \tag{1.17}$$

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

$$\operatorname{div} \mathbf{T} = \nabla \bullet \mathbf{T} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial}{\partial x_j} T_{ji} \mathbf{e}_i = \begin{bmatrix} \frac{\partial T_{11}}{\partial x_1} & + & \frac{\partial T_{21}}{\partial x_2} & + & \frac{\partial T_{31}}{\partial x_3} \\ \frac{\partial T_{12}}{\partial x_1} & + & \frac{\partial T_{22}}{\partial x_2} & + & \frac{\partial T_{32}}{\partial x_3} \\ \frac{\partial T_{13}}{\partial x_1} & + & \frac{\partial T_{23}}{\partial x_2} & + & \frac{\partial T_{33}}{\partial x_3} \end{bmatrix} . \tag{1.18}$$

The divergence operation *decreases* 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 presented now.

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

$$\nabla \bullet (\mathbf{a}\phi) = \underbrace{\mathbf{a} \bullet \nabla\phi}_{\text{Eqn. (1.8)}} + \underbrace{\phi \nabla \bullet \mathbf{a}}_{\text{simple multiplication}} . \tag{1.19}$$

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

$$\nabla \bullet (\mathbf{a} \otimes \mathbf{b}) = \underbrace{\mathbf{a} \bullet \nabla \otimes \mathbf{b}}_{\text{Eqn. (1.10)}} + \underbrace{\mathbf{b} \nabla \bullet \mathbf{a}}_{\text{Eqn. (1.7)}} . \tag{1.20}$$

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

$$\nabla \bullet (\mathbf{T} \bullet \mathbf{b}) = \underbrace{\mathbf{T} \colon \nabla \otimes \mathbf{b}}_{\text{Eqn. (1.11)}} + \underbrace{\mathbf{b} \bullet \nabla \bullet \mathbf{T}}_{\text{Eqn. (1.8)}} \ . \tag{1.21}$$

If one thinks that the product rule for the inner product of two vectors is missing, think about the result of the inner product of the two vectors and which tensor rank the result will have. After that, ask yourself how the divergence operator will change the rank.

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:

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} = \frac{\partial \phi}{\partial t} + \underbrace{\mathbf{U} \bullet \nabla \phi}_{\text{inner product}} \quad , \tag{1.22}$$

where $\mathbf{U}$ represents the velocity vector. The last term in equation (1.22) denotes the inner product. Depending on the quantity ϕ (scalar, vector, tensor, and so on), the correct mathematical expression for the second term on the right hand side (RHS) has to be applied. Example given:

- If ϕ is a scalar, we have to use equation (1.8),
- If ϕ is a vector, we have to use equation (1.10).

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 formulation 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 formulated equation to the conserved one. Personally, the better way would be to derive the conserved equation *first* and using the continuity equation *afterwards* to get the non-conserved form. *Why*? For me it was 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-conserved form of the equations, the following section should help to understand the following extension (at the moment it is not necessary to understand this equations):

- Incompressible:

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} = \underbrace{\frac{\partial \phi}{\partial t} + \mathbf{U} \bullet \nabla \phi}_{\text{non-conserved}} \boxed{+ \ \phi \ \underbrace{(\nabla \bullet (\mathbf{U}))}_{\text{continuity } = \ 0}} \ . \tag{1.23}$$

- Compressible:

$$\rho \frac{\mathrm{D}\phi}{\mathrm{D}t} = \underbrace{\rho \left[\frac{\partial \phi}{\partial t} + \mathbf{U} \bullet \nabla \phi \right]}_{\text{non-conserved}} \boxed{+ \ \phi \underbrace{\left(\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{U}) \right)}_{\text{continuity } = \ 0}} \ . \tag{1.24}$$

The reason for 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 statement 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. Therefore, some basic mathematical expressions and manipulations are introduced now.

Each matrix $\mathbf{A}$ can be split into a deviatoric $\mathbf{A}^{\text{dev}}$ and hydrostatic $\mathbf{A}^{\text{hyd}}$ part:

$$\mathbf{A} = \mathbf{A}^{\text{hyd}} + \mathbf{A}^{\text{dev}} \ . \tag{1.25}$$

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

$$A^{\text{hyd}} = \frac{1}{3}\,\text{tr}(\mathbf{A}) = \frac{1}{3}\sum_{i=1}^{n}(a_{ii}) \ . \tag{1.26}$$

The operator `tr` denotes the trace operator and is applied on the matrix. This operator simply sums up the diagonal elements. However, the correct mathematical expression for the hydrostatic part of the matrix $\mathbf{A}$ is given by:

$$\mathbf{A}^{\text{hyd}} = A^{\text{hyd}}\mathbf{I} = \frac{1}{3}\,\text{tr}(\mathbf{A})\mathbf{I} = \frac{1}{3}\sum_{i=1}^{n}(a_{ii})\mathbf{I} \ . \tag{1.27}$$

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

$$\mathbf{A}^{\text{dev}} = \mathbf{A} - \mathbf{A}^{\text{hyd}} = \mathbf{A} - \frac{1}{3}\,\text{tr}(\mathbf{A})\mathbf{I} \ . \tag{1.28}$$

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

1.3.3 The Gauss Theorem

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

$$\oint \mathbf{a}\cdot\mathbf{n}\mathrm{d}S = \int (\nabla \bullet \mathbf{a})\mathrm{d}V \ . \tag{1.29}$$

In equation (1.29), $\mathbf{n}$ represents the surface normal vector pointing outwards, $\mathrm{d}S$ the integration with respect to the surface and $\mathrm{d}V$ the integration with respect to the volume.

Note: The small dot $\cdot$ denotes the inner product of two vectors (1.8). 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 mathematical expression as the bullet.

Chapter 2

Derivations of the Governing Equations

The following chapter discusses the derivation of the continuity, momentum, total energy, mechanical (kinetic) energy, thermo (internal) energy and enthalpy equation by using a small volume element $\mathrm{d}V$. The equations are derived completely while using the Cartesian coordinate system. A summary of all discussed equations is given on page 43. 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 conserved Cartesian formulation,
- Transform the Cartesian into the vector notation,
- Perform a proof to demonstrate that the vector notation results in the Cartesian form,
- Transform the equation into the integral and non-conserved form.

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

2.1 The Continuity Equation

In the following section the derivation of the continuity equation is presented. The equation itself describes the mass balance of an arbitrary volume element $\mathrm{d}V$.

Consider the mass flow through a small control volume element $\mathrm{d}V$, c.f. figure 2.1, while 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 and leaves the volume element through its surfaces has to be equal if the mass inside the control volume does not change by means of compression or expansion — this is also named as *rate of mass accumulation*. Considering a small control volume $\mathrm{d}V$, we can say:

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

To keep clearance, we will now focus on figure 2.1. It is obvious that the quantity `mass` is transported through the surface by the velocity. This transport phenomenon is called convection or sometimes named advection. In literature we can find the different meaning of convection and advection as follows:

- Advection: Transport of mass, momentum, energy, etc. based on the fluid flow (flux) without diffusion effects.

- Convection: Transport of any property based on fluxes and diffusion.

However, personally I heard that convection and advection represents always the transport of the quantity of interest based on the fluxes, while the nomenclature of convection always if we are talking about the momentum equation (e.g. the source of fluxes) while other quantities are advected with the fluxes.

The transport of mass happens in all three space directions x (u_x), y (u_y) and z (u_z). Additionally, mass can change inside the control element $\mathrm{d}V$ which is related to compression or expansion phenomenon. Thus, the density of the fluid inside the volume must change.

Analysing figure 2.1 in more detail, we observe that the velocity vectors are aligned normal to the surface faces. The rate of mass that enters or leaves the volume element through the surface is called mass flux and is simply the density multiplied by the velocity with respect to the face area.

For the derivation of the mass conservation equation we have to build the balance of the surface fluxes at all faces of the control volume $\mathrm{d}V$. In other words, everything that is going inside has to go out, if we assume that there is no mass accumulation inside the volume (assumption: incompressible). The single terms that describe the fluxes at the surfaces are given on the right side in figure 2.1.

Considering a compressible fluid, the rate of mass change inside the control volume $\mathrm{d}V$ is related to the density ρ and will only decrease or increase with respect to the time. It is worth to mention that the quantity is defined to be **mass per unit volume**. Therefore, we can write the

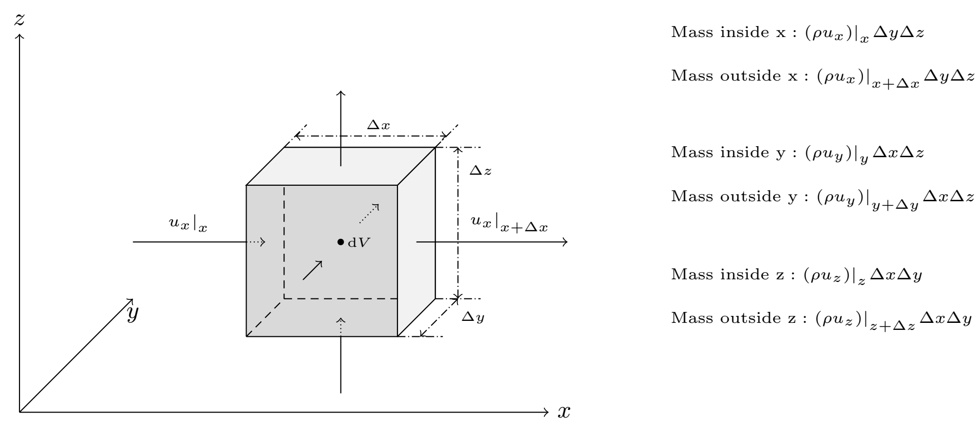


Figure 2.1: Mass balance in a small volume element $\mathrm{d}V$.

rate of change of the density as:

$$\text{Time Accumulation} = \frac{\Delta\rho}{\Delta t} \ . \tag{2.2}$$

Rewriting equation (2.1) by using the mathematical expressions given in 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 end up with the following:

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

Introducing the assumption of an infinitesimal small volume element — which means that we decrease the distance between the corners of the volume and therefore, Δ goes to the limit to become 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 infinitesimally 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:

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

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

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

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

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

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

While using 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 can assume that the density is constant and therefore, the quantity ρ can be taken out of the derivatives and the whole equation can be divide by the density ρ. It is obvious that the time derivative will vanish due to the fact that the density is a constant. In other words, there is no accumulation of mass during the time in the volume element. One may also explain it in the following way: If we assume a constant density, there is no expansion or compression phenomena and therefore, the time derivative become zero. Hence, only the mass flux that enters and/or leaves the volume element at its surface has to be taken into account.

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

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

In case of the incompressible mass conservation equation, it is evident that the vector notation results in the Cartesian form again. Thus, the transformation is not demonstrated here. If one wants to recheck it, just use equation (1.17).

Remark: In many cases incompressibility means that there is no expansion and/or compression phenomena. However, the fluid density can still be temperature depended and therefore, the quantity is not a constant. In such cases we have to be careful which mass conservation equation is used in the computational calculation. Either the incompressible or the compressible one. 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 non-constant quantities are not allowed to be taken out of the derivatives. However, if the density change is very small, we can use the incompressible mass conservation equation with limitations. The reason for that is based on numerics and the interaction with the momentum conservation equation.

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. While using the Gauss theorem (1.29), 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 $\mathrm{d}V$ itself does not change its shape with respect to the time (fixed finite volume - static mesh). 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 surfaces of the 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 arbitrary volumes such as hexaeder, tetraeder, prisms, wedges and so on. This advantage made this method popular and flexible. However, it is worth to mention that the shape of the volumes influences the numerical stability and the calculation precision in general.

OpenFOAM®

In OpenFOAM® we are using the equations (integral one) above to calculate the fluxes at the faces of each numerical cell. The flux field is named `phi` and is created by including 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 these values to the face centers. This calculation is done by calling the function `interpolate(rho*U) & mesh.Sf()`. As we can see, this will simply calculate the product of the density and the velocity vector at each cell center and interpolate the result to the face center by including the corresponding neighbor cell information. To get the fluxes, the known face values are then multiplied by the magnitude of the surface normal vector (`Sf()`). The calculation is an inner product operation of two vectors which is denoted by the ampersand sign `&` in OpenFOAM®.

2.1.2 Continuity Equation and the Total Derivative

In the first chapter, while introducing basic mathematical operation, we already mentioned the total derivative. After knowing the continuity equation, we can investigate into it in more detail.

Using the total derivative formulation (1.22), we are able to rewrite the continuity equation (2.12) by applying the product rule (1.19) 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].

2.2 The Conserved Momentum Equation

The following section discusses the derivation of the momentum equation which is also called Navier-Stokes equation.

The derivation of the conserved momentum equation is similar to the continuity equation. Again, we will use the volume element $\mathrm{d}V$. The main difference in the momentum equation compared to the mass conservation equation is as follows: The quantity of the momentum is a vector and not a scalar. Thus, the momentum is not only transported/advected via the flux through the surfaces of the volume element. Generally, we are allowed to define the momentum transport and its change inside the volume $\mathrm{d}V$ as follow:

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

Figure 2.2 shows the volume element as given in figure 2.1 but now including another transport phenomenon that acts on the surfaces (only the x direction is sketched). This transport of the momentum is based on molecular effects. The molecular transport acts always normal and tangential to the surface and is an outcome or property of the vector quantity.

Other phenomena that change the momentum inside the volume are given as a sum of forces. For example, we could have the gravitational acceleration and the pressure force acting on the volume.

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.

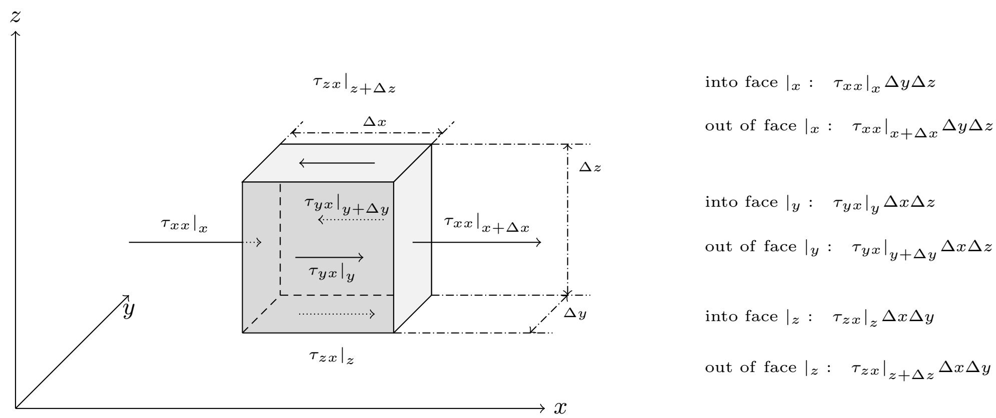


Figure 2.2: Molecular transport of the momentum in x-direction in an arbitrary small volume element $\mathrm{d}V$.

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. Therefore, the convection of the momentum can be derived similarly to the convective transport of the mass. However, now we have to take care of the **vector** quantity. Thus, the momentum in the x-direction enters the volume at the face $|_x$ and leaves the volume through the face $|_{x+\Delta x}$; identical to the continuity equation. Nevertheless, it is also possible that the x-component of the momentum is transported through the faces in y- and z-direction (molecular transport). Hence, we can write the transport of the momentum due to convection; it is merely the velocity in x-direction multiplied by the **flux** through the face we are looking at (Newton's 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 effects as demonstrated in figure 2.2. The effect is based on velocity differences (velocity gradients). As we can see in figure 2.2, different terms occur which include either the normal component τ_{xx} or the tangential component τ_{yx} or τ_{zx}. Therefore, the molecular transport of the x-momentum through the surfaces can be written as:

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

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 since they are generated concerning velocity gradients that introduce shearing.

Additional Forces that Influence the Momentum

In most scientific and engineering tasks, the only essential forces that influence the momentum are the pressure and gravity force. The pressure force acts on the surface of the volume element while the gravitational force acts on the volume directly. Hence, we can derive the change of the x-momentum based on the pressure and gravitational force:

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

Conserved Momentum Equation

After we have all terms — neglecting other influences such as surface tension and so on —, the equation (2.20) can be reconstructed with the corresponding mathematical expressions derived above. 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 infinitesimally small volume element (2.5) and time range (2.6) to rewrite the x-component of the momentum equation. The x-component of the momentum is then written as:

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

The other two space components are derived identically to the x-component. Thus, only the final formulation is given. 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 can write the conserved momentum equation in vector form:

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

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.

2.2.1 The Proof of the Transformation

The following section will investigate into the 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:

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

As we see, the time derivative term results in the same three terms that we have in the Cartesian formulation. The second term embraces the transport of momentum due to convection by the flux $\rho\mathbf{U}$. To evaluate the term, we need the mathematics (1.12) and (1.18):

$$-\nabla \bullet (\rho\mathbf{U}\otimes\mathbf{U}) = -\nabla \bullet \left\{\rho\begin{pmatrix}u_x\\ u_y\\ u_z\end{pmatrix}\otimes\begin{pmatrix}u_x\\ u_y\\ u_z\end{pmatrix}\right\} = -\nabla \bullet \left\{\rho\begin{bmatrix}u_x u_x & u_x u_y & u_x u_z\\ u_y u_x & u_y u_y & u_y u_z\\ u_z u_x & u_z u_y & u_z u_z\end{bmatrix}\right\}$$

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

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

Again, we can see 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 (1.18) for the shear-rate tensor $\boldsymbol{\tau}$, we get:

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

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

At last the pressure and gravitational acceleration term are analyzed. For the pressure term we need the definition of equation (1.14) and for the gravitational term equation (1.7). 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 8. The implementation of the momentum equation in OpenFOAM® will be discussed in chapter 10; 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 (1.29). It follows:

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

2.2.3 Non-Conserved Momentum Equation

We can manipulate the conserved momentum equation with the continuity equation (2.12). Hence, we get the non-conservative form. For that, we first consider equation (2.26) 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 (1.20). 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 (1.22), 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 investigates into 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 $\mathrm{d}V$ by:

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

The formally written equation above shows the first law of thermodynamics written for an open and unsteady system with the extension of additional heat sources which was also stated by Bird et al. [1960]. The statement is incomplete because no energy can be generated due to nuclear phenomenon. Furthermore, no radiative energy transport is included.

In the equation above, internal, kinetic and work energy is included, and therefore unsteady behavior can be captured. The kinetic energy (`per unit mass`) is given by $\frac{1}{2}\rho|\mathbf{U}|^2$ where $|\mathbf{U}|$ denotes the magnitude of the local velocity. The internal energy e (`per unit mass`) 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 $\mathrm{d}V$. The accumulation in time is clear (such as 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 the total energy – that enters and leaves the volume element $\mathrm{d}V$ based on the convection phenomenon –, we 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 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:

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

Similarly, 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 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 can rewrite equation (2.22):

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

As before, we divide the equation by the volume dV and use the assumption of expression (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. Therefore, we end up with:

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

≫ Continued on next page ≪

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

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

To get a more readable equation, we transform the above derived formulation into the vector notation. Thus, different terms can be analyzed in more detail. It follows:

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

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 (1.8) and (1.9).

Remark: Till now we did not investigate into the potential energy. This will not be discussed here. If one needs information about that, Bird et al. [1960] gives insight into the topic on p. 314.

2.3.1 The Proof of the Vector Transformation

On the next pages, we will convert the vector form of the total energy equation back into the Cartesian form. 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 formulation of equation (1.8). For the viscous force term we need equation (1.9) and (1.18).

It follows that the gravity term can be modified as:

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

The viscous force term can be changed as follows:

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

As the transformation showed us, the terms are equal. 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 formulation. 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 leads to the non-conservative form. For that, we first need to split the time and convective terms of equation (2.45) using the product rule. Hence, the time derivative can be rewritten as:

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

and the convective term will be transformed into:

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

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

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

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

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

We 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:

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

By using the definition of the total derivative (1.22), we finally can rewrite the equation in the non-conservative form:

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

OpenFOAM®

For informative purposes, the symbols used in OpenFOAM® are given now. The total energy is donated by the symbol $E = (e + \frac{1}{2}|\mathbf{U}|^2)$. The kinetic (mechanical) energy is donated by the symbol $K = \frac{1}{2}|\mathbf{U}|^2$.

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 subtract that equation from the total energy equation to get the other one. Thus, we will first derive the mechanical (kinetic) energy equation 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 by merely 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.

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

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

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 merely 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 analogously 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 $e_{\mathrm{kin,S}}$ and put the new evaluated terms into equation (2.55), we get:

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

To achieve the partial differential equation, we will divide the whole equation by the volume of the element $\mathrm{d}V$. It follows:

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

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 explicitly mentioned source term:

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

The vector notation for this equation is:

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

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

Several phenomena can influence the kinetic energy. These sources (terms) act on the volume element. To get the different source terms, we will use the momentum equation (2.26). The terms $e_{\mathrm{kin,S}}$ are merely 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 $e_{\text{kin,S}}$ by:

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

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

If we insert the source term $e_{\text{kin,S}}$ into equation (2.61), we get the conserved mechanical (kinetic) energy equation including the above mentioned source terms.

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

Analyzing the new equation, we already know the meaning of the term on the LHS and the first and last term on the RHS. The meaning of the second and third term on the RHS is not 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:

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

The pressure term can be manipulated as follows:

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

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, for the source terms get the following expression:

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

Finally, we use the new evaluated sources $e_{\mathrm{kin,S}}$ 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 process is reversible. This term will heat 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 (1.29). 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 can 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. Besides, 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:

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

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

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

As we can see, the second term on the LHS is zero due to the continuity equation, and therefore, we get the non-conserved kinetic energy equation by using the definition of the total derivative (1.22) to be:

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

Remark: It should be evident that we can use equation (2.64) and (2.65) to change/eliminate some terms or rearrange the equation.

2.5 The Conserved Thermo Energy Equation

After the total energy and the kinetic energy equations are derived, the equation for the thermo (internal) energy equation can easily be build 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:

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

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

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

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

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:

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

After sorting the terms, we get the final form:

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

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 (1.29):

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

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 always look 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:

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

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 equal to 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:

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

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

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

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

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

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. We get:

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

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 terms into 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:

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

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 literature, 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):

$$\begin{gathered}\left\{\frac{\partial}{\partial t}\rho h - \frac{\partial}{\partial t}p + \frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2\right\} - \left\{\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{U}|^2\right\} = \\ \left\{-\nabla\bullet(\rho\mathbf{U}h) - \nabla\bullet\left(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2\right) - \nabla\bullet\mathbf{q} + \rho\left(\mathbf{U}\bullet\mathbf{g}\right) - \nabla\bullet[\boldsymbol{\tau}\bullet\mathbf{U}] + \rho\mathrm{S}\right\} \\ -\left\{-\nabla\bullet(\rho\mathbf{U}\frac{1}{2}|\mathbf{U}|^2) - \nabla\bullet[\boldsymbol{\tau}\bullet\mathbf{U}] - (-\boldsymbol{\tau}\boldsymbol{:}(\nabla\otimes\mathbf{U}))\right. \\ \left. -\nabla\bullet(p\mathbf{U}) - p(-\nabla\bullet\mathbf{U}) + (\rho\mathbf{g})\bullet\mathbf{U}\right\}\ .\end{gathered} \tag{2.97}$$

The outcome of the subtraction is that many 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 widely reported and can be found in different literature.

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

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

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

This lead to the total derivative on the RHS for the pressure and we can apply the rule given by equation (1.22). The modified equation is then given by:

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

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

Chapter 3

The Governing Equations for Engineers

Typically, 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 can – *probably* – derive any equation. The general (governing) conservation equation of an arbitrary 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 sources or sinks that influence the quantity ϕ. Now we can 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 mass is not transported by diffusion effects and we further assume that the mass is not transformed 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 $\mathbf{U}$. Besides, 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 the gravitational acceleration and the pressure force. Later on, we see a more general form of this equation. Summing up, we end up with the following formulation:

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

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 already changed.

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 relevant 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 straightforward to use this equation and derive the conservative equation of interest.

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 $\mathbf{q} = -\lambda \nabla T$. Additionally, the energy of a fluid can be changed by other sources such as the pressure work, friction, and so on. These terms are given in the chapter before and are neglected now.

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

It should be mentioned that the enthalpy equation has a special characteristic because it requires the knowledge of the temperature field T. The enthalpy equation is of interest, if we are solving compressible fluids — compare the OpenFOAM® toolbox. For incompressible fluids, no information about the energy is needed commonly. However, for compressible fluid we solve an energy equation (either for the enthalpy or total energy).

Temperature equation

The temperature equation can be derived using the thermodynamic relation between the enthalpy and temperature quantity:

$$c_\mathrm{p} = \frac{\partial h}{\partial T} \quad . \tag{3.5}$$

The relation in equation 3.5 is further investigated during the derivation of the temperature equation for solid bodies.

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

$$\rho c_\mathrm{p} \frac{\partial}{\partial t} T = -\rho c_\mathrm{p} \nabla \bullet (\mathbf{U} T) + \nabla \bullet (\lambda \nabla T) \qquad \underbrace{(+S_h)}_{\text{neglected}} \quad . \tag{3.6}$$

Depending on the field we are working on, we have to take care about different phenomena that influence the temperature in the system. 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 interesting example would be as follows: Solving a fluid for incompressible fluids but using a temperature depended density. It can be shown — mathematically —, that this case can cause troubles and numerical instabilities if the implementation is not done correct.

In addition it is worth to mention, that the temperature equation looks different if the above mentioned assumptions are not fulfilled (incompressibility and constant heat capacity. Moukalled et al. [2015] give a well-done summary about the derivation of the temperature equation.

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):

$$S_{\mathrm{sh}} = \boldsymbol{\tau} : (\nabla \otimes \mathbf{U}) \ . \tag{3.7}$$

- Pressure work

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

$$S_{\mathrm{pw}} = \frac{\partial p}{\partial t} \ . \tag{3.8}$$

Note: This term can be turned on and off in the enthalpy equation by using the dpdt keyword

While using the thermodynamic relation between enthalpy, temperature, and pressure:

$$\mathrm{d}h(T,p) = \left(\frac{\partial h}{\partial T}\right)_{\mathrm{p}} \mathrm{d}T + \left(\frac{\partial h}{\partial p}\right)_{\mathrm{T}} \mathrm{d}p \ , \tag{3.12}$$

while neglecting the second term on the RHS, we get:

$$\mathrm{d}h(T) = \left(\frac{\partial h}{\partial T}\right)_{\mathrm{p}} \mathrm{d}T \ . \tag{3.13}$$

Furthermore, we know:

$$\left(\frac{\partial h}{\partial T}\right)_{\mathrm{p}} = c_{\mathrm{p}} \ . \tag{3.14}$$

Therefore, we can write (neglecting the hint of the temperature dependence of the enthalpy quantity):

$$\mathrm{d}h = c_{\mathrm{p}}\mathrm{d}T \ . \tag{3.15}$$

The next step is to rewrite the enthalpy equation by using the product rule. It follows:

$$\rho\frac{\partial h}{\partial t} + h\frac{\partial \rho}{\partial t} + \rho\mathbf{U} \bullet \nabla h + h\nabla \bullet (\rho\mathbf{U}) = -\nabla \bullet \mathbf{q} + S_h \ . \tag{3.16}$$

After sorting the terms, we get:

$$\rho\left[\frac{\partial h}{\partial t} + \mathbf{U} \bullet \nabla h\right] + h\left[\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho\mathbf{U})\right] = -\nabla \bullet \mathbf{q} + S_h \ . \tag{3.17}$$

For solids (rigid bodies) there is no motion. Therefore, the velocity vector is zero. If we further neglect the source terms, we get:

$$\rho \left[c_\mathrm{p} \frac{\partial T}{\partial t} \right] = -\nabla \bullet \mathbf{q} \ . \tag{3.23}$$

Finally, we end up with the well known equation:

$$\rho c_\mathrm{p} \frac{\partial T}{\partial t} = \nabla \bullet (\lambda \nabla T) \ . \tag{3.24}$$

It is worth to mention, that equation 3.22 can be transformed into 3.6, if the second term on the LHS is extended by $(c_\mathrm{p} T \nabla \bullet \mathbf{U})$ and the the rule 1.19 is applied.

A full derivation of the conservative temperature equation, including all terms, is given in Moukalled et al. [2015].

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 software we are using — which equation and which terms are solved — and the equation and mathematics respectively.

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

However, it is worth to mention that I have a strong personal force to keep the book up to date and extend different topics during time. Additionally, voluntary contributors are welcomed to work on that book and extend it with their topics.

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 mechanical 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
	Total Enthalpy	$\frac{\partial}{\partial t}\rho h - \frac{\partial}{\partial t}p + \frac{\partial}{\partial t}\frac{1}{2}\rho\lvert\mathbf{U}\rvert^2 = -\nabla \bullet (\rho\mathbf{U}h) - \nabla \bullet \left(\rho\mathbf{U}\frac{1}{2}\lvert\mathbf{U}\rvert^2\right) - \nabla \bullet \mathbf{q} + \rho\,(\mathbf{U} \bullet \mathbf{g}) - \nabla \bullet [\boldsymbol{\tau} \bullet \mathbf{U}] + \rho\mathrm{S}$	
	Enthalpy (Only Thermo)	$\frac{\partial}{\partial t}\rho h - \frac{\partial}{\partial t}p = -\nabla \bullet (\rho\mathbf{U}h) - \nabla \bullet \mathbf{q} + (\mathbf{U} \bullet \nabla\mathbf{p}) + [-\tau : (\nabla \otimes \mathbf{U})] + \rho\mathrm{S}$	$h = e + \frac{p}{\rho}$
	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 derived in the previous chapters allow us to investigate into engineering and scientific fluid behavior. This enables the possibility to get a better insight into the physics and lead to a better understanding of different phenomena in the flow field. Besides, it is possible to extract quantities that are not measurable in reality – imagine a liquid metal at high temperature while the pressure and velocity at certain positions should be measured.

However, if we analyze the derived equations, some quantities are not known; for example the shear-rate components τ_{ij}. These unknown quantities have to be expressed by known ones.

The shear-rate tensor $\boldsymbol{\tau}$ is expressed by differential 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 only. Further notes and information can be found in Bird et al. [1960], Ferziger and Perić [2008] and Dantzig and Rappaz [2009].

5.1 Newtonian Fluids

If we are investigating into Newtonian fluids, we use the Newtonian law for the shear-rate (viscous stress) tensor $\boldsymbol{\tau}$. Thus, the nine components of the tensor 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 quantity κ included. Bird et al. [1960] describes this variable as the bulk viscosity. However, in chapter 7, we will realize that this definition is in discrepancy to other authors. Therefore, we should describe the bulk viscosity differently. Nevertheless, as Bird et al. [1960] mentioned, the quantity κ is not important for dense gases and liquids and can be neglected; again, later on we see why. The other term in the normal stress components takes the value $\frac{2}{3}\mu$, which many authors refers to the secondary viscosity, dilatation term or first Lamés coefficient that is again in discrepancy to other authors. The main reason for that misleading definition is based on the fact that the following correlation $\lambda = -\frac{2}{3}\mu$ can be made. In chapter 7 we will investigate into this topic in more detail. It is worth to mention that Gurtin et al. [2010] also gives a good and complete overview about that. However, we will keep the quantity κ for now as it is common in literature.

Remark

In general it is sufficient to know how the shear-rate tensor is defined. However, if we are going to implement or establish new models, it is necessary to understand the different terms and their meaning. Therefore, it is an important background knowledge to know why and how we get to the shear rate tensor. Besides, it is also of importance to distinguish between the pressure and equilibrium pressure in that topic. The main reference in this field is based on Gurtin et al. [2010].

Continued

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 merged 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, which means $A_{ij} \rightarrow A_{ji}$, we can write the vector form of the above given 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:

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

The viscous stress tensor also named shear-rate or deformation-rate tensor $\boldsymbol{\tau}$ can therefore 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 define $\kappa = 0$, which comes from the Stokes hypothesis, the general Navier-Stokes equation can be presented as:

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

This form of the Navier-Stokes equation is given in many literature. Another form of the momentum equation (5.13) can be achieved after pushing the pressure gradient into the viscous stress tensor:

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

It should be obvious that the gradient of the pressure is identical to the divergence of the pressure multiplied by the identity matrix:

$$\nabla p = \nabla \bullet (p\mathbf{I}) \; . \tag{5.17}$$

All terms within the bracket are summed together to the so called Cauchy stress tensor $\boldsymbol{\sigma}$. A detailed discussion about this quantity is given in chapter 6. Finally, it should be mentioned that there are much more ways to define this equation. Especially if we distinguish between total pressure p and the equilibrium pressure p_{eq}; compare chapter 7. However, in most cases, we do not have to know all these different things. This probably of importance if new things are developed or if one wants to understand the basics in detail.

The momentum equation can also be defined for solids. In this particular case, we are using the Lamés coefficients. Things would get to complex here and the structure is not correct for the introduction of all the theory. Thus, information about *why we can use this equation for solids too* can be found in Gurtin et al. [2010]. A short overview of some constitutive relations are given in chapter 7 later on.

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 until now. The terms that we are going to investigate are the viscous 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 mathematical operation (1.18):

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

As we can see, the terms are equal for the pressure term. The analysis of the first term that includes the deformation-rate tensor $\mathbf{D}$, needs the mathematical operations (1.15) and (1.18):

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

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

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

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

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

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

At last, we 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),

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

taking the minus sign inside the bracket and 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 same terms of the y-momentum:

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

and the terms of the z-momentum:

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

The underlined terms occur in equations (5.24). That means that the vector form and Cartesian one are similar for these terms, 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 of the vector notation are equal to the Cartesian notation. Thus, both representations are identically.

5.1.2 The Term $-\frac{2}{3}\mu(\nabla\bullet\mathbf{U})$

As mentioned at the beginning of this chapter, the second term $-\frac{2}{3}\mu$ is referred in literature to be the dilatation viscosity. As already said, the choice of this nomenclature is not unique in literature. However, this term represents expansion and compression phenomena. To demonstrate the meaning of the term and the correlation to the 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 (1.19), we get:

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

Now we can sort the terms in order to get to the following formulation:

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

This expression is inserted into the shear-rate tensor $\boldsymbol{\tau}$ of equation (5.13). The outcome is the following: We 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:

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

Note: The above mentioned relation holds if the Stokes hypothesis is valid and therefore $\kappa = 0$.

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 all terms 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 a constant, we further can simplify the equation by taking out the viscosity of the divergence operator:

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

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

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

5.2 Non-Newtonian fluid

Considering non-Newtonian fluids, the shear-rate tensor has to be treated in another way due to the fact that the Newtonian law is not valid anymore. For that we can use, e.g., the equation suggested by Herschel-Bulkley. They defined the shear-rate tensor by using a power law equation:

$$\boldsymbol{\tau} = \boldsymbol{\tau}_0 + k\dot{\gamma}^n \tag{5.39}$$

This equation can be used for modelling Non-Newtonian fluids. Further simplifications are made by Ostwald and de Waele. They assume that $\boldsymbol{\tau}_0 = 0$. Therefore, we get the two parameter equation:

$$\boldsymbol{\tau} = k\dot{\gamma}^n \tag{5.40}$$

k denotes a consistency factor, $\dot{\gamma}$ the shear-rate and n the potential factor.

Using the following parameters $k = 2\mu, \dot{\gamma} = \mathbf{D}$ and $n = 1$ lead to the shear-rate tensor for incompressible Newtonian fluids.

Remark: This section was added in the first edition of the book. However, as I am not familiar with non-Newtonian fluids, I cannot proof or give further information in this particular topic. However, my former colleagues at the Montanuniversität Leoben modeled non-Newtonian fluids with a complete different viscosity model rather than just using a different strain-rate tensors.

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 be related to stresses. The correlation between the total stress, shear-rate stress and pressure is briefly discussed in this chapter.

First we start introducing 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 (1.25) 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 (1.26) or (1.27) can be related to the pressure as:

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

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

Using the definition of the deviatoric part (1.28) and the above expression, we can rewrite equation (6.2):

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

The deviatoric part is related to the shear-rate stresses and can be expressed by the shear-rate tensor $\boldsymbol{\tau}$:

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

At last, it follows:

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

Depending on the fluid of interest, $\boldsymbol{\tau}$ 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

The bulk viscosity

As we already pointed out in chapter 5 there are discrepancies in literature based on the quantity κ. Bird et al. [1960] referred the quantity κ, which is included in the normal components of the shear-rate tensor, as bulk viscosity, that is also named, dilatation, volumetric or volume viscosity. All of these names represent the same. In order to make a clear statement about the bulk viscosity, we have to go deeper into the basics of the mechanics and thermodynamics. All necessary information are given in Gurtin et al. [2010] which are summarized and compressed in the following chapter for compressible fluids that show a linear dependency in the viscosity for the shearing.

First we have to know that a linear tensor function $\mathbf{T}(\mathbf{A})$ is isotropic, if and only if there are two quantities (scalars) μ and λ (do not mix these coefficients with the first and second Lamé

Finally, after summing up, we end up with the following formulation:

$$\boldsymbol{\sigma}(\rho, \mathbf{D}) = \boldsymbol{\sigma}_{\text{vis}}(\rho, \mathbf{D}) - p_{\text{eq}}(\rho)\mathbf{I} \ . \tag{7.5}$$

Equation 7.5 is similar but not equal to 6.7 based on the the equilibrium pressure and the viscous term. Later we see why both equations are equal for some particular cases — in which we are working commonly. Using the already known definition of the total pressure p, which is given by:

$$p(\rho, \mathbf{D}) = -\frac{1}{3}\,\text{tr}(\boldsymbol{\sigma}(\rho, \mathbf{D})) \ , \tag{7.6}$$

we are able to express the total pressure by the equilibrium pressure and the viscous stress tensor:

$$p(\rho, \mathbf{D}) = -\frac{1}{3}\,\text{tr}\left[-p_{\text{eq}}(\rho)\mathbf{I} + \boldsymbol{\sigma}_{\text{vis}}(\rho, \mathbf{D})\right] \ . \tag{7.7}$$

It is trivial that this formulation leads to:

$$p(\rho, \mathbf{D}) = p_{\text{eq}}(\rho) - \frac{1}{3}\,\text{tr}\left[\boldsymbol{\sigma}_{\text{vis}}(\rho, \mathbf{D})\right] \ . \tag{7.8}$$

As the above given equation states, the total pressure for compressible fluids is based on two different contributions, the equilibrium pressure and a part, namely the isotropic part of the viscous part of the Cauchy tensor. The isotropic part can be related to internal friction.

The question that may arise now is: Where is the equilibrium pressure in all equations that we had before and why don't we have such discussions in other literature. To answer this question, we have to use the relation (7.1) for the viscous part $\boldsymbol{\sigma}_{\text{vis}}(\rho, \mathbf{D})$. It follows:

and represents the correct bulk viscosity definition. Comparing this quantity with Bird et al. [1960], we see that there is a difference in the nomenclature. Because, if we take the trace of equation (7.14), it follows (note that the trace of $\mathbf{D}_0$ is zero):

$$\mathrm{tr}\left[\boldsymbol{\sigma}_{\mathrm{vis}}(\rho, \mathbf{D})\right] = 3\kappa(\rho)\,\mathrm{tr}(\mathbf{D}) \ , \tag{7.16}$$

and put this into equation (7.8), we get:

$$p(\rho) = p_{\mathrm{eq}}(\rho) - \kappa(\rho)\,\mathrm{tr}(\mathbf{D}) \ , \tag{7.17}$$

and thus the Cauchy stress tensor can be written as:

$$\boldsymbol{\sigma}(\rho, \mathbf{D}) = 2\mu(\rho)\mathbf{D}_0 - p(\rho)\mathbf{I} \ , \tag{7.18}$$

if we replace the term on the RHS of equation 7.5 with the definitions of 7.14 and 7.17.

Again, this equation looks similar to equation (6.7) but it is in fact not equivalent. In addition the above constitutive equation for the stress tensor $\boldsymbol{\sigma}$ is only valid for compressible fluids which have a linear viscosity behavior. To get the equivalence of both equations we have to go further.

As Bird et al. [1960] already mentioned, the quantity κ is not too important and can be neglected which is also stated by Gurtin et al. [2010]. Based on that, it is common to use the Stokes relation given by the definition $\kappa = 0$. Doing that, we directly see that λ has to be equal to $-\frac{2}{3}\mu$, cf. (7.15). If we insert the outcome into equation (7.9), and express the quantity μ with the molecular viscosity of the fluid, we get the expression for the shear-rate tensor τ; cf. equation

Chapter 8

Collection of Different Notations of the Momentum Equations

In literature 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 mathematical laws to manipulate the equation as we want.

- Common conserved momentum equation (2.26):

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau} - \nabla p + \rho\mathbf{g} \ . \tag{8.1}$$

- Conserved momentum equation including the definition of the shear-rate tensor:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \left(2\mu\mathbf{D} - \frac{2}{3}\mu(\nabla \bullet \mathbf{U})\mathbf{I}\right) - \nabla p + \rho\mathbf{g} \ . \tag{8.2}$$

- Conserved momentum equation as used in chapter 7:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \left(2\mu\mathbf{D}_0 + (\lambda + \frac{2}{3}\mu)(\nabla \bullet \mathbf{U})\mathbf{I}\right) - \nabla p + \rho\mathbf{g} \ . \tag{8.3}$$

- Conserved momentum equation with bulk viscosity:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet (2\mu\mathbf{D}_0 + \kappa(\nabla \bullet \mathbf{U})\mathbf{I}) - \nabla p + \rho\mathbf{g} \ . \tag{8.4}$$

- Conserved momentum equation with trace operator:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \left(2\mu\mathbf{D} - \frac{2}{3}\mu\,\mathrm{tr}(\mathbf{D})\mathbf{I}\right) - \nabla p + \rho\mathbf{g} \ . \tag{8.5}$$

- General conserved momentum equation with Cauchy stress tensor:

$$\frac{\partial}{\partial t}\rho\mathbf{U} = -\nabla \bullet (\rho\mathbf{U} \otimes \mathbf{U}) + \nabla \bullet \boldsymbol{\sigma} + \rho\mathbf{g} \ . \tag{8.6}$$

- Non-conserved momentum equation with Cauchy stress tensor:

$$\rho\frac{\mathrm{D}\mathbf{U}}{\mathrm{D}t} = \nabla \bullet \boldsymbol{\sigma} + \rho\mathbf{g} \ . \tag{8.7}$$

- Integral form of momentum equation:

$$\frac{\partial}{\partial t}\int \rho\mathbf{U}\mathrm{d}V = -\oint (\rho\mathbf{U} \otimes \mathbf{U}) \cdot \mathbf{n}\mathrm{d}S - \oint \boldsymbol{\tau} \cdot \mathbf{n}\mathrm{d}S - \oint p\mathbf{I} \cdot \mathbf{n}\mathrm{d}S + \int \rho\mathbf{g}\mathrm{d}V \ . \tag{8.8}$$

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:

$$\nabla \bullet \mathbf{U} = \mathrm{tr}(\mathbf{D}) \ . \tag{8.9}$$

The demonstration is very simple:

$$\begin{aligned} \mathrm{tr}(\mathbf{D}) = \mathrm{tr}\left(\frac{1}{2}\left[\nabla \otimes \mathbf{U} + (\nabla \otimes \mathbf{U})^T\right]\right) & \\ = \frac{1}{2}\left[2\frac{\partial u_x}{\partial x} + 2\frac{\partial u_y}{\partial y} + 2\frac{\partial u_z}{\partial z}\right] &= \nabla \bullet \mathbf{U} \ . \end{aligned} \tag{8.10}$$

The divergence operator is evaluated by equation (1.17).

Chapter 9

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 different averaging methods. Then we are going to derive the incompressible mass and momentum equation illustrating the closure problem. After that, we discuss some hypotheses that are used to get rid of the closure problem. That leads to the derivative of the Reynolds stress equation. The outcome of this equation can be used to analyze the analogies between 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 primary literature that is used in this chapter is Ferziger and Perić [2008], Bird et al. [1960], Wilcox [1994].

9.1 Reynolds-Averaging

The investigation into flow fields is generally turbulent. 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 9.1, we can analyze that the flow has a deterministic character. That means the flow pattern is chaotic. It 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 9.1, ϕ would be the velocity u (in one direction) and could be expressed as:

$$\phi(t, x) = \bar{\phi}(x) + \phi'(t, x) \ . \tag{9.1}$$

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 9.1). 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:

$$\bar{\phi}(x)_\mathrm{T} = \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} \phi(t, x) \mathrm{d}t \ . \tag{9.2}$$

To get accurate 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 leads 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:

$$\bar{\phi}(x)_{\mathrm{V}} = \lim_{\mathrm{V}\to\infty} \frac{1}{V} \int\int\int \phi(t,x)\mathrm{d}V \ . \tag{9.3}$$

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 $\bar{\phi}(t,x)_{\mathrm{E}}$:

$$\bar{\phi}(t,x)_{\mathrm{E}} = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \phi_n(t,x) \ . \tag{9.4}$$

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.

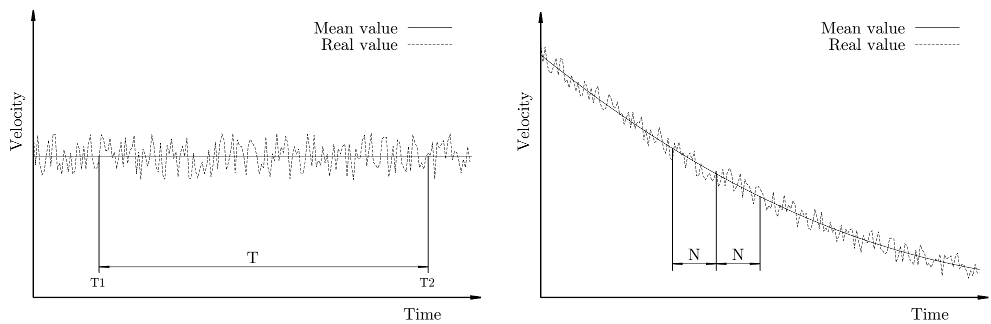


Figure 9.1: Averaging of a statistic stationary (left) and statistic non-stationary flow (right).

The averaging method that we choose for further investigation is the *time averaging* method. The reason for that is based on the fact that things can be described smoothly and precisely. Let us focus on the left part of figure 9.1 first. By replacing the instantaneous variable in equation (9.2) by the definition (9.1), we get:

$$\bar{\phi}(x) = \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \left[\bar{\phi}(x) + \phi'(t,x)\right] \mathrm{d}t \ . \tag{9.5}$$

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:

$$\bar{\phi}(x) = \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \bar{\phi}(x)\mathrm{d}t \ . \tag{9.6}$$

In addition we can see that the time averaging of the fluctuation is zero. To demonstrate that, we use equation (9.1) and replace the mean quantity on the RHS of equation by (9.6):

$$\begin{aligned}
\lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \phi'(t,x)\mathrm{d}t &= \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \left[\phi(t,x) - \bar{\phi}(x)\right] \mathrm{d}t \\
&= \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \phi(t,x)\mathrm{d}t - \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \bar{\phi}(x)\mathrm{d}t \\
&= \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \left[\bar{\phi}(x) + \phi'(t,x)\right] \mathrm{d}t - \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \bar{\phi}(x)\mathrm{d}t \\
&= \bar{\phi}(x) - \bar{\phi}(x) = 0 \ .
\end{aligned} \tag{9.7}$$

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 9.1; right), we have to modify equation (9.1) and (9.2) to:

$$\phi(t,x) = \bar{\phi}(t,x) + \phi'(t,x) \ , \tag{9.8}$$

$$\bar{\phi}(t,x) = \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} \phi(t,x)\mathrm{d}t \ . \tag{9.9}$$

Some remarks and limits to equation (9.9) 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 (9.9) to linear terms lead to linear averaged terms. To demonstrate this, we will use two linear functions $f(t,x)$ and $g(t,x)$:

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

$$= \underbrace{\overline{\bar{f}(t,x)}}_{\bar{f}(t,x)} + \underbrace{\overline{f'(t,x)}}_{=0} = \bar{f}(t,x)$$

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

$$= \underbrace{\overline{\bar{g}(t,x)}}_{\bar{\bar{g}}(t,x)} + \underbrace{\overline{g'(t,x)}}_{=0} = \bar{g}(t,x)$$

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:

$$\begin{aligned}
\overline{f(t,x) + g(t,x)} &= \frac{1}{T}\int_t^{t+T} [f(t,x) + g(t,x)]\,\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T} f(t,x)\mathrm{d}t + \frac{1}{T}\int_t^{t+T} g(t,x)\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T} \left[\bar{f}(t,x) + f'(t,x)\right]\mathrm{d}t + \frac{1}{T}\int_t^{t+T} \left[\bar{g}(t,x) + g'(t,x)\right]\mathrm{d}t \\
&= \overline{\bar{f}(t,x)} + \cancel{\overline{f'(t,x)}} + \overline{\bar{g}(t,x)} + \cancel{\overline{g'(t,x)}} \\
&= \bar{f}(t,x) + \bar{g}(t,x)\ .
\end{aligned} \tag{9.10}$$

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:

$$\begin{aligned}
\overline{f(t,x)g(t,x)} &= \frac{1}{T}\int_t^{t+T} [f(t,x)g(t,x)]\,\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T} \left[\left\{\bar{f}(t,x) + f'(t,x)\right\}\left\{\bar{g}(t,x) + g'(t,x)\right\}\right]\mathrm{d}t \\
&= \frac{1}{T}\int_t^{t+T} \left[\bar{f}(t,x)\bar{g}(t,x) + \bar{f}(t,x)g'(t,x)\right. \\
&\qquad\qquad\qquad \left. + f'(t,x)\bar{g}(t,x) + f'(t,x)g'(t,x)\right]\mathrm{d}t \\
&= \overline{\bar{f}(t,x)\bar{g}(t,x)} + \cancel{\overline{\bar{f}(t,x)g'(t,x)}} \\
&\qquad\qquad + \cancel{\overline{f'(t,x)\bar{g}(t,x)}} + \overline{f'(t,x)g'(t,x)}\ .
\end{aligned} \tag{9.11}$$

Rewriting the whole equation, we get:

$$\overline{f(t,x)g(t,x)} = \bar{f}(t,x)\bar{g}(t,x) + \underbrace{\overline{f'(t,x)g'(t,x)}}_{\text{additional terms}} \tag{9.12}$$

The reason why the second and third term cancels out is related to the fact that the fluctuation is linear in these terms, and hence, equation (9.7) 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:

$$\begin{aligned}
\overline{af(t,x)} &= \frac{1}{T}\int_t^{t+T} af(t,x)\mathrm{d}t \\
&= a\frac{1}{T}\int_t^{t+T} \left[\bar{f}(t,x) + f'(t,x)\right]\mathrm{d}t \\
&= a\overline{\bar{f}(t,x)} + a\cancel{\overline{f'(t,x)}} \\
&= a\bar{f}(t,x) \ .
\end{aligned} \tag{9.13}$$

9.2 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 leads 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 the 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.

9.2.1 Incompressible Mass Conservation Equation

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

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_x)}{\partial x} + \frac{\partial(\rho u_y)}{\partial y} + \frac{\partial(\rho u_z)}{\partial z} = 0 \ . \tag{9.14}$$

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

$$\rho\frac{\partial u_x}{\partial x} + \rho\frac{\partial u_y}{\partial y} + \rho\frac{\partial u_z}{\partial z} = 0 \ . \tag{9.15}$$

Replacing the values u_i by the assumption (9.1),

$$\rho\frac{\partial(\bar{u}_x + u'_x)}{\partial x} + \rho\frac{\partial(\bar{u}_y + u'_y)}{\partial y} + \rho\frac{\partial(\bar{u}_z + u'_z)}{\partial z} = 0 \ , \tag{9.16}$$

and apply the Reynolds time-average concept,

$$\rho\overline{\frac{\partial(\bar{u}_x + u'_x)}{\partial x}} + \rho\overline{\frac{\partial(\bar{u}_y + u'_y)}{\partial y}} + \rho\overline{\frac{\partial(\bar{u}_z + u'_z)}{\partial z}} = 0 \ , \tag{9.17}$$

we get the time-averaged incompressible mass conservation equation:

$$\boxed{\rho\frac{\partial \bar{u}_x}{\partial x} + \rho\frac{\partial \bar{u}_y}{\partial y} + \rho\frac{\partial \bar{u}_z}{\partial z} = \rho\nabla \bullet \bar{\mathbf{U}} = 0} \ . \tag{9.18}$$

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

9.2.2 Compressible Mass Conservation Equation

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

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_x)}{\partial x} + \frac{\partial(\rho u_y)}{\partial y} + \frac{\partial(\rho u_z)}{\partial z} = 0 \ , \tag{9.19}$$

$$\frac{\partial(\bar{\rho}+\rho')}{\partial t} + \frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_x+u'_x)\right]}{\partial x} + \frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_y+u'_y)\right]}{\partial y} + \frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_z+u'_z)\right]}{\partial z} = 0 \ , \tag{9.20}$$

$$\overline{\frac{\partial(\bar{\rho}+\rho')}{\partial t}} + \overline{\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_x+u'_x)\right]}{\partial x}} + \overline{\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_y+u'_y)\right]}{\partial y}} + \overline{\frac{\partial\left[(\bar{\rho}+\rho')(\bar{u}_z+u'_z)\right]}{\partial z}} = 0 \ , \tag{9.21}$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\overline{\bar{\rho}\bar{u}_x} + \cancel{\overline{\bar{\rho}u'_x}} + \cancel{\overline{\rho'\bar{u}_x}} + \overline{\rho' u'_x})}{\partial x} + \frac{\partial(\overline{\bar{\rho}\bar{u}_y} + \cancel{\overline{\bar{\rho}u'_y}} + \cancel{\overline{\rho'\bar{u}_y}} + \overline{\rho' u'_y})}{\partial y} + \frac{\partial(\overline{\bar{\rho}\bar{u}_z} + \cancel{\overline{\bar{\rho}u'_z}} + \cancel{\overline{\rho'\bar{u}_z}} + \overline{\rho' u'_z})}{\partial z} = 0 \ , \tag{9.22}$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\bar{u}_x + \overline{\rho' u'_x})}{\partial x} + \frac{\partial(\bar{\rho}\bar{u}_y + \overline{\rho' u'_y})}{\partial y} + \frac{\partial(\bar{\rho}\bar{u}_z + \overline{\rho' u'_z})}{\partial z} = 0 \ , \tag{9.23}$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i + \overline{\rho' u'_i}) = 0 \ . \tag{9.24}$$

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

$$\mathbf{U}' = \begin{pmatrix} u'_x \\ u'_y \\ u'_z \end{pmatrix} \ , \tag{9.25}$$

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

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \bullet \left(\bar{\rho}\bar{\mathbf{U}} + \overline{\rho'\mathbf{U}'}\right) = 0 \ . \tag{9.26}$$

Since 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 incompressible flow fields first.

Averaging the compressible equations will be discussed in section 9.13.

9.2.3 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 the incompressibility of the fluid. For the y and z components, the equations (5.8) and (5.9) have to be used. Because 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:

$$\begin{aligned}\rho\frac{\partial}{\partial t}u_x = &-\left(\rho\frac{\partial}{\partial x}u_x u_x + \rho\frac{\partial}{\partial y}u_y u_x + \rho\frac{\partial}{\partial z}u_z u_x\right)\\ &-\left\{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial u_x}{\partial x}\right] + \frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial u_z}{\partial x}+\frac{\partial u_x}{\partial z}\right)\right]\right\} - \frac{\partial p}{\partial x} + \rho g_x \ .\end{aligned} \tag{9.27}$$

This is the start point for the procedure. The first step is to replace the velocity quantities by equation (9.1) and apply the Reynolds time-averaging concept. For clearance, we will examine each term separately. Starting with the term on the LHS, we get:

$$\overline{\rho\frac{\partial}{\partial t}(\bar{u}_x + u'_x)} = \rho\frac{\partial}{\partial t}\bar{u}_x \ . \tag{9.28}$$

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:

$$\begin{aligned}\overline{\rho\frac{\partial}{\partial x}(\bar{u}_x+u'_x)(\bar{u}_x+u'_x)} &= \rho\frac{\partial}{\partial x}\left[\overline{\bar{u}_x\bar{u}_x} + \cancel{\overline{\bar{u}_x u'_x}} + \cancel{\overline{u'_x\bar{u}_x}} + \overline{u'_x u'_x}\right]\\ &= \rho\frac{\partial}{\partial x}(\bar{u}_x\bar{u}_x) + \rho\frac{\partial}{\partial x}(\overline{u'_x u'_x}) \ ,\end{aligned} \tag{9.29}$$

$$\begin{aligned}\overline{\rho\frac{\partial}{\partial y}(\bar{u}_y+u'_y)(\bar{u}_x+u'_x)} &= \rho\frac{\partial}{\partial y}\left[\overline{\bar{u}_y\bar{u}_x} + \cancel{\overline{\bar{u}_y u'_x}} + \cancel{\overline{u'_y\bar{u}_x}} + \overline{u'_y u'_x}\right]\\ &= \rho\frac{\partial}{\partial y}\rho(\bar{u}_y\bar{u}_x) + \rho\frac{\partial}{\partial y}(\overline{u'_y u'_x}) \ ,\end{aligned} \tag{9.30}$$

$$\begin{aligned}\overline{\rho\frac{\partial}{\partial z}(\bar{u}_z+u'_z)(\bar{u}_x+u'_x)} &= \rho\frac{\partial}{\partial z}\left[\overline{\bar{u}_z\bar{u}_x} + \cancel{\overline{\bar{u}_z u'_x}} + \cancel{\overline{u'_z\bar{u}_x}} + \overline{u'_z u'_x}\right]\\ &= \rho\frac{\partial}{\partial z}\rho(\bar{u}_z\bar{u}_x) + \rho\frac{\partial}{\partial z}(\overline{u'_z u'_x}) \ .\end{aligned} \tag{9.31}$$

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 (9.27) 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:

$$\overline{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial(\bar{u}_x+u'_x)}{\partial x}\right]}=\frac{\partial}{\partial x}\left[-2\mu\frac{\partial\bar{u}_x}{\partial x}\right] \ , \tag{9.32}$$

for the second one this expression:

$$\overline{\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial(\bar{u}_x+u'_x)}{\partial y}+\frac{\partial(\bar{u}_y+u'_y)}{\partial x}\right)\right]}=\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial\bar{u}_x}{\partial y}+\frac{\partial\bar{u}_y}{\partial x}\right)\right] \ , \tag{9.33}$$

and for the third term this one:

$$\overline{\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial(\bar{u}_z+u'_z)}{\partial x}+\frac{\partial(\bar{u}_x+u'_x)}{\partial z}\right)\right]}=\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial\bar{u}_z}{\partial x}+\frac{\partial\bar{u}_x}{\partial z}\right)\right] \ . \tag{9.34}$$

Finally, after combining all three parts, we get the following expression for the second term on the RHS of equation (9.27):

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

After we analyzed the first two terms, we will investigate into the last two terms on the RHS of equation (9.27). It follows:

$$-\overline{\frac{\partial p}{\partial x}}+\overline{\rho g_x}=-\overline{\frac{\partial(\bar{p}+p')}{\partial x}}+\rho g_x=-\frac{\partial\bar{p}}{\partial x}+\rho g_x \ . \tag{9.35}$$

Now we can rewrite the x-component of the momentum equation (9.27) as Reynolds time-averaged

x-momentum equation:

$$\boxed{\begin{aligned}\rho\frac{\partial}{\partial t}\bar{u}_x = &-\left(\rho\frac{\partial}{\partial x}\bar{u}_x\bar{u}_x + \rho\frac{\partial}{\partial y}\bar{u}_y\bar{u}_x + \rho\frac{\partial}{\partial z}\bar{u}_z\bar{u}_x\right)\\ &-\left(\rho\frac{\partial}{\partial x}(\overline{u'_x u'_x}) + \rho\frac{\partial}{\partial y}(\overline{u'_y u'_x}) + \rho\frac{\partial}{\partial z}(\overline{u'_z u'_x})\right)\\ &-\left\{\frac{\partial}{\partial x}\left[-2\mu\frac{\partial\bar{u}_x}{\partial x}\right] + \frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial\bar{u}_x}{\partial y} + \frac{\partial\bar{u}_y}{\partial x}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial\bar{u}_z}{\partial x} + \frac{\partial\bar{u}_x}{\partial z}\right)\right]\right\}\\ &-\frac{\partial\bar{p}}{\partial x} + \rho g_x\end{aligned}}\,. \tag{9.36}$$

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

$$\boxed{\begin{aligned}\rho\frac{\partial}{\partial t}\bar{u}_y = &-\left(\rho\frac{\partial}{\partial x}\bar{u}_x\bar{u}_y + \rho\frac{\partial}{\partial y}\bar{u}_y\bar{u}_y + \rho\frac{\partial}{\partial z}\bar{u}_z\bar{u}_y\right)\\ &-\left(\rho\frac{\partial}{\partial x}(\overline{u'_x u'_y}) + \rho\frac{\partial}{\partial y}(\overline{u'_y u'_y}) + \rho\frac{\partial}{\partial z}(\overline{u'_z u'_y})\right)\\ &-\left\{\frac{\partial}{\partial y}\left[-2\mu\frac{\partial\bar{u}_y}{\partial y}\right] + \frac{\partial}{\partial x}\left[-\mu\left(\frac{\partial\bar{u}_x}{\partial y} + \frac{\partial\bar{u}_y}{\partial x}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial z}\left[-\mu\left(\frac{\partial\bar{u}_z}{\partial y} + \frac{\partial\bar{u}_y}{\partial z}\right)\right]\right\} - \frac{\partial\bar{p}}{\partial y} + \rho g_y\end{aligned}}\,. \tag{9.37}$$

z-Component of Momentum

$$\boxed{\begin{aligned}\rho\frac{\partial}{\partial t}\bar{u}_z = &-\left(\rho\frac{\partial}{\partial x}\bar{u}_x\bar{u}_z + \rho\frac{\partial}{\partial y}\bar{u}_y\bar{u}_z + \rho\frac{\partial}{\partial z}\bar{u}_z\bar{u}_z\right)\\ &-\left(\rho\frac{\partial}{\partial x}(\overline{u'_x u'_z}) + \rho\frac{\partial}{\partial y}(\overline{u'_y u'_z}) + \rho\frac{\partial}{\partial z}(\overline{u'_z u'_z})\right)\\ &-\left\{\frac{\partial}{\partial z}\left[-2\mu\frac{\partial\bar{u}_z}{\partial z}\right] + \frac{\partial}{\partial x}\left[-\mu\left(\frac{\partial\bar{u}_x}{\partial z} + \frac{\partial\bar{u}_z}{\partial x}\right)\right]\right.\\ &\left.+\frac{\partial}{\partial y}\left[-\mu\left(\frac{\partial\bar{u}_y}{\partial z} + \frac{\partial\bar{u}_z}{\partial y}\right)\right]\right\} - \frac{\partial\bar{p}}{\partial z} + \rho g_z\end{aligned}} \tag{9.38}$$

If we are using the vector of fluctuations $\mathbf{U}'$ (9.25), 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:

$$\boxed{\underbrace{\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla\bullet(\bar{\mathbf{U}}\otimes\bar{\mathbf{U}}) = \nabla\bullet\underbrace{(2\mu\bar{\mathbf{D}})}_{\bar{\boldsymbol{\tau}}} - \nabla\bar{p} + \rho\mathbf{g}}_{\text{Same as equation (5.13) (with }\rho=\text{const.)}}\ \underbrace{-\rho\nabla\bullet(\overline{\mathbf{U}'\otimes\mathbf{U}'})}_{\text{Reynolds}-\text{Stresses }\bar{\boldsymbol{\sigma}}_t}}\,. \tag{9.39}$$

$\bar{\mathbf{D}}$ 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:

$$\bar{\boldsymbol{\sigma}}_{\mathrm{t}} = -\rho\overline{u_i' u_j'} = \begin{bmatrix} -\rho\overline{u_x' u_x'} & -\rho\overline{u_y' u_x'} & -\rho\overline{u_z' u_x'} \\ -\rho\overline{u_x' u_y'} & -\rho\overline{u_y' u_y'} & -\rho\overline{u_z' u_y'} \\ -\rho\overline{u_x' u_z'} & -\rho\overline{u_y' u_z'} & -\rho\overline{u_z' u_z'} \end{bmatrix} = \begin{bmatrix} \bar{\sigma}_{\mathrm{t}xx} & \bar{\sigma}_{\mathrm{t}yx} & \bar{\sigma}_{\mathrm{t}zx} \\ \bar{\sigma}_{\mathrm{t}xy} & \bar{\sigma}_{\mathrm{t}yy} & \bar{\sigma}_{\mathrm{t}zy} \\ \bar{\sigma}_{\mathrm{t}xz} & \bar{\sigma}_{\mathrm{t}yz} & \bar{\sigma}_{\mathrm{t}zz} \end{bmatrix}. \tag{9.40}$$

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

$$\boxed{\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla \bullet (\bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \bar{\boldsymbol{\tau}} - \nabla\bar{p} + \rho\mathbf{g} + \nabla \bullet \bar{\boldsymbol{\sigma}}_{\mathrm{t}}}\,. \tag{9.41}$$

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:

$$\boxed{\rho\frac{\partial}{\partial t}\bar{\mathbf{U}} + \rho\nabla \bullet (\bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \bar{\boldsymbol{\sigma}} + \rho\mathbf{g} + \nabla \bullet \bar{\boldsymbol{\sigma}}_{\mathrm{t}}}\,. \tag{9.42}$$

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 transform 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:

$$-\rho\nabla \bullet (\overline{\mathbf{U}' \otimes \mathbf{U}'}) = -\rho \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \left[\overline{\begin{pmatrix} u_x' \\ u_y' \\ u_z' \end{pmatrix} \otimes \begin{pmatrix} u_x' \\ u_y' \\ u_z' \end{pmatrix}} \right] \tag{9.43}$$

$$= -\rho \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \bullet \left[\begin{pmatrix} \overline{u_x' u_x'} & \overline{u_x' u_y'} & \overline{u_x' u_z'} \\ \overline{u_y' u_x'} & \overline{u_y' u_y'} & \overline{u_y' u_z'} \\ \overline{u_z' u_x'} & \overline{u_z' u_y'} & \overline{u_z' u_z'} \end{pmatrix} \right] \tag{9.44}$$

$$= \begin{pmatrix} -\left[\rho\frac{\partial}{\partial x}\left(\overline{u_x' u_x'}\right) + \rho\frac{\partial}{\partial y}\left(\overline{u_x' u_y'}\right) + \rho\frac{\partial}{\partial z}\left(\overline{u_x' u_z'}\right)\right] \\ -\left[\rho\frac{\partial}{\partial x}\left(\overline{u_y' u_x'}\right) + \rho\frac{\partial}{\partial x}\left(\overline{u_y' u_y'}\right) + \rho\frac{\partial}{\partial x}\left(\overline{u_y' u_z'}\right)\right] \\ -\left[\rho\frac{\partial}{\partial y}\left(\overline{u_z' u_x'}\right) + \rho\frac{\partial}{\partial x}\left(\overline{u_z' u_y'}\right) + \rho\frac{\partial}{\partial z}\left(\overline{u_z' u_z'}\right)\right] \end{pmatrix} \stackrel{!}{=} \begin{cases} \text{of } x - \text{mom.} \\ \text{of } y - \text{mom.} \\ \text{of } z - \text{mom.} \end{cases} \tag{9.45}$$

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

$$\boxed{\rho\frac{\partial}{\partial t}\bar{u}_i + \rho\frac{\partial}{\partial x_j}\left(\bar{u}_i\bar{u}_j\right) = \frac{\partial\bar{\tau}_{ij}}{\partial x_j} - \frac{\partial\bar{p}}{\partial x_i} + \rho g_i - \rho\frac{\partial}{\partial x_j}\left(\overline{u_i' u_j'}\right)}\,. \tag{9.46}$$

Furthermore, sometimes the Reynolds-Stress term is put into the convective term on the LHS.

Hence, we get:

$$\boxed{\rho\frac{\partial}{\partial t}\bar{u}_i + \rho\frac{\partial}{\partial x_j}\left(\bar{u}_i\bar{u}_j + \overline{u_i'u_j'}\right) = \frac{\partial\bar{\tau}_{ij}}{\partial x_j} - \frac{\partial\bar{p}}{\partial x_i} + \rho g_i} \,. \tag{9.47}$$

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

Note: It should be evident 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:

$$\boxed{\frac{\partial}{\partial t}\rho\bar{u}_i + \frac{\partial}{\partial x_j}\left(\rho\bar{u}_i\bar{u}_j + \rho\overline{u_i'u_j'}\right) = \frac{\partial\bar{\tau}_{ij}}{\partial x_j} - \frac{\partial\bar{p}}{\partial x_i} + \rho g_i} \,. \tag{9.48}$$

Additionally, it should be obvious, that we are allowed to divide the equations by the density ρ. For that, we 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.

9.2.4 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:

$$\underbrace{\rho\frac{\partial}{\partial t}\phi}_{\text{time accumulation}} = \underbrace{-\rho\quad\nabla\bullet(\mathbf{U}\phi)}_{\text{convective transport}} + \underbrace{\nabla\bullet(D\nabla\phi)}_{\text{diffusive transport}} \,. \tag{9.49}$$

To show the transformation to the Reynolds time-averaged equation, we will transform this equation into the Cartesian form first by using the mathematics (1.17) 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):

$$\begin{aligned}\rho\frac{\partial}{\partial t}\phi = -\left(\rho\frac{\partial}{\partial x}(u_x\phi) + \rho\frac{\partial}{\partial y}(u_y\phi) + \rho\frac{\partial}{\partial z}(u_z\phi)\right)&\\ + \frac{\partial}{\partial x}\left(D_x\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial\phi}{\partial z}\right)&\,.\end{aligned} \tag{9.50}$$

The next step is to use the expression from equation (9.1) 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:

$$\begin{aligned}\rho\frac{\partial}{\partial t}(\bar{\phi}+\phi') = &-\left(\rho\frac{\partial}{\partial x}\left[(\bar{u}_x+u'_x)(\bar{\phi}+\phi')\right]+\rho\frac{\partial}{\partial y}\left[(\bar{u}_y+u'_y)(\bar{\phi}+\phi')\right]\right.\\ &\left.+\rho\frac{\partial}{\partial z}\left[(\bar{u}_z+u'_z)(\bar{\phi}+\phi')\right]\right)+\frac{\partial}{\partial x}\left(D_x\frac{\partial}{\partial x}(\bar{\phi}+\phi')\right)\\ &+\frac{\partial}{\partial y}\left(D_y\frac{\partial}{\partial y}(\bar{\phi}+\phi')\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial}{\partial z}(\bar{\phi}+\phi')\right)\ . \end{aligned} \tag{9.51}$$

To discuss the Reynolds-Averaging procedure, we will analyze each term separately of equation (9.51). Therefore, the time term results in:

$$\overline{\rho\frac{\partial}{\partial t}(\bar{\phi}+\phi')} = \rho\frac{\partial}{\partial t}\bar{\phi}\ . \tag{9.52}$$

The first term on the RHS,

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

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

$$\begin{aligned}\overline{\rho\frac{\partial}{\partial x}\left[(\bar{u}_x+u'_x)(\bar{\phi}+\phi')\right]} &= \rho\frac{\partial}{\partial x}\left[(\overline{\bar{u}_x\bar{\phi}}+\overline{\bar{u}_x\phi'}+\overline{u'_x\bar{\phi}}+\overline{u'_x\phi'})\right]\\ &= \rho\frac{\partial}{\partial x}(\bar{u}_x\bar{\phi})+\frac{\partial}{\partial x}(\rho\overline{u'_x\phi'})\ ,\end{aligned} \tag{9.53}$$

$$\begin{aligned}\overline{\rho\frac{\partial}{\partial y}\left[(\bar{u}_y+u'_y)(\bar{\phi}+\phi')\right]} &= \rho\frac{\partial}{\partial y}\left[(\overline{\bar{u}_y\bar{\phi}}+\overline{\bar{u}_y\phi'}+\overline{u'_y\bar{\phi}}+\overline{u'_y\phi'})\right]\\ &= \rho\frac{\partial}{\partial y}(\bar{u}_y\bar{\phi})+\rho\frac{\partial}{\partial y}(\overline{u'_y\phi'})\ ,\end{aligned} \tag{9.54}$$

$$\begin{aligned}\overline{\rho\frac{\partial}{\partial z}\left[(\bar{u}_z+u'_z)(\bar{\phi}+\phi')\right]} &= \rho\frac{\partial}{\partial z}\left[(\overline{\bar{u}_z\bar{\phi}}+\overline{\bar{u}_z\phi'}+\overline{u'_z\bar{\phi}}+\overline{u'_z\phi'})\right]\\ &= \rho\frac{\partial}{\partial z}(\bar{u}_z\bar{\phi})+\rho\frac{\partial}{\partial z}(\overline{u'_z\phi'})\ .\end{aligned} \tag{9.55}$$

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:

$$\overline{\frac{\partial}{\partial x}\left(D_x\frac{\partial}{\partial x}(\bar{\phi}+\phi')\right)} = \frac{\partial}{\partial x}\left(D_x\frac{\partial\bar{\phi}}{\partial x}\right)\ , \tag{9.56}$$

$$\overline{\frac{\partial}{\partial y}\left(D_y \frac{\partial}{\partial y}(\bar{\phi}+\phi')\right)} = \frac{\partial}{\partial y}\left(D_y \frac{\partial \bar{\phi}}{\partial y}\right) \,, \tag{9.57}$$

$$\overline{\frac{\partial}{\partial z}\left(D_z \frac{\partial}{\partial z}(\bar{\phi}+\phi')\right)} = \frac{\partial}{\partial z}\left(D_z \frac{\partial \bar{\phi}}{\partial z}\right) \,. \tag{9.58}$$

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

$$\boxed{\begin{aligned} \rho\frac{\partial}{\partial t}\bar{\phi} = &-\left(\rho\frac{\partial}{\partial x}(\rho\bar{u}_x\bar{\phi}) + \rho\frac{\partial}{\partial y}(\bar{u}_y\bar{\phi}) + \rho\frac{\partial}{\partial z}(\bar{u}_z\bar{\phi})\right) \\ &+ \frac{\partial}{\partial x}\left(D_x\frac{\partial\bar{\phi}}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial\bar{\phi}}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial\bar{\phi}}{\partial z}\right) \\ &- \underbrace{\left(\rho\frac{\partial}{\partial x}(\overline{u_x'\phi'}) + \rho\frac{\partial}{\partial y}(\overline{u_y'\phi'}) + \rho\frac{\partial}{\partial z}(\overline{u_z'\phi'})\right)}_{\text{turbulent scalar flux}} \end{aligned}} \,, \tag{9.59}$$

and is given in vector form by:

$$\boxed{\underbrace{\rho\frac{\partial}{\partial t}\bar{\phi} = -\rho\nabla\bullet\left(\bar{\mathbf{U}}\bar{\phi}\right) + \nabla\bullet\left(D\nabla\bar{\phi}\right)}_{\text{same as before}} - \underbrace{\rho\nabla\bullet\left(\overline{\mathbf{U}'\phi'}\right)}_{\text{turbulent scalar flux}}} \,. \tag{9.60}$$

Equation (9.60) 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:

$$\boxed{\underbrace{\frac{\partial}{\partial t}\rho\bar{\phi} = -\nabla\bullet\left(\rho\bar{\mathbf{U}}\bar{\phi}\right) + \nabla\bullet\left(D\nabla\bar{\phi}\right)}_{\text{same as before}} - \underbrace{\nabla\bullet\left(\rho\overline{\mathbf{U}'\phi'}\right)}_{\text{turbulent scalar flux}}} \,. \tag{9.61}$$

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:

$$\boxed{\frac{\partial}{\partial t}\rho\bar{\phi} + \nabla\bullet\left(\rho\bar{\mathbf{U}}\bar{\phi} + \rho\overline{\mathbf{U}'\phi'}\right) = \nabla\bullet\left(D\nabla\bar{\phi}\right) + S_\phi} \,. \tag{9.62}$$

9.3 The Closure Problem

The Reynolds-Averaged procedure leads 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 cannot be calculated. Hence, the set of equations is 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 these assumptions, we try to correlate the unknown quantities with known ones.

For the **Reynolds-Stresses** and **turbulent scalar fluxes**, we can use several theories that try approximately 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 (a 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.

9.4 Boussinesq Eddy Viscosity

The most used hypothesis is the theory postulated by Joseph Boussinesq that relates the turbulence of a flow to higher fluid viscosity. The thought behind is as follows: If we have a higher turbulence flow, the flow gets more chaotic, and we get many vortexes that can transport, for example, heat in addition to the already existing transport phenomena. Therefore, it is clear and evident 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 gives 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, higher mixing rates $\longrightarrow$ additional transport). However, this means that a higher disspation of the kinetic energy into heat occurs. 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:

$$\underbrace{-\rho\overline{u_i'u_j'}}_{\bar{\boldsymbol{\sigma}}_{\mathrm{t}}} = \mu_t \underbrace{\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3}\left(\nabla \bullet \bar{\mathbf{U}}\right)\delta_{ij}\right)}_{2\bar{\mathbf{D}} - \frac{2}{3}\,\mathrm{tr}(\bar{\mathbf{D}})\mathbf{I}} - \underbrace{\frac{2}{3}\rho\delta_{ij}k}_{\frac{2}{3}\rho\mathbf{I}k}\,, \tag{9.63}$$

$$\bar{\boldsymbol{\sigma}}_{\mathrm{t}} = \underline{2\mu_{\mathrm{t}}\bar{\mathbf{D}} - \frac{2}{3}\mu_{\mathrm{t}}\,\mathrm{tr}(\bar{\mathbf{D}})\mathbf{I}} - \frac{2}{3}\rho\mathbf{I}k\,, \tag{9.64}$$

$$\bar{\boldsymbol{\sigma}}_{\mathrm{t}} = \bar{\boldsymbol{\tau}}_{\mathrm{t}} - \frac{2}{3}\rho\mathbf{I}k\,. \tag{9.65}$$

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 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:

$$k = \frac{1}{2}\overline{u_i'u_i'} = \frac{1}{2}\left(\overline{u_x'u_x'} + \overline{u_y'u_y'} + \overline{u_z'u_z'}\right) \ . \tag{9.66}$$

New we need to take the trace of the Reynolds-Stress tensor $\bar{\boldsymbol{\sigma}}_\mathrm{t}$ (9.40). It follows:

$$\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t}) = \mathrm{tr}(-\rho\overline{u_i'u_j'}) = \mathrm{tr}\left(\begin{bmatrix} -\rho\overline{u_x'u_x'} & -\rho\overline{u_y'u_x'} & -\rho\overline{u_z'u_x'} \\ -\rho\overline{u_x'u_y'} & -\rho\overline{u_y'u_y'} & -\rho\overline{u_z'u_y'} \\ -\rho\overline{u_x'u_z'} & -\rho\overline{u_y'u_z'} & -\rho\overline{u_z'u_z'} \end{bmatrix}\right) \ , \tag{9.67}$$

$$= \underbrace{(-\rho\overline{u_x'u_x'}) + (-\rho\overline{u_y'u_y'}) + (-\rho\overline{u_z'u_z'})}_{=\,-2\rho k} \ . \tag{9.68}$$

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 (9.66):

$$-2\rho k = -2\rho\left[\frac{1}{2}\left(\overline{u_x'u_x'} + \overline{u_y'u_y'} + \overline{u_z'u_z'}\right)\right] = \underbrace{(-\rho\overline{u_x'u_x'}) + (-\rho\overline{u_y'u_y'}) + (-\rho\overline{u_z'u_z'})}_{\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t})} \ . \tag{9.69}$$

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 (9.65) 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:

$$\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t}) = \mathrm{tr}\left(\bar{\boldsymbol{\tau}}_\mathrm{t} - \frac{2}{3}\rho\mathbf{I}k\right) = -2\rho k \ , \tag{9.70}$$

$$\mathrm{tr}(\bar{\boldsymbol{\sigma}}_\mathrm{t}) = \mathrm{tr}\left(2\mu_\mathrm{t}\bar{\mathbf{D}} - \frac{2}{3}\mu_\mathrm{t}\,\mathrm{tr}(\bar{\mathbf{D}})\mathbf{I} - \frac{2}{3}\rho\mathbf{I}k\right) = -2\rho k \ . \tag{9.71}$$

If we use the definition of the deformation rate tensor (5.11) with respect to the mean quantities and apply the transformation (8.9), it follows:

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

$$= \operatorname{tr}\left(\underbrace{\mu_\mathrm{t}\left[\begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix} \otimes \begin{pmatrix}\bar{u}_x\\ \bar{u}_y\\ \bar{u}_z\end{pmatrix} + \left\{\begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix} \otimes \begin{pmatrix}\bar{u}_x\\ \bar{u}_y\\ \bar{u}_z\end{pmatrix}\right\}^T\right]}_{\text{Term 1}} \right.$$

$$\underbrace{-\frac{2}{3}\mu_\mathrm{t}\begin{bmatrix} \frac{\partial \bar{u}_x}{\partial x} + \frac{\partial \bar{u}_y}{\partial y} + \frac{\partial \bar{u}_z}{\partial z} & 0 & 0 \\ 0 & \frac{\partial \bar{u}_x}{\partial x} + \frac{\partial \bar{u}_y}{\partial y} + \frac{\partial \bar{u}_z}{\partial z} & 0 \\ 0 & 0 & \frac{\partial \bar{u}_x}{\partial x} + \frac{\partial \bar{u}_y}{\partial y} + \frac{\partial \bar{u}_z}{\partial z} \end{bmatrix}}_{\text{Term 2}}$$

$$\left. \underbrace{-\begin{bmatrix} -\frac{2}{3}\rho k & 0 & 0 \\ 0 & -\frac{2}{3}\rho k & 0 \\ 0 & 0 & -\frac{2}{3}\rho k \end{bmatrix}}_{\text{Term 3}} \right) . \tag{9.72}$$

Applying the dyadic product rule (1.12) to term 1, add both matrices and multiply everything by the eddy viscosity, we end up with term 1 as:

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

Since we are only interested in the main diagonal elements (trace), we 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:

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

$$-\underbrace{3\frac{2}{3}\rho k}_{\text{Term 3}} = -2\rho k \,. \tag{9.73}$$

The result of the trace operator to the Boussinesq hypothesis is $-2\rho k$. Hence, the trace of the RHS and LHS of equation (9.63) is equal. If we would remove the term $-\frac{2}{3}\rho\delta_{ij}k$ on the RHS of equation (9.63), 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 many people were asking about the term $-\frac{2}{3}\rho\delta_{ij}k$ in public forums. Finally, we cannot find this term in OpenFOAM®, which is related to a straightforward 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 confuse 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 (9.65), we can evaluate the same kind of behavior:

$$\underbrace{\boldsymbol{\sigma}}_{\text{(Cauchy)}-\text{Stress tensor}} = \underbrace{\boldsymbol{\tau}}_{\text{shear}-\text{rate tensor (traceless)}} + \underbrace{-p\mathbf{I}}_{\text{pressure (=trace)}} , \tag{9.74}$$

$$\underbrace{\bar{\boldsymbol{\sigma}}_{\text{t}}}_{\text{(Reynolds)}-\text{Stress tensor}} = \underbrace{\bar{\boldsymbol{\tau}}_{\text{t}}}_{\text{(RA)}-\text{shear}-\text{rate tensor (traceless)}} + \underbrace{-\frac{2}{3}\rho\mathbf{I}k}_{\text{add. term (=trace)}} , \tag{9.75}$$

$$\underbrace{\mathbf{A}}_{\text{complete matrix}} = \underbrace{\mathbf{A}^{\text{dev}}}_{\text{deviatoric part (traceless)}} + \underbrace{\mathbf{A}^{\text{hyd}}}_{\text{hydro. part (=trace)}} . \tag{9.76}$$

$$\rho \frac{\partial}{\partial t} \bar{\mathbf{U}} + \rho \nabla \bullet (\bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left(\left[\mu_{\mathrm{l}} \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} \left(\nabla \bullet \bar{\mathbf{U}} \right) \mathbf{I} \right\} \right] \right.$$
$$\left. + \left[\mu_{\mathrm{t}} \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} \left(\nabla \bullet \bar{\mathbf{U}} \right) \mathbf{I} \right\} \right] \right) + \rho \mathbf{g} - \nabla \bullet (p^* \mathbf{I}) \ , \quad (9.81)$$

$$\frac{\partial}{\partial t} \rho \bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left([\mu_{\mathrm{l}} + \mu_{\mathrm{t}}] \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} \left(\nabla \bullet \bar{\mathbf{U}} \right) \mathbf{I} \right\} \right) + \rho \mathbf{g} - \nabla \bullet (p^* \mathbf{I}) \ . \quad (9.82)$$

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

$$\mu_{\mathrm{eff}} = \mu_{\mathrm{l}} + \mu_{\mathrm{t}} \ , \quad (9.83)$$

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

$$\frac{\partial}{\partial t} \rho \bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left(\mu_{\mathrm{eff}} \left\{ 2\bar{\mathbf{D}} - \frac{2}{3} \left(\nabla \bullet \bar{\mathbf{U}} \right) \mathbf{I} \right\} \right) + \rho \mathbf{g} - \nabla \bullet (p^* \mathbf{I}) \ , \quad (9.84)$$

$$\frac{\partial}{\partial t} \rho \bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \left(\underbrace{2\mu_{\mathrm{eff}} \bar{\mathbf{D}} - \frac{2}{3} \mu_{\mathrm{eff}} \left(\nabla \bullet \bar{\mathbf{U}} \right) \mathbf{I}}_{\bar{\boldsymbol{\tau}}_{\mathrm{eff}}} \right) + \rho \mathbf{g} - \nabla \bullet (p^* \mathbf{I}) \ . \quad (9.85)$$

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

$$\boxed{\frac{\partial}{\partial t} \rho \bar{\mathbf{U}} + \nabla \bullet (\rho \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = \nabla \bullet \bar{\boldsymbol{\tau}}_{\mathrm{eff}} - \nabla \bullet (p^* \mathbf{I}) + \rho \mathbf{g}} \ . \quad (9.86)$$

9.5 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 relate the eddy viscosity to known quantities. Commonly the turbulent (eddy) viscosity is characterized by 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 $q = \sqrt{k}$. These 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:

$$\boxed{\mu_\mathrm{t} \approx C_\mu \rho q L} \, . \tag{9.89}$$

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.

9.6 Algebraic Models

At the beginning of computational fluid dynamics, the power of personal and supercomputers was restricted. 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 produce non-physical values for the eddy viscosity.

9.7 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 two-equation models. Since 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 approximation 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. (9.70). 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 these equations are discussed in the following sections.

9.8 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:

$$\rho\frac{\partial u_i}{\partial t} + \rho\frac{\partial}{\partial x_j}\left(u_j u_i\right) = \frac{\partial}{\partial x_j}\left[2\mu\left\{\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right\}\right] - \frac{\partial p}{\partial x_i}\ . \tag{9.90}$$

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:

$$\rho\frac{\partial}{\partial x_j}(u_j u_i) = \rho u_j\frac{\partial u_i}{\partial x_j} + \underbrace{\cancel{\rho u_i\frac{\partial u_j}{\partial x_j}}}_{\text{continuity}}\ . \tag{9.91}$$

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

$$\rho\frac{\partial u_i}{\partial t} + \rho u_j\frac{\partial u_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left[2\mu\left\{\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right\}\right] + \frac{\partial p}{\partial x_i} = \mathcal{N}(u_i)\ . \tag{9.92}$$

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

$$\mathcal{N}(u_i) = 0\ . \tag{9.93}$$

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:

$$u'_i\mathcal{N}(u_j) + u'_j\mathcal{N}(u_i) = 0\ . \tag{9.94}$$

The next step is to apply the expression (9.1) to the Navier-Stokes operator $\mathcal{N}(u_i)$ and average the whole equation by using the Reynolds time-averaging method (9.9). This leads to the following equation:

$$\overline{u'_i\mathcal{N}(\bar{u}_j + u'_j) + u'_j\mathcal{N}(\bar{u}_i + u'_i)} = 0\ . \tag{9.95}$$

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 14.1.

Operations and relations

For the derivation of the Reynolds-Stress equation we need to build the following tensor equation with formula (9.95):

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

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:

$$\boxed{\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial u_k} = -\bar{\sigma}_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \bar{\sigma}_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k} + C_{ijk}\right) + \epsilon_{ij} - \Pi_{ij}} \, . \tag{9.96}$$

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.

9.9 The Incompressible Kinetic Energy Equation

The derivation of the kinetic energy equation of the turbulence (per unit mass) for incompressible flows is straightforward after knowing the Reynolds-Stress equation due to the fact of the relation given by equation (9.66). To get the equation, we have to take the trace of equation (9.96). It follows:

$$\begin{aligned}
&\mathrm{tr}\left\{\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial u_k}\right\} \\
&\qquad = \mathrm{tr}\left\{-\bar{\sigma}_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \bar{\sigma}_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k} + C_{ijk}\right) + \epsilon_{ij} - \Pi_{ij}\right\} .
\end{aligned} \tag{9.97}$$

After applying the trace operator to each term we get:

For the time derivation we get:

$$\begin{aligned}
\mathrm{tr}\left\{\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t}\right\} &= \frac{\partial \bar{\sigma}_{\mathrm{t}_{xx}}}{\partial t} + \frac{\partial \bar{\sigma}_{\mathrm{t}_{yy}}}{\partial t} + \frac{\partial \bar{\sigma}_{\mathrm{t}_{zz}}}{\partial t} = -\rho \frac{\partial \overline{u_x' u_x'}}{\partial t} - \rho \frac{\partial \overline{u_y' u_y'}}{\partial t} - \rho \frac{\partial \overline{u_z' u_z'}}{\partial t} \\
&= -\rho \frac{\partial}{\partial t} \underbrace{\left(\overline{u_x' u_x'} + \overline{u_y' u_y'} + \overline{u_z' u_z'}\right)}_{(9.66) \rightarrow 2k} = \boxed{-2\rho \frac{\partial k}{\partial t}} \, .
\end{aligned} \tag{9.98}$$

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

$$\begin{aligned}\mathrm{tr}\left\{\bar{u}_k\frac{\partial\bar{\sigma}_{\mathrm{t}_{ij}}}{\partial u_k}\right\} &= \bar{u}_k\frac{\partial\bar{\sigma}_{\mathrm{t}_{xx}}}{\partial u_k}+\bar{u}_k\frac{\partial\bar{\sigma}_{\mathrm{t}_{yy}}}{\partial u_k}+\bar{u}_k\frac{\partial\bar{\sigma}_{\mathrm{t}_{zz}}}{\partial u_k}\\ &= -\rho\bar{u}_k\frac{\partial\overline{u'_xu'_x}}{\partial u_k}-\rho\bar{u}_k\frac{\partial\overline{u'_yu'_y}}{\partial u_k}-\rho\bar{u}_k\frac{\partial\overline{u'_zu'_z}}{\partial u_k}\\ &= -\rho\bar{u}_k\frac{\partial}{\partial u_k}(\overline{u'_xu'_x}+\overline{u'_yu'_y}+\overline{u'_zu'_z}) = \boxed{-2\rho\bar{u}_k\frac{\partial k}{\partial u_k}}\ .\end{aligned} \tag{9.99}$$

The first and second term of equation (9.96) lead to:

$$\mathrm{tr}\left\{-\bar{\sigma}_{\mathrm{t}_{jk}}\frac{\partial\bar{u}_i}{\partial x_k}-\bar{\sigma}_{\mathrm{t}_{ik}}\frac{\partial\bar{u}_j}{\partial x_k}\right\} = -\bar{\sigma}_{\mathrm{t}_{ik}}\frac{\partial\bar{u}_i}{\partial x_k}-\bar{\sigma}_{\mathrm{t}_{ik}}\frac{\partial\bar{u}_i}{\partial x_k} = \boxed{2\rho\overline{u'_iu'_k}\frac{\partial\bar{u}_i}{\partial x_k}}\ . \tag{9.100}$$

The first part of the third term results in:

$$\begin{aligned}\mathrm{tr}\left\{\frac{\partial}{\partial x_k}\left(\nu\frac{\partial\bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k}\right)\right\} &= \frac{\partial}{\partial x_k}\left(\nu\frac{\partial\bar{\sigma}_{\mathrm{t}_{xx}}}{\partial x_k}\right)+\frac{\partial}{\partial x_k}\left(\nu\frac{\partial\bar{\sigma}_{\mathrm{t}_{yy}}}{\partial x_k}\right)+\frac{\partial}{\partial x_k}\left(\nu\frac{\partial\bar{\sigma}_{\mathrm{t}_{zz}}}{\partial x_k}\right)\\ &= -\frac{\partial}{\partial x_k}\left(\rho\nu\frac{\partial\overline{u'_xu'_x}}{\partial x_k}\right)-\frac{\partial}{\partial x_k}\left(\rho\nu\frac{\partial\overline{u'_xu'_x}}{\partial x_k}\right)-\frac{\partial}{\partial x_k}\left(\rho\nu\frac{\partial\overline{u'_xu'_x}}{\partial x_k}\right)\\ &= -\frac{\partial}{\partial x_k}\left(\mu\frac{\partial}{\partial x_k}(\overline{u'_xu'_x}+\overline{u'_yu'_y}+\overline{u'_zu'_z})\right)\\ &= \boxed{-2\frac{\partial}{\partial x_k}\left(\mu\frac{\partial k}{\partial x_k}\right)}\ .\end{aligned} \tag{9.101}$$

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

$$\mathrm{tr}\left\{\frac{\partial}{\partial x_k}\rho\overline{u'_iu'_ju'_k}+\frac{\partial}{\partial x_k}\left[\overline{p'u'_j}\delta_{ik}+\overline{p'u'_i}\delta_{jk}\right]\right\} = \boxed{\underline{\frac{\partial}{\partial x_j}\rho\overline{u'_ju'_iu'_i}}+2\frac{\partial}{\partial x_j}\overline{p'u'_j}}\ . \tag{9.102}$$

The evaluation of the second term that includes the pressure can be done in an easy way. It is merely 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:

$$\mathrm{tr}\left(\rho\overline{u'_xu'_ju'_k}\right) = \mathrm{tr}\begin{bmatrix}\rho\overline{u'_xu'_xu'_x} & \rho\overline{u'_xu'_xu'_y} & \rho\overline{u'_xu'_xu'_z}\\ \rho\overline{u'_xu'_yu'_x} & \rho\overline{u'_xu'_yu'_y} & \rho\overline{u'_xu'_yu'_z}\\ \rho\overline{u'_xu'_zu'_x} & \rho\overline{u'_xu'_zu'_y} & \rho\overline{u'_xu'_zu'_z}\end{bmatrix} = \rho\overline{u'_xu'_iu'_i}\ . \tag{9.103}$$

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

$$\mathrm{tr}\left\{2\mu\overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}}\right\} = \boxed{2\mu\overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_i}{\partial x_k}}}\ . \tag{9.104}$$

The last term of equation (9.96), Π_{ij}, is zero due to the fact that $\frac{\partial u'_i}{\partial x_i} = 0$:

$$\mathrm{tr}\left\{\overline{p'\left[\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}\right]}\right\} = \overline{p'\left[\cancel{\frac{\partial u'_x}{\partial x}} + \cancel{\frac{\partial u'_x}{\partial x}}\right]} + \overline{p'\left[\cancel{\frac{\partial u'_z}{\partial y}} + \cancel{\frac{\partial u'_y}{\partial y}}\right]} + \overline{p'\left[\cancel{\frac{\partial u'_z}{\partial z}} + \cancel{\frac{\partial u'_z}{\partial z}}\right]} = 0\,. \qquad (9.105)$$

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

$$-2\rho\frac{\partial k}{\partial t} - 2\rho\bar{u}_k\frac{\partial k}{\partial u_k} = 2\rho\overline{u'_i u'_k}\frac{\partial \bar{u}_i}{\partial x_k} - 2\frac{\partial}{\partial x_k}\left(\mu\frac{\partial k}{\partial x_k}\right) + \frac{\partial}{\partial x_k}\rho\overline{u'_j u'_i u'_i} + 2\frac{\partial}{\partial x_k}\overline{p' u'_i} + 2\mu\overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_i}{\partial x_k}}\,. \qquad (9.106)$$

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

$$\rho\frac{\partial k}{\partial t} + \rho\bar{u}_k\frac{\partial k}{\partial u_k} = \underbrace{-\rho\overline{u'_i u'_k}\frac{\partial \bar{u}_i}{\partial x_k}}_{P_k} + \frac{\partial}{\partial x_k}\left(\mu\frac{\partial k}{\partial x_k}\right) \underbrace{-\frac{\partial}{\partial x_k}\frac{\rho}{2}\overline{u'_j u'_i u'_i} - \frac{\partial}{\partial x_j}\overline{p' u'_j}}_{\text{turbulent diffusion}} - \underbrace{\mu\overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_i}{\partial x_k}}}_{\text{dissipation }\epsilon}\,. \qquad (9.107)$$

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 ordinary kinetic energy equation as:

$$\boxed{\rho\frac{\partial k}{\partial t} + \rho\bar{u}_k\frac{\partial k}{\partial u_k} = \frac{\partial}{\partial x_k}\left(\mu\frac{\partial k}{\partial x_k}\right) + P_k - \frac{\partial}{\partial x_k}\left[\frac{\rho}{2}\overline{u'_j u'_i u'_i} + \overline{p' u'_j}\right] - \epsilon}\,. \qquad (9.108)$$

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

$$-\left[\frac{\rho}{2}\overline{u'_j u'_i u'_i} + \overline{p' u'_j}\right] \approx \frac{\mu_{\mathrm{t}}}{\mathrm{Pr_t}}\frac{\partial k}{\partial x_j}\,. \qquad (9.109)$$

Here, $\mathrm{Pr_t}$ denotes the turbulent Prandtl number and is assumed to be one. In literature, it is common to denote the turbulent Prandtl number by σ_k. Since we use sigma to describe any stress tensor, we avoid the usage of another sigma quantity here.

The production rate is modeled with the assumption given by equation (9.63), 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:

$$P_k = -\rho\overline{u'_i u'_j}\frac{\partial \bar{u}_i}{\partial x_j} \approx \mu_{\mathrm{t}}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\frac{\partial \bar{u}_i}{\partial x_j}\,. \qquad (9.110)$$

The dissipation ϵ that describes 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 $\bar{\boldsymbol{\sigma}}_{\mathrm{t}}$. 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 that both quantities can be related.

9.10 The Relation between ϵ and L

The 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. 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:

$$\epsilon \approx \frac{k^{\frac{3}{2}}}{L} \; . \tag{9.111}$$

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 (these vortexes are named Kolmogorov vortexes), the viscous effect will transfer the energy of motion into internal energy. This phenomenon is called dissipation.

9.11 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:

$$\rho \frac{\partial \epsilon}{\partial t} + \rho \bar{u}_j \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon_1} P_k \frac{\epsilon}{k} - \rho C_{\epsilon_2} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left(\frac{\mu_{\mathrm{t}}}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right) \tag{9.112}$$

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 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 (9.89) with the new quantities:

$$\mu_{\mathrm{t}} = \rho C_\mu \sqrt{k} L = \rho C_\mu \sqrt{k} \frac{\sqrt{k^3}}{\epsilon} = \rho C_\mu \frac{k^2}{\epsilon} \; . \tag{9.113}$$

The model parameters of the equations above are:

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

9.12 Coupling of the Parameters

As we could see in the last sections, turbulence modeling is a complex topic. The most comfortable 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 of turbulent flows is exceptionally 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). Useful references for further investigations into the turbulence modeling are the books of Ferziger and Perić [2008], Bird et al. [1960] and Wilcox [1994].

9.13 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 the derivation for compressible fluids. Therefore, we get:

$$\rho = \bar{\rho} + \rho' \ . \tag{9.114}$$

This lead to more unknown terms that will make the problem even more complicated; compare the already derived Reynolds time-averaged compressible mass conservation equation (9.24) which is given again:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i + \overline{\rho' u_i'}) = 0 \ . \tag{9.115}$$

Here we need approximations for the correlation between ρ' and u_i', which is 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 physically correct. What we do is simple. We add a mass-averaged velocity field $\tilde{u}_i$, that is defined as:

$$\tilde{u}_i = \frac{1}{\bar{\rho}} \lim_{T \to \infty} \int_t^{t+T} \rho(t,x) u_i(t,x) \mathrm{d}\tau \ . \tag{9.116}$$

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:

$$\bar{\rho}\tilde{u}_i = \overline{\rho u_i} \ . \tag{9.117}$$

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

$$\bar{\rho}\tilde{u}_i = \overline{(\bar{\rho} + \rho')(\bar{u}_i + u'_i)} = \overline{\bar{\rho}\bar{u}_i} + \cancel{\overline{\bar{\rho} u'_i}} + \cancel{\overline{\rho' \bar{u}_i}} + \overline{\rho' u'_i} = \bar{\rho}\bar{u}_i + \overline{\rho' u'_i} \ . \tag{9.118}$$

If we use this expression for equation (9.115), we end up with:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i) = 0 \ . \tag{9.119}$$

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 in to 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 method 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 10

Calculation of the Shear-Rate Tensor in OpenFOAM®

In this chapter we discuss the implementation of the calculation of the shear-rate tensor $\boldsymbol{\tau}$, $\bar{\boldsymbol{\tau}}_\mathrm{t}$ or $\tilde{\boldsymbol{\tau}}_\mathrm{t}$ which represents the real, Reynolds-averaged or Favre-averaged quantities. In OpenFOAM® the shear-rate tensor is calculated by calling the either the function `divDevReff` for incompressible or `divDevRhoReff` for compressible fluids.

The discussion is based on OpenFOAM® version 7. Be prepared that the code can look different in former versions. The reason is related to code maintenance and improvements as well as sustainability. The following chapter discusses the shear-rate tensor for liquids with a linear viscous stress relation named Newtonian fluids.

10.1 The incompressible Shear-Rate Tensor (divDevReff)

For incompressible fluids, the momentum equation that is used in OpenFOAM® can be analyzed in the *UEqn.H* files of e.g. `pimpleFoam, pisoFoam, simpleFoam`. The c++ code of the momentum equation is presented in the code snippet above:

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

Listing 10.1: $FOAM_SOLVERS/incompressible/pimpleFoam/UEqn.H

There are different numerical terms included inside the matrix which are marked by using the symbol (I) to (V). The first term (I) is the time derivation. The second term (II) represents the convective term. After that, an additional correction term (III) is added due to the usage of the Multi-Reference-Frame (MRF) assumption; this term is zero if no MRF approach is used in the simulation. The next term (IV) is related to the the shear-rate tensor and finally, we see the last term (V) that handles additional sources/sinks/manipulations that act on the equation. The last term is controlled with the `fvOptions` dictionary in the `system` folder.

For now on, we only focus onto the shear-rate (diffusion) term (IV) `turbulence->divDevReff(U)` and its implementation.

First of all, we will discuss the meaning of the name `divDevReff`. 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 calculate the effective diffusion transport which includes laminar and turbulent transport phenomena. Therefore, we get the name `divDevReff` for incompressible and `divDevRhoReff` for compressible fluids. The equation below gives the mathematical expression:

$$\nabla \bullet \boldsymbol{\tau} = \nabla \bullet \boldsymbol{\sigma}^{\text{dev}} \tag{10.1}$$

The analysis of the c++ function can be checked with the source code guide named Doxygen or directly in the source and header files of the code. For the following explanations, it is assumed that basic object oriented programming concepts are known.

Starting with the code line `turbulence->divDevReff(U)` in the `UEqn.H` file, it can be seen that the word `turbulence` is an object that calls the function named `divDevReff`. The function itself takes an argument namely the velocity field `U`. To analyze the c++ function, it is necessary to know the class of the object `turbulence`. For incompressible solvers, the object is based on the general *turbulenceModel* class which is derived from the *IncompressibleTurbulenceModel* class. The

The new called function **divDevRhoReff(U)** depends on the transport model we are using. Commonly, in engineering and in most scientific areas we are dealing with Newtonian fluids following the linear viscosity assumption. Hence, the turbulence models are then referring to the *linearViscouseStress* class. Based on that, the function **divDevRhoReff(U)** calls the function definition in the *linearViscousStress* class. The code snipped is presented below.

Note, in the extended book (red color), there is a detailed explanation on how the turbulence model class hierarchy is

```
template<class BasicTurbulenceModel>
Foam::tmp<Foam::fvVectorMatrix>
Foam::linearViscousStress<BasicTurbulenceModel>::divDevRhoReff
(
    volVectorField& U
) const
{
    return
    (
      - fvc::div((this->alpha_*this->rho_*this->nuEff())*dev2(T(fvc::grad(U))))
      - fvm::laplacian(this->alpha_*this->rho_*this->nuEff(), U)
    );
}
```

Listing 10.4: turbulenceModels/linearViscousStress/linearViscousStress.C

In the above given snipped, we see the divergence and laplacian function in the return statement.

The `dev2` function thus calculates and returns the deviatoric part given as:

$$\mathbf{T}^{\text{dev}} = \mathbf{T} - \begin{bmatrix} \frac{2}{3} & 0 & 0 \\ 0 & \frac{2}{3} & 0 \\ 0 & 0 & \frac{2}{3} \end{bmatrix} \text{tr}(\mathbf{T}) \ . \tag{10.2}$$

The Laplacian part

As before, the variables `this->alpha_` and `this->rho_` are equal to one. therefore, the second part in the return statement of the `divDevRhoReff(U)` is simply the laplacian operator:

$$\nabla \bullet (\nu_{\text{eff}} \nabla \otimes \mathbf{U})$$

Summing up

Adding the mathematical expressions into the analyzed c++ functions we get the following formulation for the first part. The `dev2` function returns equation (10.2), that is similar to (1.28) except, that the trace is further multiplied by the factor two. The argument of that function is the transposed gradient of the velocity vector $\mathbf{U}$. Thus, the RHS of equation (10.2) becomes the following form ($\mathbf{T} = (\nabla \otimes \mathbf{U})^T$):

$$(\nabla \otimes \mathbf{U})^T - \frac{2}{3} \,\text{tr}\left[(\nabla \otimes \mathbf{U})^T\right] \mathbf{I} \ .$$

The above formulation is multiplied by the effective viscosity:

underbraced terms with their expressions, it follows:

$$- \nabla \boldsymbol{\tau} = -\nabla \bullet \left[2\nu_{\text{eff}} \mathbf{D} - \frac{2}{3}\nu_{\text{eff}} (\nabla \bullet \mathbf{U}) \mathbf{I} \right] \ . \tag{10.5}$$

As for each time step, the continuity should be fulfilled, the last term on the RHS vanishes and we end up with the following incompressible shear-rate tensor equation:

$$- \nabla \boldsymbol{\tau} = -\nabla \bullet \left[2\nu_{\text{eff}} \mathbf{D} \right] \ . \tag{10.6}$$

As we could see, the implementation of the shear-rate tensor in OpenFOAM® is correct and valid. The sign difference in the equation refers to the position at the LHS in OpenFOAM® whereas in equation (5.36) the shear-rate tensor stands on the RHS.

Stability

During the analysis of the c++ functions, we figured out that the term $\frac{2}{3}\nu_{\text{eff}} \operatorname{tr}(\nabla \otimes \mathbf{U})$ is included in the calculation of the diffusion term of the momentum equation. As the continuity equation is not zero in numerics, this term stabilizes the calculation as the continuity error is taken into account in the momentum equation. Furthermore, if the continuity is fulfilled, this term becomes zero and we end up with the derived equation (5.36).

10.2 The Compressible Shear-Rate Tensor (divDevRhoReff)

- The function call `turbulence->divDevRhoReff(U)` is similar to the incompressible one. The only difference here is, that the `divDevRhoReff(U)` function is only implemented as virtual function within the *compressible* class. Thus, we directly call the corresponding function in the *linearViscouseStress* class.
- While calling the same function, the quantity `this->rho_` is not equal to one anymore. Now it represents the density field in the domain.

As shown in the previous section, the end equation that one can derive from the source code is equal to equation (5.14). Thus, the correct mathematical expression for the shear-rate tensor in density based solvers is correctly implemented in OpenFOAM®.

10.3 A Hint to Turbulence Models vs Laminar

If one runs a simulation case using the turbulence model laminar and recalculate the same case while using a RAS model, e.g. kEpsilon and turning off the keyword `turbulence off;` within the `turbulenceProperties` file, the results do not have to be identical.

Why? As we use a turbulence model, we calculate the effective viscosity by summing up the laminar and turbulent one. While using the laminar turbulence model, the turbulent viscosity is zero while it is not, if we set-up a RAS model. Even though, if we are setting the `turbulence` keyword to off. The reason for this is related to the initialization of the turbulence quantities and the first initialization of the turbulent viscosity based on the initial data.

The keyword `turbulence off;` just do not execute the recalculation of the turbulent fields

Chapter 11

The numerical algorithms: SIMPLE, PISO and PIMPLE

Solving the Navier-Stokes equations requires numerical techniques to solve the coupled pressure-momentum system. This is done by the well-known algorithms named: `SIMPLE`, `PISO`, and `PIMPLE`.

The different algorithms are based on various problems. Therefore, we will understand these algorithms better after we introduced the difficulties that come into handy when we solve the Navier-Stokes equations or any other coupled system. Further information about the algorithms presented in this chapter can be found in Ferziger and Perić [2008] and Moukalled et al. [2015]

Considering the general momentum equation (2.26) and applying the incompressible assumption — the density is constant and can be taken out of the derivatives —, we get:

$$\rho \frac{\partial \mathbf{U}}{\partial t} = -\rho \nabla \bullet (\mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau} - \nabla p + \rho \mathbf{g} \; . \tag{11.1}$$

Note: In the equation above, the definition of the shear-rate tensor was not introduced. That is why a negative sign is applied here.

Now, we divide the equation by the density ρ. Hence, $\boldsymbol{\tau}$ has to be expressed by equation (5.36), thus, it follows:

$$\frac{\partial \mathbf{U}}{\partial t} = -\nabla \bullet (\mathbf{U} \otimes \mathbf{U}) - \nabla \bullet \boldsymbol{\tau}_{\text{inco}} - \nabla \frac{p}{\rho} + \mathbf{g} \; . \tag{11.2}$$

Based on the fact that the density is constant, there is no need to solve the 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 the velocity vector $\mathbf{U}$. However, there are four unknowns and only three equations (the momentum formulation in x, y, and z). Therefore, we need an additional equation, which is the mass conservation equation (2.13). Based on the fact that this equation does not include the pressure quantity, special techniques are needed to solve the coupled pressure-momentum system. 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* and use its meaning to get a further equation that includes the pressure.

Thus, we apply the divergence operator onto the left- and right-hand side of 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. The derivation is not presented in the green version of the book.

Now, there exist four equations for four unknown quantities. Therefore, the linear system of equations can be solved.

In general, these equations are solved sequentially. 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 we are solving the Poisson equation for the pressure p. It is worth to note that the momentum equation does not have to be solved. It is sufficient to build the velocity matrix and use it in the pressure calculation.

The strategy for the numerical algorithm is to find a pressure and momentum field that fulfills the mass conservation equation.

The sequential solving procedure is achieved by using the algorithms mentioned above, namely: `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 analysis.

- `PISO` := Pressure-Implicit-of-Split-Operations.
  In OpenFOAM® we are using this algorithm for transient calculation. The calculation is limited to the time step which is related to the Courant number (Co < 1).

- `PIMPLE` := Merged `PISO`–`SIMPLE`.
  The algorithm combines both algorithms (`SIMPLE` and `PISO`) which enables the usage of larger time-steps (Co $\gg 1$).

Note: There is a family of different algorithms available. For example, the `SIMPLE` algorithm is not consistent in terms of the mathematical formulation. During the derivation of the `SIMPLE` formulation, one term is neglected. Therefore, different algorithms were derived while the missing term is approximated, and the formulation gets consistent again. These algorithms are known as `SIMPLER`, `SIMPLEM`, or `SIMPLEC` algorithm. OpenFOAM® includes the `SIMPLE` and `SIMPLEC` (Consistent) algorithms. An overview is presented in Moukalled et al. [2015].

11.1 The SIMPLE algorithm in OpenFOAM®

Each SIMPLE based solver in OpenFOAM®, do not contain any time derivation in the equations. It is worth to mention that the time derivation is a natural limiter for the solution. That means, for a particular time interval of Δt, the solution can only *move on* by this time-step. Based on the fact that we do not have the time derivation within that algorithm, we can only calculate the steady-state solution. Regarding the missing natural limiter Δt and the fact that the SIMPLE algorithm is not consistent, under-relaxation has to be performed to the equations and/or fields in order to achieve stability and convergence. Otherwise, the solver might blow up while throwing a *floating point exception* (dividing by zero), or the result does not represent a physical behavior.

While using the SIMPLE algorithm, the time-step Δt should be modified and set to 1 within the controlDict file. Thus, the simulation time now corresponds to the numbers of iterations within the SIMPLE loop. Changing the time step to other values will not influence the solution. The only effect of changing the time-step in the controlDict will let us reach the *pseudo end time* faster or not, and therefore, we are performing more or fewer iterations.

Of course, one may think that changing Δt affects the result, but this is not true if we reach the steady-state solution at the end of the simulation.

For the SIMPLE algorithm it is important to estimate the relaxation factors for the field and equation relaxation to reach

- numerical stability ,
- and a fast convergence rate .

If for any reason, the user sets tiny relaxation factors, the stability might be excellent, but the convergence rate is prolonged. This increases the computational costs and might lead to a convergence indication while the solution is not even close the steady-state value.

11.1.1 The SIMPLEC algorithm in OpenFOAM®

Since OpenFOAM® 3.0, the SIMPLEC algorithm is implemented and can be used in all SIMPLE and PIMPLE operating algorithms. For that purpose, we have to add the special keyword `consistent true;` to the SIMPLE or PIMPLE control dictionary as given in the fvSolutions file below.

```
SIMPLE
{
    consistent   true;
}

PIMPLE
{
    consistent   true;
}
```

Listing 11.1: SIMPLE operating in SIMPLEC mode

As already mentioned in the previous section, the SIMPLEC algorithm includes the missing pressure term, which is neglected in the SIMPLE algorithm. The added character C stands for consistent.

Using the SIMPLEC method will require more iterations for each single segregated calculation step, but the convergence rate will increase drastically. The release notes report a speed-up of three times. Furthermore, larger values for the under-relaxation factors can be applied. It is worth to note that the pressure field should not be relaxed too much. A relaxation factor of 0.95 is already considered small.

Note: Again, the `consistent` keyword can be added to the `PIMPLE` dictionary too, but will only affect the algorithm, if we operate in the real `PIMPLE` mode. Otherwise, this keyword will not influence the numerical calculation. The correct usage of the `PIMPLE` algorithm, will be discussed later.

11.2 The PISO algorithm in OpenFOAM®

The two main differences to the SIMPLE algorithm are the included time derivation term sand the consistency of the pressure-velocity coupling equation. Based on those 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 imagined 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 limited to be less than one. Generally, it is common practice to start with a Courant number at the start of the beginning, which is increased during the run-time to some case depended value. The stability criterion is defined as:

$$\mathrm{Co} = \frac{\mathbf{U}\Delta t}{\Delta x} \ . \tag{11.3}$$

The Courant number depends on the local cell velocity $\mathbf{U}$, the time-step Δt, and the distance between the cell centers Δx. In OpenFOAM®, the calculation is based on the cell volume rather than the distance Δx.

```
scalar CoNum = 0.0;
scalar meanCoNum = 0.0;

{
    scalarField sumPhi
    (
        fvc::surfaceSum(mag(phi))().primitiveField()
    );

    CoNum = 0.5*gMax(sumPhi/mesh.V().field())*runTime.deltaTValue();

    meanCoNum =
        0.5*(gSum(sumPhi)/gSum(mesh.V().field()))*runTime.deltaTValue();
}

Info<< "Courant Number mean: " << meanCoNum
    << " max: " << CoNum << endl;
```

Listing 11.2: Courant number calculation coded in the CourantNo.H file

Based on formula (11.3), 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 cell volume ΔV, the larger the Courant number.

The central aspect here is, that if we refine the mesh, increase the velocity or the time-step, the Courant number will increase. To fulfill the criterion given in equation (11.3), the time-step has to be adjusted based on the mesh size and the velocity.

Note: The Courant number criterion has to be fulfilled for each numerical cell. Hence, any bad cell can limit the whole simulation.

11.3 The PIMPLE algorithm in OpenFOAM®

The `PIMPLE` algorithm is one of the most used ones if we have transient problems because it combines the `PISO` and `SIMPLE` (`SIMPLEC`) one. The advantage is that we can use Courant numbers larger than one (Co >> 1), and thus, the time-step can be increased drastically.

The principal of the algorithm is as follows. Within a single time-step, a steady-state solution is searched while an under-relaxation strategy is applied. After the solution is found, we go to the next time-step. For this, we need the so-called outer correction loops, to ensure that all explicit parts of the equations are converged. After a user-defined tolerance criterion is reached — within the steady-state calculation — the outer correction loop is left, and we move on in time. This is done until the simulation end time is reached.

Note: The `PIMPLE` algorithm in OpenFOAM® can also work in `PISO` mode, if we set the `nOuterCorrectors` to one. Setting the value to zero ignores the whole pimple loop, and hence, no calculation is performed. 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 11.3: The output of the pimple algorithm

11.4 The correct usage of the PIMPLE algorithm

The usage of the `PIMPLE` algorithm is explained and discussed in the next pages. 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 11.4: The control dictionary within the fvSolution file

The keyword has to be added to the `fvSolution` file. Otherwise, the solver will throw out an error. Nevertheless, it is sufficient to create an empty dictionary because OpenFOAM® uses default values based on the constructor of the class `pimpleControl`. Since OpenFOAM® 5, and the implementation of the `chtMultiRegionFoam` residual control, the classes were restructured. Thus, new classes were introduced. While starting a `PIMPLE` based solver, the constructor for the `pimpleControl` class is called.

```
// * * * * * * * * * * * * * * * * Constructors  * * * * * * * * * * * * * * * //

Foam::pimpleControl::pimpleControl(fvMesh& mesh, const word& algorithmName)
:
    pimpleNoLoopControl(mesh, algorithmName, *this),
    pimpleLoop(static_cast<solutionControl&>(*this))
```

Listing 11.5: The constructor of the pimpleControl class

The constructor of the **pimpleControl** class calls two further constructors. The first one is the constructor of the **pimpleNoLoopControl** and the second one of the **pimpleLoop** class. Within the **pimpleNoLoopControl**, the constructor is as follows:

```
// * * * * * * * * * * * * * * * * * Constructors  * * * * * * * * * * * * * * * //

Foam::pimpleNoLoopControl::pimpleNoLoopControl
(
    fvMesh& mesh,
    const word& algorithmName,
    const pimpleLoop& loop
)
:
    pisoControl(mesh, algorithmName),
    singleRegionConvergenceControl
    (
        static_cast<singleRegionSolutionControl&>(*this)
    ),
    singleRegionCorrectorConvergenceControl
    (
        static_cast<singleRegionSolutionControl&>(*this),
        "outerCorrector"
    ),
    loop_(loop),
    simpleRho_(false),
    turbOnFinalIterOnly_(true)
{
    read();
}
```

After the `pisoControl` constructor was called, the `singleRegionConvergenceControl` is called. Here, steady-state convergence control data are read from the `fvSolution` file. The corresponding entry is named `residualControl`.

Subsequently, the `singleRegionCorrectorConvergenceControl` class constructor is called. This class stores the residual control data related to the outer correction loops. The class checks the availability of the keyword `outerCorrectorResidualControl` inside the `fvSolution` file and stores the given data.

```
bool Foam::pisoControl::read()
{
    if (!fluidSolutionControl::read())
    {
        return false;
    }

    const dictionary& solutionDict = dict();

    nCorrPiso_ = solutionDict.lookupOrDefault<label>("nCorrectors", 1);

    return true;
}
```

Listing 11.8: The constructor of the pisoControl class

Following, the `loop_` variable is set which is of class type `pimpleLoop`. This class stores the information of the outer corrector status. The amount of outer correction that have to be performed

At the end of the `pimpleNoLoopControl` constructor, the class function `read()` is called. In the function, the `simpleRho` and `tubOnFinalIterOnly` keywords are looked-up in the `PIMPLE` dictionary and set accordingly.

Following, the actual object (`*this`) which already stores a solution control section, is casted to the `pimpleLoop` constructor. After that, the initialization is finished and the `read()` function of the `pimpleControl` class is called. Within this function the `nCorrPimple_` variable is reset with the search value named `nOuterCorrectors`.

Finally, some output information is printed, and the user gets information about the algorithm mode that is activated. The following possible modes can be achieved using the `PIMPLE` algorithm:

- `nOuterCorrectors` = 1
  - SIMPLE
  - PISO
- `nOuterCorrectors` > 1
  - steady-state
    If the ddt scheme is steady-state ⟶ `mesh.steady()`
  - transient
    If the ddt scheme is not steady-state ⟶ `mesh.transient()`
  - mixed steady-state/transient
    If both schemes are available

After analyzing the code, it is obvious that the `pimpleControl` object stores the following information:

- Information about the amount of `PISO` iterations (nCorrectors) ,
- Information about the amount of `PIMPLE` iterations (nOuterCorrectors) ,
- Information if the turbulence properties are updated in each outer iteration or only at the last one ,
- Information about the convergence criterion for the steady-state solution (stopping the solver) and the transient solution (stopping the steady-state calculation within one time-step) .

It is worth to mention that the `pisoControl` inherits the `fluidSolutionControl` class which inherits the `nonOrthogonalSolutionControl`. The `fluidSolutionControl` class stores information about the setting for the:

- momentumPredictor ,

  Solve the momentum equation; default ⟶ true

- frozenFlow ,

  Only solve the energy equation ⟶ used in the `chtMultiRegionFoam` solver ; default ⟶ false

- transonic ,

  Change the pressure calculation for transonic behaviors; default ⟶ false

- consistent ,

  Use the `SIMPLEC` algorithm rather than the `SIMPLE` one; default ⟶ false

while the `nonOrthogonalSolutionControl` further stores the information about the number of non-orthogonal correction loops. The non-orthogonal correction loop is used to converge the explicit added non-orthogonal correction term. It is important for high non-orthogonal meshes.

For the further analysis, we investigate into a simple non-steady test case while the key-idea of the `PIMPLE` algorithm is illustrated.

11.4.1 The test case

In order to demonstrate the influence of different parameters that control the `PIMPLE` algorithm within the `fvSolution` file, a simple 2D transient pipe flow will be considered. It is worth to mention that this case is not suited best for describing the `PIMPLE` algorithm. The advantages of the `PIMPLE` method come with complex geometries. Thus, the test case is just a demonstration.

The pipe geometry suddenly reduces its cross-section to accelerate the fluid in order to create some vortex shedding behavior. This creates an unstable flow that has to be handled by the algorithm. Compare figure (11.1).

The kinematic viscosity ν is set to $1e^{-6}$ and the extrusion of the 2D mesh in z-direction is equal to 0.01m. The analysis was performed using OpenFOAM® 7.x.

For own investigations, the test case is provided at https://Holzmann-cfd.de/ in the Free Material section named Pimple Investigations.

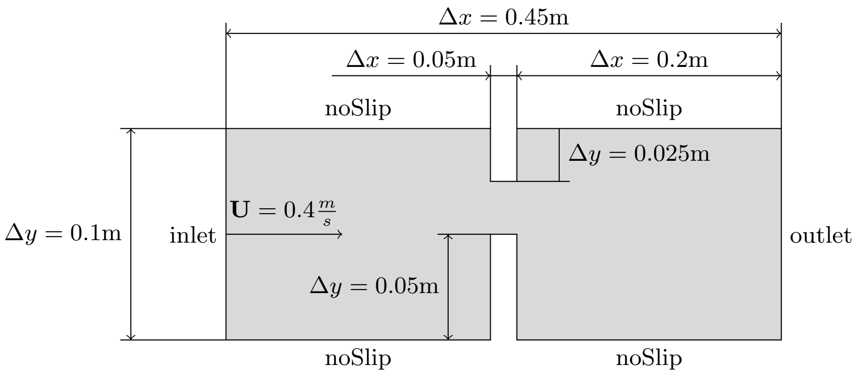


Figure 11.1: The 2D pipe flow domain for the analyze of the PIMPLE algorithm.

Another example and further explanation about the equations that are solved can be found in Holzmann [2014]. Furthermore, a detailed introduction into the method and how the pressure-momentum coupling is constructed in OpenFOAM® is presented in Moukalled et al. [2015].

The momentum-pressure coupling equations are not derived in the green version of the book.

11.4.2 First considerations

In the following, we are using the domain indicated above using the boundary conditions to demonstrate the usage of the `PIMPLE` algorithm. In the beginning, some necessary investigations into the problem are done to get more familiar with the numerical analysis.

By using the continuity equation, the maximum time-step for the simulation can be estimated. The area at the inlet is given as $A = 0.1\ \text{m} \cdot 0.01\ \text{m} = 0.001\ \text{m}^2$. Therefore, we get a volumetric flux of $\phi = U \cdot A = 0.4\ \frac{\text{m}}{\text{s}} \cdot 0.001\ \text{m}^2 = 0.0004\ \frac{\text{m}^3}{\text{s}}$. This flux has to pass the small cross section in the middle of the domain and thus, the velocity has to increase, while the pressure will drop (Bernoulli). The cross section area is given as $A_{\text{cross}} = 0.025\ \text{m} \cdot 0.01\ \text{m} = 0.00025\ \text{m}^2$. Hence, the velocity in the cross section increases to around $U_{\text{cross}} = 1.6\ \frac{\text{m}}{\text{s}}$. Based on the fact that the flow will be contracted in the cross section, the velocity will further increase. Considering the maximum velocity to be around $1.8\ \frac{\text{m}}{\text{s}}$, the resulting time-step, while using a cell distance of $\Delta x = 0.002$ m, can be evaluated by using equation (11.3):

$$\Delta t \leq \frac{1 \cdot 0.002\ \text{m}}{1.8\ \frac{\text{m}}{\text{s}}} = 0.00111\ \text{s}\ .$$

The generated mesh is a pure hexahedral mesh, and thus, no orthogonal correction scheme has to be applied in the `fvSchemes` file.

First, we will use the `pisoFoam` solver and the previously calculated time-step. After that, we will use the `pimpleFoam` solver and apply all keywords subsequently in order to illustrate its functionality and influence to the solution.

To make the investigation more sophisticated, we use the `Gauss linear` discretization scheme for the convective scheme. This scheme tends to produce non-physical results if the stability criterion is not satisfied or the mesh quality is pure.

For each numerical analysis, the residuals for the pressure and velocities are plotted against the time. Furthermore, the velocity profile is shown always at the simulation end time (1 s). However, if the simulation will crash, the results before the floating-point exception will be shown. The scaling for the velocity plot is set to min/max: 0 ms^{-1}/1.2 ms^{-1}.

11.4.3 Using the PISO algorithm

The analysis with the `PISO` algorithm is used as reference. As previously mentioned, the `pisoFoam` solver is used here. Furthermore, no turbulence model is used which lead to natural vortexes, and thus, lead to a high transient flow character. This will make the system more stiff and, from a numerical point of view, harder to converge. Lastly, based on the transient behavior, some interesting numerical phenomena are visible during the `PIMPLE` algorithm analysis.

After the calculation finishes, the simulation results that are shown in figure 11.2 and 11.3 can be generated. As already mentioned, a fixed time-step is used. Therefore, as the velocity changes during the simulation, the Courant number will change too, cf. (11.3).

During the simulation, a maximum Courant number of around 1.5 and a maximum velocity (magnitude) of around 2.8 ms^{-1} are achieved. Both quantities indicate that the time-step approximation done before works well. Although a larger Courant number than one is reached, the simulation runs stable. It is obvious that the time-step approximation based on equation (11.3) can only be used for simple geometries. Moreover, it is common practice to adjust the time-step automatically during the runtime rather than using a fixed time-step Δt.

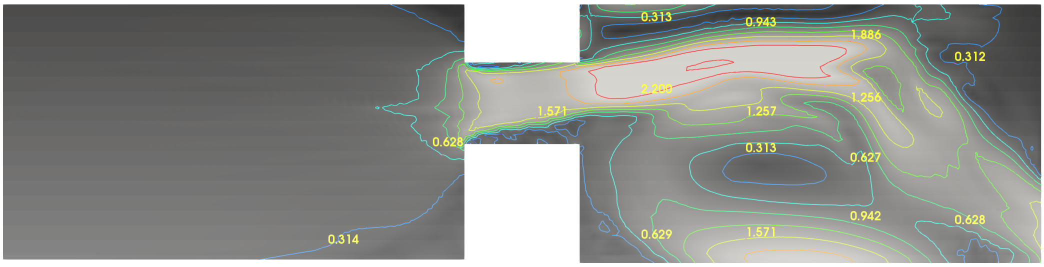


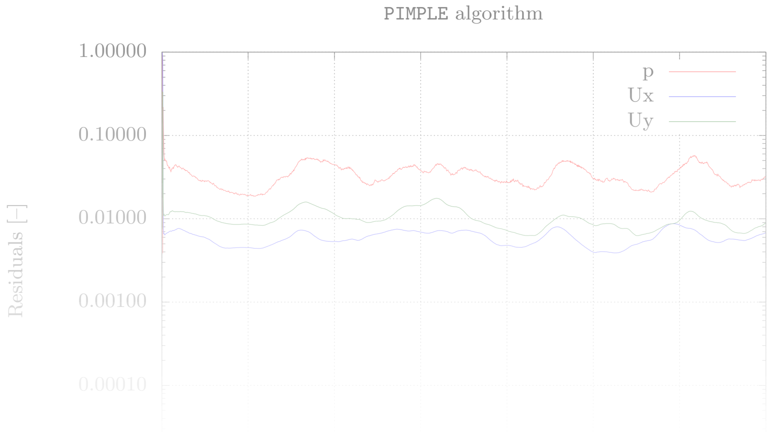
Figure 11.3: Velocity contours for the `pisoFoam` solver at $t = 1.4$ s; fixed time-step $\Delta t = 0.001$ s.

numerical instabilities in that region. Therefore, the `PISO` algorithm is close to the instability border; mainly related to the Gauss linear scheme.

11.4.4 The PIMPLE algorithm set-up to work in PISO mode

Using the existing case while changing the `fvSolution` file to enable the usage of the `pimpleFoam` solver in `PISO` mode, lead to identical numerical results.

For the calculation, the `PIMPLE` dictionary inside the `fvSolution` file is kept empty. Hence, the application control uses the default values, and thus, the `pimpleFoam` solver operates in `PISO` mode and is equal to the `pisoFoam` solver. The numerical results are presented in figure 11.4 and 11.5.



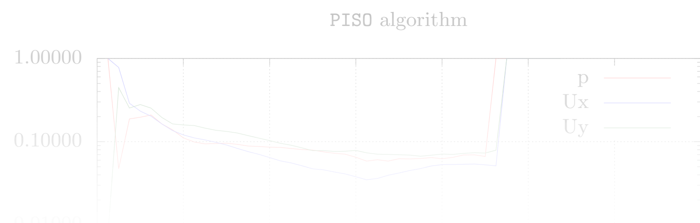
11.4.5 `PIMPLE` algorithm set-up to work in `PISO` mode with large Δt

The next investigation is similar to the previous one but now we increase the time-step to $\Delta t = 0.025$ s. While increasing the time-step, the end time of the simulation is within fewer time iterations. However, subsequently, the Courant number has to increase too, based on equation (11.3), and hence, the simulation should crash, if the stability is not satisfied anymore.

Running the case with the `pimpleFoam`, that is running in `PISO` mode while increasing the time-step, the algorithm crashes with a floating point exception after 1.175 s.

The residual plot illustrates that after the simulation time of 0.9 s is reached, the residuals of each quantity blow-up. The analysis of the flow results in critical velocities and numerical instabilities; cf. figure 11.6.

The velocity contours show high-velocity spots at the outlet and close to the upper wall. Furthermore, numerical problems occur additionally after the reduced cross-section at the upper and lower corner.



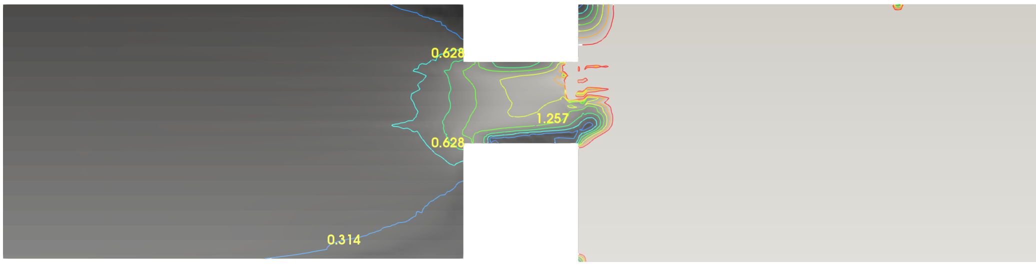


Figure 11.7: Velocity contours of the PIMPLE algorithm working in PISO mode at 1.125 s using an increased time-step $\Delta t = 0.025$ s.

Furthermore, figure 11.7 shows the time-step of the numerical instability initialization. The velocities increase until OpenFOAM® shows the nan value (total gray areas). Within the next two time steps, the instability accelerates, and the algorithm crashes. As the velocities are coupled to the pressure, all fields blow-up (as indicated in the residual plot).

11.4.6 The PIMPLE algorithm modified (adding outer corrections)

Up to now, the `PIMPLE` algorithm was used in `PISO` mode. Now the merged `PISO-SIMPLE` method is set-up step by step. Thus, the appropriate keywords inside the `PIMPLE` dictionary have to be adjusted and set. In the following investigation, the following dictionary set-up is used.

```
PIMPLE
{
    // Outer Loops (Pressure-Momentum Correction)
    nOuterCorrectors     5;
}
```

Listing 11.11: The control dictionary within the fvSolution file

The `nOuterCorrectors` will set the `nCorrPIMPLE_` variable to five and hence, the algorithm makes five (pressure-momentum correction loop). The outer correction includes 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 data. Finally, we correct the velocities and repeat the above steps until five outer corrections were performed. In order to get instabilities in that case, we have to set the simulation end-time to 2 s.

First of all, one may think that using the outer corrector loop will improve the numerical calculation and makes the algorithm more robust and stable. In fact the solver crashes as the residual and contour plot indicate.

In figure 11.9, the whole right part has already incredible large velocities which will move on to the left, until the solver crashes. However, in this case it can be derived that the crash

Figure 11.9: Velocity contours of the PIMPLE algorithm and `nOuterCorrectors = 5`.

SIMPLE method. Moreover, it is known that the SIMPLE algorithm is not stable (in most situations) without under-relaxation. The outer corrector loops can be considered as a SIMPLE loop, and thus, without under-relaxation, the procedure can get unstable; the outer correctors may accelerate the divergence of a solution. It is worth to mention that the solution between 1 s and 1.6 s seems to be stable without any indication of an upcoming crash. Nevertheless, as the stability criterion is not satisfied (Courant number larger than 30), a simple numerical instability may result in a domino-effect while the instability accelerates while the calculation errors increase to infty.

The difference with nOuterCorrectors

The difference using the outer loop correction is, that the algorithm recalculates the fluxes, pressure

However, it is worth to mention that we are not operating in a pure `SIMPLE` algorithm as the time derivative is included, which acts as a limiter which stabilizes the whole solution procedure.

As one can see, within one time-step, five `SIMPLE` iteration steps are performed. If one combines the highest peaks of the residual using a line, the result would be figure 11.8.

11.4.7 The PIMPLE algorithm with further modifications (adding inner corrections)

It is common practice to recalculate the pressure with the newly updated fluxes while keeping the old momentum matrix. The pressure correction is known as the `PISO` correction. The pressure loop might help to stabilize the algorithm (if more than one iteration is done) as under-relaxation is performed to the pressure field (except for the last iteration). To activate the pressure correction loop, the **`nCorrectors`** keyword has to be set. The following `PIMPLE` dictionary is used for the subsequent analysis.

```
PIMPLE
{
    // Outer Loops (Pressure-Momentum Correction)
    nOuterCorrectors     5;

    // Inner Loops (Pressure Correction)
    nCorrectors          2;
}
```

Listing 11.12: The control dictionary within the fvSolution file

As before, instead of getting a more stable algorithm, the solver already crashes in the third time step. Therefore, the analysis of the common residual plot will not give detailed information. Nevertheless, it is possible to evaluate the residuals within the the outer and inner iterations.

Recall: For one time-step, we calculate five outer loops and within one outer loop, we perform two inner loops.

consists of 5 outer loops. The residual log-scale was removed to show that the residuals of the velocities are close to 1.

It can be observed that within the first time-step, the solution tends already to diverge. This trend is continued within the second time-step until the solver crashes in the third time-step evaluation. The velocity profile is not presented here, as the velocity quantity values are already within a range of $1e24$ ms^{-1}. Thus, the plot is just white.

A further increase in the number of performed outer loops would speed-up the divergence of the solution. This is related to the fact that within the first time-step, the solution tends already to diverge. Therefore, applying more outer iterations will destabilize the solution as it increases the calculation of the wrong solution.

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 until now. The first step for the correct usage of the algorithm is discussed in the next section.

11.4.8 The `PIMPLE` algorithm with under-relaxation

To make the `PIMPLE` algorithm stable and robust, one has to think about the `SIMPLE` method in more detail (outer correction loop). As already mentioned in section 11.1, the method is not consistent (missing pressure term) and hence, the user has to apply the under-relaxation technique.

For the next investigation, the outer loops are increased to 100 and a field relaxation for the pressure and a matrix relaxation for the momentum is set.

In the code snipped, one can see that two relaxation factors are set. The first one is used for all outer iterations. The relaxation factors marked with `Final` is applied for the last outer correction loop.

There are many discussions about the correct value of the *Final* relaxation factor. Here, the question arises if we are allowed to under-relax the final inner/outer loop iteration. Fact is: If we under-relax the final inner/outer loop, we might lose some information, and we are not consistent. However, if the linear system of equations reaches already a small tolerance criterion, an under-relaxation of the final loop can be performed without problems.

It is worth to mention, that OpenFOAM® has the following behavior:

- If no relaxation factor is set, the default value of one is used for all outer/inner iterations.
- If only the relaxation factor for p and/or $\mathbf{U}$ is specified without setting the *Final* one explicitly, the final relaxation factors are set to one.

Starting the numerical analysis using the relaxation factors given in the code snippet above, lead to the results shown in figure 11.12, 11.13 and 11.14.

First of all, for each time-step 100 outer corrections and within one outer loop, two inner corrections are performed. Thus, for one time-step, 100 momentum-pressure coupling and 200 pressure correction calculations are completed.

Analyzing the time-depended residual plots, we get similar graphs compared to the `PISO` algorithm, but now there is one essential difference. Within one time-step, a lot more momentum-pressure iterations are performed, including under-relaxation, cf. figure 11.14. Therefore, it is

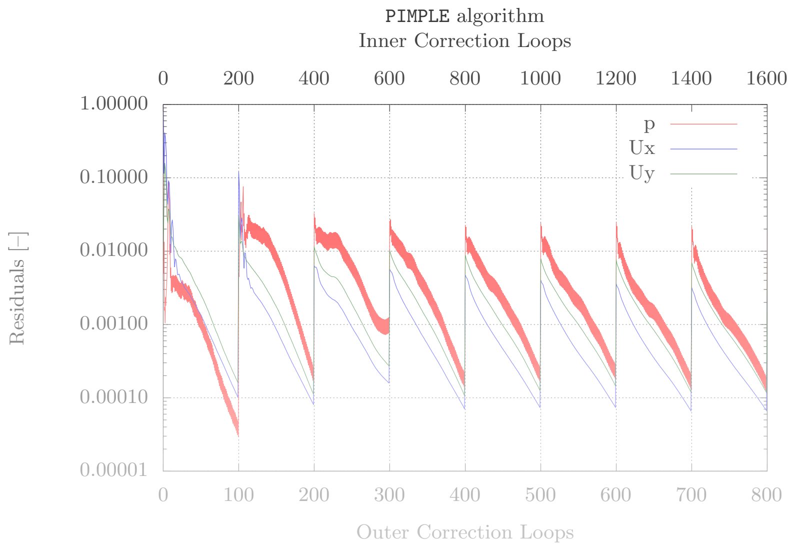


Figure 11.13: Residuals of the iterations of the inner and outer correction loops; `nOuterCorrectors = 100` and `nCorrectors = 2`. Each 100 outer correction represents one time-step.

algorithm in that mode allows us, in the presented case, to get Courant numbers larger than 30

- Using a `Final` relaxation factor smaller than one

If the flow pattern is highly transient, large Courant number can also lead to wrong solutions as important and essential transient information might be ignored (not resolved within the time-step), which influences the flow pattern significantly.

In the presented case, it is related to the last mentioned hypothesis. Based on the large time-step, the natural vortexes are not resolved which lead to a different flow pattern.

If the current case is modified to restrict the maximum Courant number to Co = 5, the result presented in figure 11.15 is achieved. The new calculation is now comparable to the `PISO` calculation; cf. figure 11.3.

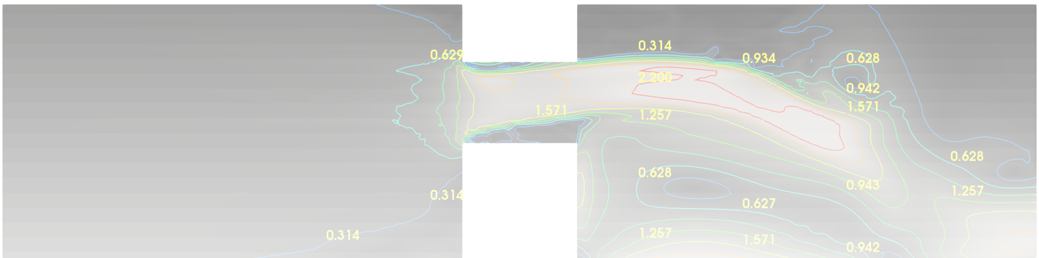


Figure 11.15: Velocity contours; `nOuterCorrectors = 100` and `nCorrectors = 2`; additional residual control added and Courant number controlled Co = 5

11.4.9 The PIMPLE algorithm speed-up

During the latest investigations, the numerical effort increased drastically. While performing 100 outer correctors is not sufficient, especially if the reached tolerance is already to accurate, the algorithm should stop performing the outer iterations after a defined tolerance criterion is reached. Thus, while using the `PIMPLE` algorithm in `PIMPLE` mode, the residual control set-up is essential to limit the computational costs.

While setting a residual control for the outer corrections, OpenFOAM® will check the initial residuals of each quantity that is specified inside the residual control. After all, quantities fulfill the residual control, the outer loop will be stopped, and the new time-step calculation starts. This approach reduces the calculation time massively while ensuring the accuracy set by the user.

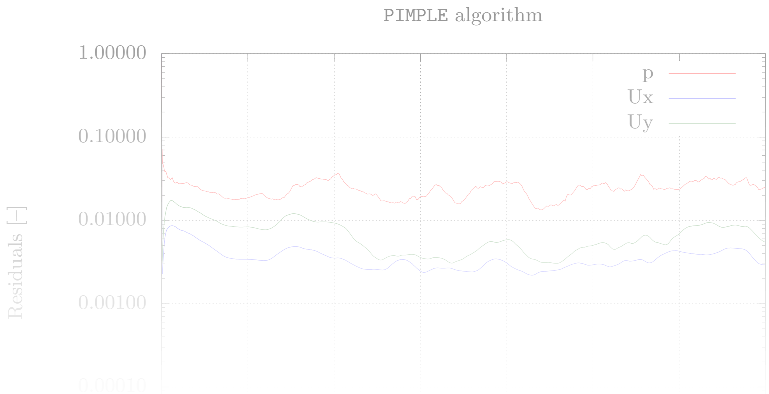
The next listing shows the correct usage of the `PIMPLE` algorithm. Of course, one can also add other switches that control the algorithm, such as the `momentumPredictor` or `consistent`.

```
PIMPLE
{
    // Outer Loops (Pressure-Momentum Correction)
    nOuterCorrectors     100;

    // Inner Loops (Pressure Correction)
    nCorrectors          2;

    // Residual control for the outer loops
    outerCorrectorResidualControl
    {
        p
```

The new numerical data are presented in the next figures. It is worth to mention that the Courant number is kept to be lower than Co ≤ 4. Comparing the computational costs from the prior calculation (without residual control) to the latest one it follows:

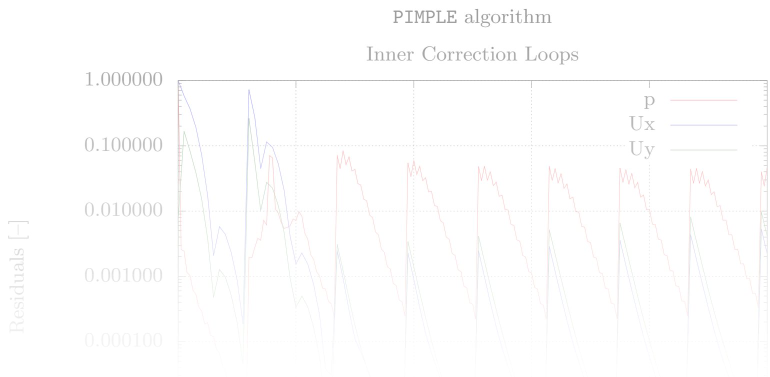
- Calculation time without residual control $\longrightarrow$ 714 s ,
- Calculation time with residual control $\longrightarrow$ 225 s .

It is obvious that using the residual control reduces the numerical costs. The residual plot is presented in figure 11.16.



The influence of the residual control cannot be analyzed within the typical residual plot. Therefore, the inner and outer corrections are presented for the first time steps. The main difference here is that we do not perform all 100 outer loops per time-step anymore. As figure 11.18 illustrates, after 100 outer loops, already eight time-steps were calculated. Analyzing the plots in more detail (especially the pressure), it seems that the `PIMPLE` algorithm does not stop at $1e^{-3}$ for the pressure. This is related to the principal how OpenFOAM® stops the outer loop.

OpenFOAM® analysis the `initial residual` of the field. If all fields fulfill the residual control, the `Final` outer loop is performed using the `Final` relaxation factors. Therefore, even though the fields satisfy the residual control, a further outer loop is performed.



11.4.10 The PIMPLE algorithm conclusion

As demonstrated in the prior sections, the PIMPLE algorithm can be used to increase the time-step and go beyond the stability criterion $\mathrm{Co} \leq 1$. 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 too many advantages. For more complex geometries, skewed, non-orthogonal meshes that include different kinds of cells and intricate flow patterns or if one has to solve stiff systems, the PIMPLE algorithm provides more advantages (compared to the PISO algorithm), and can stabilize the simulation.

In advance, the PIMPLE algorithm has to be applied correctly, and the time-step cannot be set individually large. For the numerical investigation one should know the time-scale of the problem. However, commonly the PIMPLE algorithm is used by limiting the Courant number while adopting the time-step automatically.

Furthermore, different algorithm settings lead to different solutions, if the numerics are not considered probably, e.g. setting the Courant number to 30.

Additionally, one should keep in mind that OpenFOAM® is continuously updated. Therefore, the given results might be different or not reproducible with other version.

11.5 The PIMPLE algorithm flowchart

In the following flowchart, one can see how the PIMPLE algorithm is working within the OpenFOAM® version 7.x. Once the idea of the algorithm is understood, the whole pressure-momentum coupling

Chapter 12

The relaxation methods

Relaxation methods are used for steady-state simulations or if one uses a large time-step and the PIMPLE algorithm. The problem in such cases is that the solution might be not stable because the quantities change to much. E.g. we do not take care about numerical limits like the Courant number. To stabilize or even get a solution, we need to use relaxation methods. There are two different ways to do that known as field relaxation and matrix relaxation.

12.1 Field relaxation

The field relaxation is simple to understand and limits the new values of the field as follows:

the matrix, each row has to be at least diagonal equal and one of the rows has to be diagonal dominant. What does that mean?

- Diagonal equality is given if the diagonal element is equal to the sum of the magnitude of the off-diagonals,
- Diagonal dominant is given if the diagonal element is larger than the sum of the magnitude of the neighbor elements.

The main difference between matrix and field relaxation is based on the fact that we do not cut off too much information, if ever - it is based on the method of how we relax.

Relaxing the matrix means to make it more diagonal dominant, and therefore, the linear solvers are happier and will find the solution easier and faster. However, there are some things that we have to keep in mind.

Relaxing the matrix means actually to divide all diagonal elements by the relaxation factor α. Based on the fact that α is between $0 < \alpha < 1$, the diagonal elements increase its value. If we would only change the values of the diagonal elements, the whole procedure is not consistent. To be consistent, we have to add the changes to the source vector $\mathbf{b}$ in order to keep consistency. The whole procedure makes a better matrix system for the linear solvers but on the other hand, makes it more explicit. The result is that we need more outer corrections to get all terms converged. Important is the pre-requirement for the matrix relaxation which introduces inconsistency.

The implementation is given in the `fvMatrix` class.

Chapter 13

OpenFOAM® tutorials

For those who want to learn OpenFOAM® and search for special tutorials, you can checkout https://Holzmann-cfd.de. The site offers a wide range of free material 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®,
- Summary of different voluntary projects.

Furthermore, you can find different libraries and publications.

For OpenFOAM® beginners

If you are not familiar with OpenFOAM®, it is recommended to check the following website, wiki.openfoam.com. Here, one finds a new wiki page that shares a lot of information. The work is based on voluntary OpenFOAM® experts listed in the contributers list. It is highly recommended to check the three weeks series in which you will learn a lot of OpenFOAM® and CFD related stuff. Furthermore, the User-Guide of OpenFOAM® should be read.

Chapter 14

Appendix

14.1 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 9.8 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)

$$\overline{u_x'\rho\frac{\partial(\bar{u}_x + u_x')}{\partial t} + u_y'\rho\frac{\partial(\bar{u}_z + u_z')}{\partial t}} = \cancel{\overline{u_x'\rho\frac{\partial\bar{u}_x}{\partial t}}} + \overline{u_x'\rho\frac{\partial u_x'}{\partial t}} + \cancel{\overline{u_y'\rho\frac{\partial\bar{u}_z}{\partial t}}} + \overline{u_y'\rho\frac{\partial u_z'}{\partial t}} = \overline{u_x'\rho\frac{\partial u_x'}{\partial t}} + \overline{u_y'\rho\frac{\partial u_z'}{\partial t}} \ . \tag{14.1}$$

b)

$$\overline{u_x'\rho\frac{\partial(\bar{u}_y + u_y')}{\partial t} + u_y'\rho\frac{\partial(\bar{u}_x + u_x')}{\partial t}} = \cancel{\overline{u_x'\rho\frac{\partial\bar{u}_y}{\partial t}}} + \overline{u_x'\rho\frac{\partial u_y'}{\partial t}} + \cancel{\overline{u_y'\rho\frac{\partial\bar{u}_x}{\partial t}}} + \overline{u_y'\rho\frac{\partial u_x'}{\partial t}} = \overline{u_x'\rho\frac{\partial u_y'}{\partial t}} + \overline{u_y'\rho\frac{\partial u_x'}{\partial t}} \ . \tag{14.2}$$

c)

$$\overline{u_x'\rho\frac{\partial(\bar{u}_z + u_z')}{\partial t} + u_y'\rho\frac{\partial(\bar{u}_y + u_y')}{\partial t}} = \cancel{\overline{u_x'\rho\frac{\partial\bar{u}_z}{\partial t}}} + \overline{u_x'\rho\frac{\partial u_z'}{\partial t}} + \cancel{\overline{u_y'\rho\frac{\partial\bar{u}_y}{\partial t}}} + \overline{u_y'\rho\frac{\partial u_y'}{\partial t}} = \overline{u_x'\rho\frac{\partial u_z'}{\partial t}} + \overline{u_y'\rho\frac{\partial u_y'}{\partial t}} \ . \tag{14.3}$$

d)

$$\overline{u_y'\rho\frac{\partial(\bar{u}_x + u_x')}{\partial t} + u_z'\rho\frac{\partial(\bar{u}_z + u_z')}{\partial t}} = \cancel{\overline{u_y'\rho\frac{\partial\bar{u}_x}{\partial t}}} + \overline{u_y'\rho\frac{\partial u_x'}{\partial t}} + \cancel{\overline{u_z'\rho\frac{\partial\bar{u}_z}{\partial t}}} + \overline{u_z'\rho\frac{\partial u_z'}{\partial t}} = \overline{u_y'\rho\frac{\partial u_x'}{\partial t}} + \overline{u_z'\rho\frac{\partial u_z'}{\partial t}} \ . \tag{14.4}$$

e)

$$\overline{u_y'\rho\frac{\partial(\bar{u}_y + u_y')}{\partial t} + u_z'\rho\frac{\partial(\bar{u}_x + u_x')}{\partial t}} = \cancel{\overline{u_y'\rho\frac{\partial\bar{u}_y}{\partial t}}} + \overline{u_y'\rho\frac{\partial u_y'}{\partial t}} + \cancel{\overline{u_z'\rho\frac{\partial\bar{u}_x}{\partial t}}} + \overline{u_z'\rho\frac{\partial u_x'}{\partial t}} = \overline{u_y'\rho\frac{\partial u_y'}{\partial t}} + \overline{u_z'\rho\frac{\partial u_x'}{\partial t}} \ . \tag{14.5}$$

f)

$$\overline{u_y'\rho\frac{\partial(\bar{u}_z + u_z')}{\partial t} + u_z'\rho\frac{\partial(\bar{u}_y + u_y')}{\partial t}} = \cancel{\overline{u_y'\rho\frac{\partial\bar{u}_z}{\partial t}}} + \overline{u_y'\rho\frac{\partial u_z'}{\partial t}} + \cancel{\overline{u_z'\rho\frac{\partial\bar{u}_y}{\partial t}}} + \overline{u_z'\rho\frac{\partial u_y'}{\partial t}} = \overline{u_y'\rho\frac{\partial u_z'}{\partial t}} + \overline{u_z'\rho\frac{\partial u_y'}{\partial t}} \ . \tag{14.6}$$

g)

$$\overline{u'_z\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}+u'_x\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}}$$
$$=\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}+\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}=\overline{u'_z\rho\frac{\partial u'_x}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_z}{\partial t}}\ . \tag{14.7}$$

h)

$$\overline{u'_z\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}+u'_x\rho\frac{\partial(\bar{u}_x+u'_x)}{\partial t}}$$
$$=\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}+\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_x}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}=\overline{u'_z\rho\frac{\partial u'_y}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_x}{\partial t}}\ . \tag{14.8}$$

i)

$$\overline{u'_z\rho\frac{\partial(\bar{u}_z+u'_z)}{\partial t}+u'_x\rho\frac{\partial(\bar{u}_y+u'_y)}{\partial t}}$$
$$=\cancel{\overline{u'_z\rho\frac{\partial\bar{u}_z}{\partial t}}}+\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}+\cancel{\overline{u'_x\rho\frac{\partial\bar{u}_y}{\partial t}}}+\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}=\overline{u'_z\rho\frac{\partial u'_z}{\partial t}}+\overline{u'_x\rho\frac{\partial u'_y}{\partial t}}\ . \tag{14.9}$$

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:

$$\rho\overline{\frac{\partial u'_x u'_x}{\partial t}}+\rho\overline{\frac{\partial u'_y u'_y}{\partial t}}+\rho\overline{\frac{\partial u'_z u'_z}{\partial t}}+\rho\overline{\frac{\partial u'_x u'_y}{\partial t}}+\rho\overline{\frac{\partial u'_x u'_z}{\partial t}}$$
$$+\rho\overline{\frac{\partial u'_y u'_z}{\partial t}}+\rho\overline{\frac{\partial u'_y u'_x}{\partial t}}+\rho\overline{\frac{\partial u'_z u'_y}{\partial t}}+\rho\overline{\frac{\partial u'_z u'_x}{\partial t}}\ .$$

The above expression can be written in one single term by using the Einsteins summation convention:

$$\boxed{\rho\frac{\partial\overline{u'_j u'_i}}{\partial t}=\frac{\partial\rho\overline{u'_j u'_i}}{\partial t}}\ . \tag{14.10}$$

The Convective Term

First we will focus on the convective term of part a)

$$
\begin{aligned}
&\overline{u'_x\left[\rho\left(\bar{u}_x+u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_x+u'_x\right)+\rho\left(\bar{u}_y+u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_x+u'_x\right)+\rho\left(\bar{u}_z+u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_x+u'_x\right)\right]}\\
&+\overline{u'_y\left[\rho\left(\bar{u}_x+u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_z+u'_z\right)+\rho\left(\bar{u}_y+u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_z+u'_z\right)+\rho\left(\bar{u}_z+u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_z+u'_z\right)\right]}
\end{aligned}
$$

$$
\begin{aligned}
&=\overline{\left(u'_x\rho\bar{u}_x+u'_x\rho u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_x+u'_x\right)+\left(u'_x\rho\bar{u}_y+u'_x\rho u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_x+u'_x\right)}\\
&\qquad+\overline{\left(u'_x\rho\bar{u}_z+u'_x\rho u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_x+u'_x\right)}\\
&+\overline{\left(u'_y\rho\bar{u}_x+u'_y\rho u'_x\right)\frac{\partial}{\partial x}\left(\bar{u}_z+u'_z\right)+\left(u'_y\rho\bar{u}_y+u'_y\rho u'_y\right)\frac{\partial}{\partial y}\left(\bar{u}_z+u'_z\right)}\\
&\qquad+\overline{\left(u'_y\rho\bar{u}_z+u'_y\rho u'_z\right)\frac{\partial}{\partial z}\left(\bar{u}_z+u'_z\right)}
\end{aligned}
$$

$$
\begin{aligned}
&=\cancel{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}\bar{u}_x}}+\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}+\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}+\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}+\cancel{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}\bar{u}_x}}+\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}\\
&+\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}+\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}+\cancel{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}\bar{u}_x}}+\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}+\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}+\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}\\
&+\cancel{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}\bar{u}_z}}+\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}+\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}+\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}+\cancel{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}\bar{u}_z}}+\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}\\
&+\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}+\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}+\cancel{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}\bar{u}_z}}+\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}+\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}+\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}
\end{aligned}
$$

$$
\begin{aligned}
=\;&\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{1}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{2}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}}_{3}+\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{4}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{5}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}}_{6}\\
+\;&\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{7}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{8}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}}_{9}+\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{10}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{11}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}}_{12}\\
+\;&\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{13}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{14}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}}_{15}+\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{16}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{17}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}}_{18}\;.
\end{aligned}
\tag{14.11}
$$

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 (14.11) 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)

$$
\begin{aligned}
&\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{73}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{74}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_y}}_{75}+\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{76}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{77}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_y}}_{78}\\
+&\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{79}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{80}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_y}}_{81}+\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{82}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{83}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_x}}_{84}\\
+&\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{85}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{86}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_x}}_{87}+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{88}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{89}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_x}}_{90}\ ,
\end{aligned}
$$

f)

$$
\begin{aligned}
&\underbrace{\overline{u'_y\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{91}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{92}+\underbrace{\overline{u'_y\rho u'_x\frac{\partial}{\partial x}u'_z}}_{93}+\underbrace{\overline{u'_y\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{94}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{95}+\underbrace{\overline{u'_y\rho u'_y\frac{\partial}{\partial y}u'_z}}_{96}\\
+&\underbrace{\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{97}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{98}+\underbrace{\overline{u'_y\rho u'_z\frac{\partial}{\partial z}u'_z}}_{99}+\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{100}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{101}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_y}}_{102}\\
+&\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{103}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{104}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_y}}_{105}+\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{106}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{107}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_y}}_{108}\ ,
\end{aligned}
$$

g)

$$
\begin{aligned}
=&\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{109}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{110}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_x}}_{111}+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{112}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{113}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_x}}_{114}\\
+&\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{115}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{116}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_x}}_{117}+\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{118}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{119}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_z}}_{120}\\
+&\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{121}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{122}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_z}}_{123}+\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{124}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{125}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_z}}_{126}\ ,
\end{aligned}
$$

h)

$$
\begin{aligned}
&\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{127}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{128}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_y}}_{129}+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{130}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{131}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_y}}_{132}\\
+&\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{133}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{134}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_y}}_{135}+\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_x}}_{136}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_x}}_{137}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_x}}_{138}\\
+&\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_x}}_{139}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_x}}_{140}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_x}}_{141}+\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}}_{142}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_x}}_{143}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_x}}_{144}\ ,
\end{aligned}
$$

i)

$$
\begin{aligned}
&\underbrace{\overline{u'_z\rho\bar{u}_x\frac{\partial}{\partial x}u'_z}}_{145}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}\bar{u}_z}}_{146}+\underbrace{\overline{u'_z\rho u'_x\frac{\partial}{\partial x}u'_z}}_{147}+\underbrace{\overline{u'_z\rho\bar{u}_y\frac{\partial}{\partial y}u'_z}}_{148}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}\bar{u}_z}}_{149}+\underbrace{\overline{u'_z\rho u'_y\frac{\partial}{\partial y}u'_z}}_{150}\\
+&\underbrace{\overline{u'_z\rho\bar{u}_z\frac{\partial}{\partial z}u'_z}}_{151}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}\bar{u}_z}}_{152}+\underbrace{\overline{u'_z\rho u'_z\frac{\partial}{\partial z}u'_z}}_{153}+\underbrace{\overline{u'_x\rho\bar{u}_x\frac{\partial}{\partial x}u'_y}}_{154}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}\bar{u}_y}}_{155}+\underbrace{\overline{u'_x\rho u'_x\frac{\partial}{\partial x}u'_y}}_{156}\\
+&\underbrace{\overline{u'_x\rho\bar{u}_y\frac{\partial}{\partial y}u'_y}}_{157}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}\bar{u}_y}}_{158}+\underbrace{\overline{u'_x\rho u'_y\frac{\partial}{\partial y}u'_y}}_{159}+\underbrace{\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}}_{160}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}\bar{u}_y}}_{161}+\underbrace{\overline{u'_x\rho u'_z\frac{\partial}{\partial z}u'_y}}_{162}\ .
\end{aligned}
$$

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:

$$
\overline{\rho \frac{\partial}{\partial x} u'_y u'_z u'_x} = \overline{\rho u'_z u'_x \frac{\partial}{\partial x} u'_y} + \overline{\rho u'_y u'_x \frac{\partial}{\partial x} u'_z} + \overline{\rho u'_y u'_z \frac{\partial}{\partial x} u'_x} \ . \tag{14.12}
$$

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:

$$
\overline{\rho u'_i u'_j \cancel{\frac{\partial}{\partial x_k} u'_k}} = 0 \ . \tag{14.13}
$$

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:

$$
\boxed{\overline{\rho\frac{\partial}{\partial x_k}u'_i u'_j u'_k} = \frac{\partial}{\partial x_k}\rho\overline{u'_i u'_j u'_k}} \ . \tag{14.14}
$$

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:

$$\boxed{\overline{\rho u'_i u'_k\frac{\partial}{\partial x_k}\bar{u}_j}=\rho\overline{u'_i u'_k}\frac{\partial}{\partial x_k}\bar{u}_j}\ . \tag{14.15}$$

and the second 27 terms could be written as:

$$\boxed{\overline{\rho u'_j u'_k\frac{\partial}{\partial x_k}\bar{u}_i}=\rho\overline{u'_j u'_k}\frac{\partial}{\partial x_k}\bar{u}_i}\ . \tag{14.16}$$

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:

$$\overline{\rho\bar{u}_z\frac{\partial}{\partial z}u'_xu'_y}=\overline{u'_y\rho\bar{u}_z\frac{\partial}{\partial z}u'_x}+\overline{u'_x\rho\bar{u}_z\frac{\partial}{\partial z}u'_y}\;. \tag{14.17}$$

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:

$$\boxed{\overline{\rho\bar{u}_k\frac{\partial}{\partial x_k}u'_iu'_j}=\bar{u}_k\frac{\partial}{\partial x_k}\rho\overline{u'_iu'_j}}\;. \tag{14.18}$$

Now, the convective term is manipulated and derived. Combining all terms, we end up with:

$$\boxed{\bar{u}_k\frac{\partial\rho\overline{u'_iu'_j}}{\partial x_k}+\rho\overline{u'_ju'_k}\frac{\partial\bar{u}_i}{\partial x_k}+\rho\overline{u'_iu'_k}\frac{\partial\bar{u}_j}{\partial x_k}+\frac{\partial}{\partial x_k}\rho\overline{u'_iu'_ju'_k}}\;. \tag{14.19}$$

The Shear-Rate Term

a)

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

$$= -\cancel{\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial\bar{u}_x}{\partial x}\right)}}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\cancel{\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial\bar{u}_x}{\partial x}\right)}}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\cancel{\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial\bar{u}_x}{\partial y}\right)}}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_x}{\partial y}\right)}$$
$$-\cancel{\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial\bar{u}_y}{\partial x}\right)}}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\cancel{\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial\bar{u}_x}{\partial z}\right)}}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\cancel{\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial\bar{u}_z}{\partial x}\right)}}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial x}\right)}$$
$$-\cancel{\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial\bar{u}_z}{\partial x}\right)}}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}-\cancel{\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial\bar{u}_x}{\partial z}\right)}}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\cancel{\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial\bar{u}_z}{\partial y}\right)}}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_z}{\partial y}\right)}$$
$$-\cancel{\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial\bar{u}_y}{\partial z}\right)}}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\cancel{\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial\bar{u}_z}{\partial z}\right)}}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}-\cancel{\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial\bar{u}_z}{\partial z}\right)}}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}$$

$$= -\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial x}\right)}$$
$$-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_z}{\partial y}\right)}-\overline{u'_y\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}-\overline{u'_y\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}$$

For the parts b) to i) we will just write the final terms:

b)

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

c)

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

d)

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

e)

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

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)

$$\begin{aligned}
&-\underbrace{\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}}_{**}-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial y}\right)}\\
&-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial x}\right)}
\end{aligned}$$

i)

$$\begin{aligned}
&-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_z}{\partial y}\right)}-\overline{u'_z\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}-\overline{u'_z\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial z}\right)}\\
&-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}-\overline{u'_x\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_x}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial y}\left(\mu\frac{\partial u'_y}{\partial y}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_y}{\partial z}\right)}-\overline{u'_x\frac{\partial}{\partial z}\left(\mu\frac{\partial u'_z}{\partial y}\right)}
\end{aligned}$$

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:

$$-\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}-\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}\,. \tag{14.20}$$

This two terms cannot be merged, hence we need two terms in addition:

$$\begin{aligned}
&-\overbrace{\overline{u'_y\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_z}{\partial x}\right)}}^{1}\underbrace{-\overbrace{\overline{\mu\frac{\partial u'_y}{\partial x}\frac{\partial u'_z}{\partial x}}}^{2}+\overbrace{\overline{\mu\frac{\partial u'_y}{\partial x}\frac{\partial u'_z}{\partial x}}}^{3}}_{\text{added}}-\overbrace{\overline{u'_z\frac{\partial}{\partial x}\left(\mu\frac{\partial u'_y}{\partial x}\right)}}^{4}\\
&\qquad\underbrace{-\overbrace{\overline{\mu\frac{\partial u'_z}{\partial x}\frac{\partial u'_y}{\partial x}}}^{5}+\overbrace{\overline{\mu\frac{\partial u'_z}{\partial x}\frac{\partial u'_y}{\partial x}}}^{6}}_{\text{added}}\,.
\end{aligned} \tag{14.21}$$

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:

$$-\underbrace{\overline{\frac{\partial}{\partial x} u'_y \left(\mu \frac{\partial u'_z}{\partial x}\right)}}_{7} - \underbrace{\overline{\frac{\partial}{\partial x} u'_z \left(\mu \frac{\partial u'_y}{\partial x}\right)}}_{8} + 2\mu \overline{\frac{\partial u'_z}{\partial x} \frac{\partial u'_y}{\partial x}} \ . \tag{14.22}$$

Now we see that the term 7 and 8 can be combined using the product rule again. Finally we end up with:

$$-\overline{\frac{\partial}{\partial x} \left(\mu \frac{\partial u'_y u'_z}{\partial x}\right)} + 2\mu \overline{\frac{\partial u'_z}{\partial x} \frac{\partial u'_y}{\partial x}} \ . \tag{14.23}$$

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:

$$\boxed{-\overline{\frac{\partial}{\partial x_k} \left(\mu \frac{\partial u'_i u'_j}{\partial x_k}\right)} = -\frac{\partial}{\partial x_k} \left(\mu \frac{\partial \overline{u'_i u'_j}}{\partial x_k}\right)} \ . \tag{14.24}$$

The new introduced terms (due to the trick), can be expressed as:

$$\boxed{\overline{2\mu \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k}} = 2\mu \overline{\frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k}}} \ . \tag{14.25}$$

Summing up, the shear-rate terms can be written as:

$$\boxed{-\frac{\partial}{\partial x_k} \left(\mu \frac{\partial \overline{u'_i u'_j}}{\partial x_k}\right) + 2\mu \overline{\frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k}}} \ . \tag{14.26}$$

The pressure derivative

a)

$$\overline{u'_x \frac{\partial (\bar{p} + p')}{\partial x}} + \overline{u'_y \frac{\partial (\bar{p} + p')}{\partial z}} = \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_x \frac{\partial p'}{\partial x}} + \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_y \frac{\partial p'}{\partial z}} = \overline{u'_x \frac{\partial p'}{\partial x}} + \overline{u'_y \frac{\partial p'}{\partial z}} \ , \tag{14.27}$$

b)

$$\overline{u'_x \frac{\partial (\bar{p} + p')}{\partial y}} + \overline{u'_y \frac{\partial (\bar{p} + p')}{\partial x}} = \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_x \frac{\partial p'}{\partial y}} + \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_y \frac{\partial p'}{\partial x}} = \overline{u'_x \frac{\partial p'}{\partial y}} + \overline{u'_y \frac{\partial p'}{\partial x}} \ , \tag{14.28}$$

c)

$$\overline{u'_x \frac{\partial (\bar{p} + p')}{\partial z}} + \overline{u'_y \frac{\partial (\bar{p} + p')}{\partial y}} = \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_x \frac{\partial p'}{\partial z}} + \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_y \frac{\partial p'}{\partial y}} = \overline{u'_x \frac{\partial p'}{\partial z}} + \overline{u'_y \frac{\partial p'}{\partial y}} \ , \tag{14.29}$$

d)

$$\overline{u'_y \frac{\partial (\bar{p} + p')}{\partial x}} + \overline{u'_z \frac{\partial (\bar{p} + p')}{\partial z}} = \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_y \frac{\partial p'}{\partial x}} + \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_z \frac{\partial p'}{\partial z}} = \overline{u'_y \frac{\partial p'}{\partial x}} + \overline{u'_z \frac{\partial p'}{\partial z}} \ , \tag{14.30}$$

e)

$$\overline{u'_y \frac{\partial (\bar{p} + p')}{\partial y}} + \overline{u'_z \frac{\partial (\bar{p} + p')}{\partial x}} = \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_y \frac{\partial p'}{\partial y}} + \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_z \frac{\partial p'}{\partial x}} = \overline{u'_y \frac{\partial p'}{\partial y}} + \overline{u'_z \frac{\partial p'}{\partial x}} \ , \tag{14.31}$$

f)

$$\overline{u'_y \frac{\partial(\bar{p}+p')}{\partial z}} + \overline{u'_z \frac{\partial(\bar{p}+p')}{\partial y}} = \cancel{\overline{u'_y \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_y \frac{\partial p'}{\partial z}} + \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_z \frac{\partial p'}{\partial y}} = \overline{u'_y \frac{\partial p'}{\partial z}} + \overline{u'_z \frac{\partial p'}{\partial y}} \ , \tag{14.32}$$

g)

$$\overline{u'_z \frac{\partial(\bar{p}+p')}{\partial x}} + \overline{u'_x \frac{\partial(\bar{p}+p')}{\partial z}} = \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_z \frac{\partial p'}{\partial x}} + \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_x \frac{\partial p'}{\partial z}} = \overline{u'_z \frac{\partial p'}{\partial x}} + \overline{u'_x \frac{\partial p'}{\partial z}} \ , \tag{14.33}$$

h)

$$\overline{u'_z \frac{\partial(\bar{p}+p')}{\partial y}} + \overline{u'_x \frac{\partial(\bar{p}+p')}{\partial x}} = \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_z \frac{\partial p'}{\partial y}} + \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial x}}} + \overline{u'_x \frac{\partial p'}{\partial x}} = \overline{u'_z \frac{\partial p'}{\partial y}} + \overline{u'_x \frac{\partial p'}{\partial x}} \ , \tag{14.34}$$

i)

$$\overline{u'_z \frac{\partial(\bar{p}+p')}{\partial z}} + \overline{u'_x \frac{\partial(\bar{p}+p')}{\partial y}} = \cancel{\overline{u'_z \frac{\partial \bar{p}}{\partial z}}} + \overline{u'_z \frac{\partial p'}{\partial z}} + \cancel{\overline{u'_x \frac{\partial \bar{p}}{\partial y}}} + \overline{u'_x \frac{\partial p'}{\partial y}} = \overline{u'_z \frac{\partial p'}{\partial z}} + \overline{u'_x \frac{\partial p'}{\partial y}} \ . \tag{14.35}$$

Summing up and sorting:

$$\begin{aligned}
&\overline{u'_x \frac{\partial p'}{\partial x}} + \overline{u'_x \frac{\partial p'}{\partial y}} + \overline{u'_x \frac{\partial p'}{\partial z}} + \overline{u'_y \frac{\partial p'}{\partial x}} + \overline{u'_y \frac{\partial p'}{\partial y}} + \overline{u'_y \frac{\partial p'}{\partial z}} + \overline{u'_z \frac{\partial p'}{\partial x}} + \overline{u'_z \frac{\partial p'}{\partial y}} + \overline{u'_z \frac{\partial p'}{\partial z}} \\
&+ \overline{u'_x \frac{\partial p'}{\partial x}} + \overline{u'_y \frac{\partial p'}{\partial x}} + \overline{u'_z \frac{\partial p'}{\partial x}} + \overline{u'_x \frac{\partial p'}{\partial y}} + \overline{u'_y \frac{\partial p'}{\partial y}} + \overline{u'_z \frac{\partial p'}{\partial y}} + \overline{u'_x \frac{\partial p'}{\partial z}} + \overline{u'_y \frac{\partial p'}{\partial z}} + \overline{u'_z \frac{\partial p'}{\partial z}} \ .
\end{aligned} \tag{14.36}$$

leads to the following expression:

$$\overline{u'_i \frac{\partial p'}{\partial x_j}} + \overline{u'_j \frac{\partial p'}{\partial x_i}} \ . \tag{14.37}$$

Finally we use the product rule,

$$\overline{u'_i \frac{\partial p'}{\partial x_j}} = -\overline{p' \frac{\partial u'_i}{\partial x_j}} + \overline{\frac{\partial p' u'_i}{\partial x_j}} \ , \tag{14.38}$$

$$\overline{u'_j \frac{\partial p'}{\partial x_i}} = -\overline{p' \frac{\partial u'_j}{\partial x_i}} + \overline{\frac{\partial p' u'_j}{\partial x_i}} \ , \tag{14.39}$$

$$-\overline{p' \frac{\partial u'_i}{\partial x_j}} + \overline{\frac{\partial p' u'_i}{\partial x_j}} - \overline{p' \frac{\partial u'_j}{\partial x_i}} + \overline{\frac{\partial p' u'_j}{\partial x_i}} \ . \tag{14.40}$$

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:

$$\boxed{-\overline{p' \left[\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}\right]} + \frac{\partial}{\partial x_k}\left[\overline{p' u'_j}\delta_{ik} + \overline{p' u'_i}\delta_{jk}\right]} \ . \tag{14.41}$$

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:

$$\begin{aligned}
&\frac{\partial \rho \overline{u'_j u'_i}}{\partial t} + \bar{u}_k \frac{\partial \rho \overline{u'_i u'_j}}{\partial x_k} + \rho \overline{u'_j u'_k} \frac{\partial \bar{u}_i}{\partial x_k} + \rho \overline{u'_i u'_k} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k} \rho \overline{u'_i u'_j u'_k} - \frac{\partial}{\partial x_k}\left(\mu \frac{\partial \overline{u'_i u'_j}}{\partial x_k}\right) \\
&\qquad + 2\mu \overline{\frac{\partial u'_i}{\partial x_k}\frac{\partial u'_j}{\partial x_k}} - \overline{p' \left[\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}\right]} + \frac{\partial}{\partial x_k}\left[\overline{p' u'_j}\delta_{ik} + \overline{p' u'_i}\delta_{jk}\right] = 0 \ .
\end{aligned} \tag{14.42}$$

Applying the definition of the Reynolds-Stress tensor (9.40), 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:

$$\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k} = -\bar{\sigma}_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \bar{\sigma}_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k}\right) + \underbrace{2\mu \overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_j'}{\partial x_k}}}_{\epsilon_{ij}}$$
$$- \underbrace{\overline{p'\left[\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right]}}_{\Pi_{ij}} + \underbrace{\frac{\partial}{\partial x_k}\rho\overline{u_i'u_j'u_k'} + \frac{\partial}{\partial x_k}\left[\overline{p'u_j'}\delta_{ik} + \overline{p'u_i'}\delta_{jk}\right]}_{\frac{\partial}{\partial x_k}\underbrace{\left(\rho\overline{u_i'u_j'u_k'} + \overline{p'u_j'}\delta_{ik} + \overline{p'u_i'}\delta_{jk}\right)}_{C_{ijk}}} \;. \tag{14.43}$$

Finally, we can write the common Reynolds-Stress equation:

$$\boxed{\frac{\partial \bar{\sigma}_{\mathrm{t}_{ji}}}{\partial t} + \bar{u}_k \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k} = -\bar{\sigma}_{\mathrm{t}_{jk}} \frac{\partial \bar{u}_i}{\partial x_k} - \bar{\sigma}_{\mathrm{t}_{ik}} \frac{\partial \bar{u}_j}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\nu \frac{\partial \bar{\sigma}_{\mathrm{t}_{ij}}}{\partial x_k} + C_{ijk}\right) + \epsilon_{ij} - \Pi_{ij}} \;. \tag{14.44}$$

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About the Author

Hello everybody, my name is Tobias Holzmann from Germany (Bavaria). Since 2009 I am working in the field of numerical simulations. During my studies at the Fachhochschule Augsburg, I decided to write my Bachelor thesis in the field of heat transfer while using numerical tools such as OpenFOAM® while validating the results against measurements. During my Master's study, my personal focus was set on all topics, including numerical simulations. During that time, I started to compare the quantitative results of different phenomena using ANSYS® CFX and OpenFOAM®. I finished my master's study by writing a thesis about biomass combustion using the flamelet model in OpenFOAM®. After that, I started to publish my knowledge in the field of numerical simulations and OpenFOAM® on my private website to support other people. In 2014 I started my Ph.D. at the Montanuniversität Leoben investigating into local heat treatments of aluminium alloys. The main topics were thermal stress analysis, the material calculation for local heat treatment in 3D, and optimization. The result was a newly developed framework that handles all these three topics automatically.

After I started my Ph.D. in 2014, I decided to investigate more into the field of numerical mathematics, matrix algebra, derivations, and advanced programming in C++. Additionally, I always tried to go beyond the limits of OpenFOAM® while publishing script based tutorials on my personal website. In 2017 I became an official contributor to the OpenFOAM Foundation toolbox, mainly in the conjugated heat transfer section. However, I am also active in the bug-tracking system as well as generating feature patches.

Additionally, I am a moderator in the German OpenFOAM® forum, namely cad.de as well as in the known cfd-online.com forum. All my recent projects and investigations can be found on my website https://holzmann-cfd.de.

Keep Foaming...
Dr. mont. Tobias Holzmann