RADIATIVE HEAT TRANSFER, FAVRE-AVERAGING AND TURBULENCE CLOSURE MODELS FOR COMBUSTION APPLICATIONS

J.B. de Vos

Delft/Rijswijk, The Netherlands

May 1983
Delft University of Technology
Faculty of Aerospace Engineering
Delft

Prins Maurits Laboratory
Organization for Applied Scientific Research TNO
Rijswijk

Report LR - 383
Report PML 1983 - 114

SFCC Publication no. 6

RADIATIVE HEAT TRANSFER, FAVRE-AVERAGING AND TURBULENCE CLOSURE MODELS FOR COMBUSTION APPLICATIONS

J.B. de Vos

Delft/Rijswijk, The Netherlands

May 1983
SUMMARY

This report continues the theoretical description of the flow through a Solid Fuel Combustion Chamber. As mentioned in [1] this report pays attention to radiative heat transfer, 'Favre'-averaging of the conservation equations and to choosing a turbulence closure model which will be used in a computational model describing the flow through a SFCC. At the end of the report a list of further investigations is given.

This report is part of the investigation of the flow and combustion in a solid fuel combustion chamber. The investigation is supported by the Netherlands Foundation for Technical Research, S.T.W. under projectnumber DLR 11.0120, and the Project Office for Energy Research, PBE, and is carried out by the Department of Aerospace Engineering of the Delft University of Technology and the Prins Maurits Laboratory of the Netherlands Organization for Applied Scientific Research (TNO).
<table>
<thead>
<tr>
<th>CONTENTS</th>
<th>page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Summary</td>
<td>1</td>
</tr>
<tr>
<td>Contents</td>
<td>2</td>
</tr>
<tr>
<td>Nomenclature</td>
<td>3</td>
</tr>
<tr>
<td>1. Introduction</td>
<td>6</td>
</tr>
<tr>
<td>2. Radiative Heat Transfers</td>
<td></td>
</tr>
<tr>
<td>2.1 Blackbody Radiation</td>
<td>7</td>
</tr>
<tr>
<td>2.2 Non-luminous Radiation</td>
<td>11</td>
</tr>
<tr>
<td>2.3 Radiation from Solid Particles</td>
<td>17</td>
</tr>
<tr>
<td>3. Favre-Averaging</td>
<td></td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>19</td>
</tr>
<tr>
<td>3.2 The Favre-Averaged Equation for Conservation of Mass</td>
<td>23</td>
</tr>
<tr>
<td>3.3 The Favre-Averaged Momentum Equation</td>
<td>23</td>
</tr>
<tr>
<td>3.4 The Favre-Averaged Energy Equation</td>
<td>25</td>
</tr>
<tr>
<td>3.5 The Favre-Averaged Equation for Conservation of Angular Momentum</td>
<td>27</td>
</tr>
<tr>
<td>3.6 The Favre-Averaged Equation for Conservation of Species</td>
<td>28</td>
</tr>
<tr>
<td>3.7 Compilation of the Favre-Averaged Conservation Equations</td>
<td>28</td>
</tr>
<tr>
<td>4. Turbulence Modelling</td>
<td></td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>31</td>
</tr>
<tr>
<td>4.2 The ( k - \varepsilon ) model</td>
<td>34</td>
</tr>
<tr>
<td>4.3 Reynolds-Stress Closure Models</td>
<td>42</td>
</tr>
<tr>
<td>4.4 Algebraic Stress/Flux Models</td>
<td>49</td>
</tr>
<tr>
<td>4.5 Multiple-Scale Turbulence Modelling</td>
<td>52</td>
</tr>
<tr>
<td>4.6 Selecting a Turbulence Closure Model for use in a Computational Model</td>
<td>55</td>
</tr>
<tr>
<td>5. Future Investigations</td>
<td>56</td>
</tr>
<tr>
<td>6. References</td>
<td>57</td>
</tr>
<tr>
<td>Appendix A: The Derivation of the Equation for Entropy Balance</td>
<td>60</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
</tr>
<tr>
<td>A</td>
<td>Constant in the Van Driest hypothesis</td>
</tr>
<tr>
<td>a</td>
<td>constant</td>
</tr>
<tr>
<td>B</td>
<td>equilibrium specific intensity</td>
</tr>
<tr>
<td>( b_f )</td>
<td>specific angular momentum</td>
</tr>
<tr>
<td>c</td>
<td>velocity of light</td>
</tr>
<tr>
<td>( C_s )</td>
<td>empirical constant in the equation for the flame emissivity (Chapter 2)</td>
</tr>
<tr>
<td>( C_{L} )</td>
<td>empirical constant in the equation for the turbulent viscosity</td>
</tr>
<tr>
<td>( C_{e1}, C_{e2} )</td>
<td>empirical constants in the equation for the dissipation rate</td>
</tr>
<tr>
<td>( C_s )</td>
<td>empirical constant (Chapter 4)</td>
</tr>
<tr>
<td>( C_{1c}, C_{2c}, C_{3c}, C_{4c} )</td>
<td>empirical constants in the equation for the Reynolds stresses</td>
</tr>
<tr>
<td>( C_{\phi 1}, C_{\phi 2} )</td>
<td>the scalar fluxes</td>
</tr>
<tr>
<td>( C_{\lambda c}, C_{\lambda 2c} )</td>
<td>the fluctuating velocity</td>
</tr>
<tr>
<td>( C_e )</td>
<td>the dissipation rate</td>
</tr>
<tr>
<td>( C_{p1}, C_{p2} )</td>
<td>the dissipation from the production region</td>
</tr>
<tr>
<td>( C_{T1}, C_{T2} )</td>
<td>empirical constants in the equation for the dissipation from the transfer region</td>
</tr>
<tr>
<td>( \text{D}_j )</td>
<td>Diffusion vector</td>
</tr>
<tr>
<td>E</td>
<td>Energy</td>
</tr>
<tr>
<td>( f_R )</td>
<td>photon distribution function</td>
</tr>
<tr>
<td>f</td>
<td>probability density function</td>
</tr>
<tr>
<td>g</td>
<td>mass-weighted probability density function</td>
</tr>
<tr>
<td>g</td>
<td>acceleration due to gravity = 9.80665 m/sec²</td>
</tr>
<tr>
<td>h</td>
<td>Planck's constant = 6.626196 × 10⁻³⁴ Jsec</td>
</tr>
<tr>
<td>h</td>
<td>specific enthalpy</td>
</tr>
<tr>
<td>I</td>
<td>specific intensity</td>
</tr>
<tr>
<td>j</td>
<td>mass-emission coefficient</td>
</tr>
<tr>
<td>k</td>
<td>Boltzmann's constant = 1.3805 × 10⁻²³ eV/molecule K</td>
</tr>
<tr>
<td>k</td>
<td>turbulent kinetic energy</td>
</tr>
<tr>
<td>L</td>
<td>path length</td>
</tr>
<tr>
<td>( \lambda_i )</td>
<td>unit vector</td>
</tr>
<tr>
<td>( \lambda_m )</td>
<td>mixing length</td>
</tr>
<tr>
<td>M</td>
<td>molar mass</td>
</tr>
<tr>
<td>n</td>
<td>number density</td>
</tr>
<tr>
<td>( n_{ij} )</td>
<td>component of the stress tensor defined in Eq. (3.30)</td>
</tr>
</tbody>
</table>
\( P_{ij} \) - pressure tensor
\( P_{ij} \) - production rate of Reynolds stresses (Chapter 4)
\( P_k \) - production rate of turbulent kinetic energy
\( p \) - hydrostatic pressure
\( Q \) - heat
\( q_i \) - heat transfer vector
\( R_o \) - coordinate
\( r \) - position vector
\( S \) - Source term
\( S \) - entropy
\( s \) - specific entropy
\( T \) - temperature
\( t \) - time
\( U \) - internal energy
\( u \) - specific internal energy
\( u^R \) - radiative energy density
\( V \) - volume
\( V_{Si} \) - Diffusion velocity vector
\( V_i \) - velocity vector
\( X \) - molar fraction
\( Y \) - mass fraction
\( \alpha \) - volumetric absorption coefficient (Chapter 2)
\( \alpha \) - arbitrary property (Chapter 3)
\( \alpha_p \) - Planck emission mean absorption coefficient
\( \alpha_R \) - Rosseland mean absorption coefficient
\( \delta \) - flamezone thickness
\( \varepsilon \) - emissivity
\( \varepsilon \) - turbulent dissipation function
\( k_u \) - mass absorption coefficient
\( \kappa \) - Von Kármán constant
\( \lambda \) - wave length
\( \lambda \) - coefficient of thermal conductivity
\( \mu \) - dynamic viscosity
\( \nu \) - frequency
\( \nu \) - kinematic viscosity
\( \rho \) - density
\( \sigma \) - Stefan-Boltzmann constant = \( 5.6697 \times 10^{-8} \text{ W/(m}^2 \text{ K}^4) \)
\( \sigma \) - Prandtl number
\( \tau_\nu \) - optical depth
\( \tau_{ij} \) - stress tensor
\( \phi \) - scalar flux
\( \Omega \) - solid angle
\( \omega \) - mass rate of production

subscripts
\( f \) - flame
\( i \) - coordinate direction
\( j \) - coordinate direction
\( k \) - coordinate direction
\( p \) - production region
\( s \) - soot (Chapter 2)
\( s \) - species
\( T \) - transfer region
\( t \) - turbulent
\( w \) - wall
\( \lambda \) - wave length
\( \nu \) - frequency

superscripts
\( (\cdot) R \) - radiation
\( (\cdot) ' \) - fluctuation from conventional- or Reynolds-mean
\( (\cdot) " \) - fluctuation from mass-weighted- or Favre-mean
\( (\cdot)^* \) - mass-weighted or Favre-average mean
\( (\cdot) \) - conventional- or Reynolds-averaged mean
1. INTRODUCTION

In a solid fuel combustion chamber a solid fuel, for instance waste material or coal, is burnt with air. Because the combustion temperatures are high (from 2000 to 3000 K), the thermal efficiency is high and the combustion gases are relatively clean. Toxic molecules, such as for instance PCB's etc. are expected not to exist at these temperatures. The formation of nitrogen oxides may strongly be reduced by operating at or just below stoichiometric conditions. Solid fuel combustion chambers may find applications for waste combustion, energy conversion systems and aerospace propulsion. The scope of the SFCC-project is to obtain a thorough understanding of the flow and combustion processes in a SFCC, and to get a mathematical description of these processes. This report is a continuation of the theoretical foundations of this project. In this report, attention is given to radiative heat transfer, mass-weighted or Favre-averaging and turbulence modelling. In a SFCC radiative heat transfer is especially important when the regression rate of the solid fuel is studied because the regression rate depends on the total heat transfer to the solid fuel. In this report blackbody radiation, non-luminous radiation and radiation from solid particles are discussed; Mass-weighted or Favre-averaging of the conservation equations yields, in comparison with unweighted- or Reynolds-averaging, a set of equations which is simpler in form and has a clearer physical meaning. The mathematical and physical background of mass-weighted averaging is discussed in Chapter 3 and applied to the conservation equations derived in [1]. The Favre-averaged conservation equations have to be completed by a turbulence closure model in which terms involving turbulent fluctuations are modelled. The k - ε model, the Reynolds stress model, the algebraic stress model and the multiple scale model are discussed in Chapter 4. At the end of this chapter, the choice of the k - ε model to be applied in a computational model is explained.
2. RADIATIVE HEAT TRANSFER

According to the atomic model of Rutherford and Bohr, an atom consists of a nucleus with electrons moving in orbits around it. If a certain amount of energy \( E \) is supplied to an atom, an electron may jump to another orbit with a higher energy level at greater distance to the nucleus. After a short time this electron falls back to its original orbit (with a lower energy level) and emits the amount of energy \( E \) as radiative energy. This assumed to be, depending on the kind of problem under consideration, in the form of photons or electromagnetic waves. All bodies with a temperature above 0 K emit energy in the form of radiation, but the amount of transmitted radiative energy becomes significant only at high temperatures.

To include energy gained and lost by gases at high temperatures through radiative transfer, the equations for conservation of momentum and of energy must be extended with terms accounting for of radiation. In the first Section of this Chapter, attention is given to blackbody radiation. In the second Section the phenomenon of (non-luminous) gaseous radiation is studied. This leads to an expression for the radiative heat flux vector involving a multiple integral over the spectrum of radiation and over all space involving emission. This expression is simplified into two limiting cases. Radiation from soot or solid particles is studied in the last Section.

2.1. BLACKBODY RADIATION

A blackbody is defined as a substance that absorbs all incident radiation. On the other hand, the equilibrium radiant energy emitted from a blackbody per unit area and per unit time represents an upper limit for the emitted radiant energy from any substance at the same temperature as the blackbody [2]. Consider a volume, enclosed by walls which all have the same temperature. Assume that there is a small hole in one of the walls, and assume that the radiation field in the volume is in thermodynamic equilibrium with the walls, and that the radiation field is not disturbed by the hole. Such a volume is called a \('hohlräum', and all radiation that enters the volume will be absorbed [3]. Therefore, the small hole in the walls may be regarded as a blackbody. A radiation field consists of electromagnetic waves, and each wavelength is related to a certain amount of energy. If an object is placed in a radiation field, it will change his temperature. If this object is in thermodynamic equilibrium with the radiation field, it is said that the radiation field has the same temperature as the object. It can be shown that the radiation field inside a \('hohlräum' only depends on the temperature of the walls, and not on the gas inside the volume, or the composition of the walls (Kirchhoff's law) [4]. Because the walls enclosing the \('hohlräum' all have the same temperature and because the radiation fields inside the \('hohlräum' is in thermodynamic equilibrium with the walls, the radiation field will be isotropic. If the total radiative energy density of the radiation field is denoted by \( u^R (T) \), it can be shown that the radiative pressure equals [3] (Maxwell's equations)

\[
p^R = \frac{1}{3} u^R (T) .
\]  

(2.1)

From the second law of thermodynamics the following relation can be derived [4]

\[
\left( \frac{\partial u}{\partial V} \right)_T = T \left( \frac{\partial p}{\partial T} \right)_V - p.
\]  

(2.2)
This relation applied to the radiation field inside the 'hohlraum', where

\[ U = u^R(T) \nu, \]  

(2.3)

and \( p \) is given by Eq. (2.1) yields

\[ u^R(T) = \frac{T}{3} \frac{\partial}{\partial T} u^R(T) - \frac{u^R(T)}{3}, \]

or

\[ \frac{4}{3} u^R(T) = \frac{T}{3} \frac{3u^R(T)}{\partial T}. \]  

(2.4)

Integrating this equation yields

\[ u^R(T) = a T^4 \]  

(2.5)

where \( a \) is an integration constant. The total radiative energy density is thus proportional to \( T^4 \).

The relation between the energy of an electromagnetic wave and the wavelength is given by

\[ E_\nu = h \nu = h \frac{c}{\lambda} \]  

(2.6)

where \( \nu \) is the frequency, \( c \) the velocity of light and \( h \) Planck's constant. If \( u^R_\nu \) is defined as the radiative energy density with frequency \( \nu \) then it is possible to write \( u^R \) as

\[ u^R = \int_0^\infty u^R_\nu \, d\nu. \]  

(2.7)

If the 'hohlraum' is considered as a harmonic oscillator, one can find the energy distribution function \( u^R_\nu \) which is given by [4], [5].

\[ u^R_\nu = \frac{8\pi h \nu^3}{c^3} \frac{1}{e^{h \nu/kT} - 1}. \]  

(2.8)
Substitution of Eq. (2.8) into Eq. (2.7) and subsequent integrating yields

\[ u_R = \frac{8\pi^5 k^4}{15 \frac{h^3}{c^3}} T^4 = \frac{4}{c} \sigma T^4, \quad (2.9) \]

where the Stefan-Boltzmann constant \( \sigma \) is given by

\[ \sigma = \frac{2\pi^5 k^4}{15 \frac{h^3}{c^2}} = 5.6697 \times 10^{-8} \text{ W/m}^2\text{K}^4. \quad (2.10) \]

(Note that \( a = \frac{4\sigma}{c} \).)

The relations (2.8) and (2.9) are derived for an isotropic radiation field inside a volume which can be considered as a 'hohlräum'. Often one is not only interested in the radiation field inside a 'hohlräum' but also in the outward radiative energy flux through the hole into a solid angle. This hole may then be seen as a blackbody radiator. The relation between the volume energy distribution function \( u_0 \) and the energy distribution function for radiation into a solid angle is given by [2], [6]

\[ u_R^o = \frac{4\pi}{c} B_\nu. \quad (2.11) \]

\( B_\nu \) is often called the equilibrium specific intensity and may be written as

\[ B_\nu = \frac{2\nu^3}{c^2} \frac{1}{e^{\nu/kT} - 1}. \quad (2.12) \]

Integrating this equation over all frequencies and over a sphere yields the radiative energy flux into all directions in space [6]

\[ q_R = \sigma T^4. \quad (2.13) \]

Equation (2.12) is called the Planck-function, and Eq. (2.13) the Stefan-Boltzmann law. If the frequency \( \nu \) is small, Eq. (2.12) may be approximated by

\[ B_\nu = \frac{2 \nu^2 k T}{c^2}, \quad (2.14) \]

and this is the Rayleigh-Jeans radiation law. For high frequencies may Eq. (2.13) be approximated by
\[ B_\nu = \frac{2}{c^2} \nu^3 e^{-\nu/kT} , \quad (2.15) \]

and this is the Wien radiation law. This equation shows that if the frequency goes to infinity \( B_\nu \) becomes zero. From Eq. (2.14) it follows that \( B_\nu \) goes to zero as \( \nu \) goes to zero, and one may conclude that there will be a frequency (or wavelength) where \( B_\nu \) reaches a maximum. To find this maximum it is convenient to write Eq. (2.12) as function of the wavelength \( \lambda \). The radiative energy flux \( q^R \) is defined as

\[ q^R = \int_0^\infty B_\nu d\nu = \int_0^\infty B_\lambda d\lambda . \quad (2.16) \]

From this equation, it follows that

\[ B_\nu d\nu = - B_\lambda d\lambda , \quad (2.17) \]

and substituting the relation \( \nu = c/\lambda \) into this equation and Eq. (2.12) yields

\[ B_\lambda = \frac{2}{\lambda^5} \frac{1}{\frac{hc}{\lambda kT}-1} . \quad (2.18) \]

Define \( Y \) as

\[ Y = \frac{hc}{\lambda mkT} . \quad (2.19) \]

Differentiating Eq. (2.18) with respect to \( \lambda \) and setting the result equal to zero yields

\[ \lambda_m T = \frac{hc}{kY} = 2898 \times 10^{-6} \text{ m K} , \quad (2.20) \]

where \( Y \) equals [2]

\[ Y = 4.9651 \quad (2.21) \]

Equation (2.20) is called the Wien displacement law. Substitution of Eq. (2.20) into Eq. (2.18) yields
\[
B_{\lambda_{\text{max}}} = \frac{2 \pi c^2}{b^5} T^5 \frac{1}{\pi c/kb e^{-1}} = c T^5 ,
\]

where \( b = 2898 \times 10^{-6} \). The maximum energy density hence is proportional to \( T^5 \).

2.2. NON-LUMINOUS RADIATION

To simplify the description of radiative heat transfer in gases, it is common to make the following idealizations [7].

a) Neglect radiative stresses. Suppose the temperature of the gas is 3000 K. From Eq. (2.9) and (2.1) it follows that the radiative pressure in this case equals \( pR = 6.12 \times 10^{-2} \text{ N/m}^2 \), which is small in comparison with the hydrostatic pressure \( p = 10^5 \text{ N/m}^2 \).

b) Neglect the scattering of photons by gas molecules. With scattering is meant the change of propagation direction of photons through interaction with gas molecules where the energy of the photons remains the same. This effect can in most problems of gasdynamics be neglected [3] because the wavelengths of radiative energy in gases is in the order of \( 10^{-6} \text{ m} \), while the molecular size is in the order of \( 10^{-9} - 10^{-10} \text{ m} \). The probability that a photon is scattered by a molecule therefore is small.

c) assume local thermodynamic equilibrium.

![Diagram](image)

**Fig. 1: Radiation into a solid angle dΩ**

Consider Fig. 1, and consider a radiation field that is composed of \( n^R \) photons per unit volume. All photons have the same speed, the velocity of light \( c \), but have different propagation directions and different energies. The relation between the energy of a photon and the frequency is given by Eq. (2.6). The photon distribution function \( f^R \) is a function of time, position, direction of propagation and the energy or frequency of the photons. The number of photons having a direction of propagation into the solid angle \( d\Omega \) and with a frequency within the range \( \nu \) to \( \nu + d\nu \) is now given by

\[
n^R_{\nu d\Omega} = n^R f^R d\Omega d\nu .
\]

Integration this equation over all frequencies and over the whole space yields the number of photons per unit volume \( n^R \).
\[
\begin{align*}
\int_{\nu=0}^{\infty} \int_{\Omega=0}^{4\pi} n^R_{\nu\Omega} \, d\Omega d\nu &= \int_{\nu=0}^{\infty} \int_{\Omega=0}^{4\pi} n^R \, f^R \, d\Omega d\nu = \int_{\nu=0}^{\infty} \int_{\Omega=0}^{4\pi} f^R \, d\Omega d\nu \\
(2.24)
\end{align*}
\]

The photon velocity vector can be defined as \( c \hat{\nu}_i \) \((\nu = 1, 2, 3)\), where \( \hat{\nu}_i \) is a unit vector specifying the direction of propagation of the photons. The number flux of photons across a surface normal to the corresponding coordinate axis, \( Z \), is given by [2]

\[
Z = c \, l_j \, n^R \, f^R \, d\Omega d\nu \\
(2.25)
\]

Each photon has a momentum \( \frac{h \nu}{c} \, \hat{\nu}_i \) \((i = 1, 2, 3)\) and an energy \( h \nu \), and the momentumflux and radiative energy flux are respectively given by

\[
P^R_{\nu\Omega} = h \nu \, \nu l_i \, l_j \, n^R \, f^R \, d\Omega d\nu \\
(2.26)
\]

and

\[
q^R_{\nu\Omega} = c \, h \nu \, \nu l_j \, n^R \, f^R \, d\Omega d\nu \\
(2.27)
\]

The specific intensity \( I_\nu \) is now defined as:

\[
I_\nu = c \, h \nu \, n^R \, f^R \\
(2.28)
\]

and is related to the radiative energy flux with frequency \( \nu \). Integrating Eq. (2.27) over all frequencies and over the whole sphere gives the radiative heat flux vector:

\[
q_i^R = \int_{\nu=0}^{\infty} \int_{\Omega=0}^{4\pi} \nu l_i \, I_\nu \, d\Omega d\nu \\
(2.29)
\]

The radiative energy density with frequency \( \nu \) is given by

\[
\nu^R = \int_{\nu=0}^{4\pi} h \nu \, n^R \, f^R \, d\Omega = \frac{1}{c} \int_{\nu=0}^{4\pi} I_\nu \, d\Omega \\
(2.29)
\]
and the total radiative energy density yields

$$u^R = \frac{1}{c} \int \int \int I_{\nu} d\Omega d\nu = \frac{4}{c} \sigma T^4,$$

where use has been made of Eq. (2.9).

It is possible to write down an equation for radiative transfer which is a continuity equation for the number of photons having a direction into the solid angle $d\Omega$ and a frequency in the range $\nu$ to $\nu + d\nu$. The time rate of change of the number of photons in an arbitrary volume element $dV$ equals the transport of photons through the surfaces plus the net change of photons due to emission and absorption by the gas molecules (Scattering of photons is neglected). Thus

$$\frac{\partial}{\partial t} (n^R f^R d\Omega d\nu) dV = \frac{\partial}{\partial x_j} (n^R f^R d\Omega d\nu) dV + \left[ \frac{\partial}{\partial t} (n^R f^R d\Omega d\nu) \right]_{e,a} dV,$$

where $e, a$ denotes respectively emission and absorption. This equation may be written as

$$\frac{\partial}{\partial t} n^R f^R + c \frac{\partial}{\partial x_j} n^R f^R = \left[ \frac{\partial}{\partial t} n^R f^R \right]_{e,a}$$

or, after multiplication with $h\nu$ and substitution of Eq. (2.28)

$$\frac{1}{c} \frac{\partial}{\partial t} I_{\nu} + \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_j} I_{\nu} = \left[ \frac{\partial}{\partial t} h\nu n^R f^R \right]_{e,a}$$

The right hand side of this equation contains the contributions of emission and absorption of photons, and may be written as [3]

$$\left[ \frac{\partial}{\partial t} h\nu n^R f^R \right]_{e,a} = \rho (j_{\nu} - k_{\nu} I_{\nu})$$

where $j_{\nu}$ is the mass emission coefficient, $k_{\nu}$ the mass absorption coefficient and $\rho$ the gas density. The first term on the left hand side of Eq. (2.32) contains the velocity of light in the denominator, and is therefore, for almost all problems, in gas-dynamics negligibly small [3]. This term will be omitted. The assumption of local thermodynamic equilibrium means that the atomic and molecular states that participate in the emission and absorption are given by their equilibrium values. Equation (2.32) can now be written as
\[ \frac{\partial}{\partial x_j} I_{\nu} = \alpha_{\nu} (B_{\nu}(T) - I_{\nu}) \]  

(2.34)

The volumetric absorption coefficient \( \alpha_{\nu} \) is given by

\[ \alpha_{\nu} = \rho \kappa_{\nu} \left( 1 - e^{-\frac{-h\nu}{\kappa T}} \right) \]  

(2.35)

The equilibrium specific intensity \( B_{\nu} \) is given by Eq. (2.12). The derivation of Eq. (2.34) requires a rather detailed knowledge of the internal states of an atom or molecule and can be found in ref. 3. The right hand side of Eq. (2.34) now contains the sum of the following contributions

\[ \alpha_{\nu} B_{\nu} = \rho \kappa_{\nu} \left( 1 - e^{-\frac{h\nu}{\kappa T}} \right) B_{\nu} = \rho \kappa_{\nu} e^{-\frac{h\nu}{2c^2}} \]  

(2.36)

from spontaneous emission,

\[ \rho \kappa_{\nu} e^{-\frac{h\nu}{\kappa T}} I_{\nu} \]  

(2.37)

from induced emission (i.e. in the presence of radiation the emission in a given direction and of a given frequency can be increased above and beyond that resulting from spontaneous emission) and

\[ - \rho \kappa_{\nu} I_{\nu} \]  

(2.38)

from absorption. Comparing Eq. (2.36) with Eq. (2.15) shows that spontaneous emission mainly occurs at high frequencies, which is in agreement with the idealizations mentioned at the beginning of this section. Taking the divergence of Eq. (2.29), and subsequent substitution of Eq. (2.34) yields

\[ - \frac{\partial}{\partial x_i} q_i^R = \int_{\nu=0}^{\infty} \int_{\Omega=0}^{4\pi} \frac{1}{2} \frac{\partial}{\partial x_i} I_{\nu} \, d\Omega d\nu = \int_{\nu=0}^{\infty} \int_{\Omega=0}^{4\pi} \alpha_{\nu} (I_{\nu} - B_{\nu}) \, d\Omega d\nu \]  

(2.39)

This is the equation of radiative energy or heat transfer. Substitution of this expression into the equation for conservation of energy leads to a partial-integro-differential equation which is difficult to handle. There are two limiting cases which greatly simplify this equation. Before studying these two cases, it is useful to define a coordinate \( r \), which is measured from the point in question in the direction of propagation of the radiation. Equation (2.34) can be written as
\[
\frac{3}{4r} I_\nu = - \alpha_\nu (I_\nu - B_\nu) \quad .
\] (2.40)

The solution of this first order differential equation can be obtained with standard methods, and is [6]

\[
I_\nu (r) = I_\nu (0) \exp \left( - \int_0^r \alpha_\nu \, dr \right) + \int_0^r \alpha_\nu (r') B_\nu (r') \exp \left( - \int_{r'}^r \alpha_\nu \, dr' \right) \, dr' .
\] (2.41)

\(I_\nu (0)\) denotes the intensity at \(r = 0\). The meaning of this equation can be explained with the help of Figure 2. The first term on the right hand side of

![Figure 2: Emission and absorption of radiation](image)

this equation expresses the fact that the intensity decreases by absorption in its travel through the distance \(r\). This term goes to zero if \(r\) goes to infinity, which was to be expected. The second term describes the increase of the intensity by emission of radiative energy along the path length \(r\). The optical depth is now defined by

\[
\tau_\nu = \int_0^r \alpha_\nu \, dr \quad ,
\] (2.42)

and is a measure for the attenuation of the intensity by absorption. In the case of an optically thin medium, i.e.

\[
\tau_\nu \ll 1 \quad \text{or} \quad \alpha_\nu L \ll 1 \quad ,
\] (2.43)

Eq. (2.41) changes into

\[
I_\nu (r) = I_\nu (0) + \int_0^r \alpha_\nu B_\nu \, dr \quad .
\] (2.44)
In this case the emission processes dominate over the absorption processes, i.e.

\[ I_\nu \ll B_\nu \quad , \quad (2.45) \]

and Eq. (2.40) reduces to

\[ \frac{3}{2} \frac{\partial}{\partial r} I_\nu = \alpha_\nu B_\nu \quad . \quad (2.46) \]

In this special case, the equation of radiative heat transfer becomes

\[ - \frac{3}{2} \frac{\partial}{\partial x_1} q^R_i = - 4\pi \int_0^\infty \alpha_\nu B_\nu \, d\nu \equiv 4\alpha_p \sigma T^4 , \quad (2.47) \]

where the Planck- or emission mean absorption coefficient \( \alpha_p \) is given by

\[ \alpha_p = \frac{\pi}{\int_0^\infty \frac{\alpha_\nu B_\nu \, d\nu}{\int_0^\infty B_\nu \, d\nu}} = \pi \frac{\int_0^\infty \alpha_\nu B_\nu \, d\nu}{\sigma T^4} . \quad (2.48) \]

Use has been made of the assumption that the radiation field is homogeneous and isotropic, i.e. \( \alpha_\nu \) and \( B_\nu \) are independent of the direction. The characteristic mean free path is defined as \( \alpha^{-1} \), and in the case of an optically thin gas, it follows from Eq. (2.43) that \( \Lambda \) \( \mu \) is much larger than a characteristic dimension \( L \) of the region in question [3].

The limiting case of an optically thin medium may be applied to turbulent combustion free from solid particles [8]. This form of radiation is called (non-luminous) gaseous radiation. The opposite limiting case is the optically thick approximation,

\[ \tau_\nu \gg 1 \quad . \quad (2.49) \]

In this case the characteristic radiative mean free path is much smaller than the characteristic dimension of the flowfield. It can be shown [6] that in this case, the radiative heat transfer becomes diffuse, and the radiative heat transfer vector can be written as [3]

\[ q^R_i = - \frac{16}{3} \frac{\sigma}{\alpha_R} \frac{T^3}{\nabla T} \quad , \quad (2.50) \]
where

\[
\frac{1}{\alpha_R} = \int_0^\infty \frac{1}{\alpha_\nu} \frac{d B_\nu}{dT} \, d\nu. \tag{2.51}
\]

\(\alpha_R\) is called the Rosseland mean absorption coefficient, and \(\Lambda_R = \alpha_R^{-1}\) the Roseland mean free path for radiation.

The emission mean absorption coefficient \(\alpha_\nu\) and the Rosseland mean absorption coefficient \(\alpha_R\) both depend on the composition of the gas mixture. To calculate the total radiation from gases, one often uses Hottel's emissivity charts [9], which plot the emissivity of a homogeneous gas for each ray in terms of the gas-temperature and a partial-pressure path length product. These charts are available for each of the important radiating species, but, unfortunately, are not suitable for most situations involving mixtures of two or more radiating species. Other methods to calculate gaseous radiation are given in [10].

2.3. RADIATION FROM SOLID PARTICLES

In most practical combustion systems solid particles, for instance soot, which is formed in fuel rich portions of the flow, or (unburnt) fuel particles are the main emitters and absorbers of radiation. In most cases the soot is situated in the full-rich side of the flame-zone. These zones are highly non-homogeneous in temperature and species concentrations and therefore the soot distribution in these zones is difficult to determine. Usually one assumes that these flame-zones have homogeneous soot and species concentrations at some effective temperature.

As derived in Section (2.1) an ideal radiator emits energy according to the Stefan-Boltzmann law

\[
q^R = \sigma T^4. \tag{2.13}
\]

In most situations, however, a radiator emits less energy, and this is accounted for by the emittance \(\varepsilon\), \(\varepsilon < 1\), which is defined as the ratio of the actual radiative energy flux to the blackbody radiation heat flux from an ideal radiator at the same temperature. The radiative heat flux then equals

\[
q^R = \varepsilon \sigma T^4. \tag{2.52}
\]

If it is assumed that the soot is spectrally gray, i.e. the soot absorption coefficient \(\alpha_s\) is independent of the frequency \(\nu\) (or wavelength \(\lambda\)) it is possible to approximate the emissivity of the flamezone by [11]

\[
\varepsilon_s = 1 - e^{-\alpha_s L} = 1 - e^{-C_s X_s L}, \tag{2.53}
\]

where \(L\) is the path length, \(C_s\) is a dimensionless constant and \(X_s\) the soot con-
centration. According to ref. 10, the assumption of a spectrally gray gas may be applied to flames from most typical plastic fuels, for instance Polymethyl Methacrylate (PMMA), Polypropylene (PP) and Polystyrene (PS). The radiative heat flux from a cloud of soot in a flame zone with thickness $\delta$ can now be approximated by

$$q^R = \varepsilon_f \sigma T_f^4,$$  \hspace{1cm} (2.54)

where

$$\varepsilon_f = 1 - e^{-C_s X s \delta}.$$  \hspace{1cm} (2.55)

$T_f$ is the effective flame temperature.

The calculation of the radiative heat flux from a cloud of soot in a flame zone is especially important when the regression rate of a solid fuel is studied. The regression rate of a solid fuel depends on the total heat transfer to the surface. This heat transfer can be divided into two interdependent parts, convection and radiation. The convective heat transfer mainly depends on the airtemperature and the air mass flow rate per unit area. The net radiative heat flux to the fuel surface can be approximated by [11]

$$q^R = \varepsilon_w \sigma \varepsilon_f T_f^4 - \sigma \varepsilon_w T_w^4 = \sigma \varepsilon_w (\varepsilon_f T_f^4 - T_w^4),$$  \hspace{1cm} (2.56)

where $T_w$ is the wall temperature and $\varepsilon_w$ the emissivity and absorptivity of the wall. The first term on the left hand side of this equation denotes the radiative heat flux emitted from the flame zone and absorbed by the wall, the second term denotes the radiative energy emitted from the wall. It was assumed that the gases between the flame and the wall were optically thin, and that the gas phase radiation was negligible small in comparison with the soot radiation.
3. FAVRE-AVERAGING

In this Chapter, the technique of mass-weighted averaging developed by Favre [12] is treated and applied to the conservation equations derived in ref. 1. In the first Section the mathematical and physical background of Favre- or mass-weighted averaging is discussed and compared with conventional or unweighted averaging. In the following Sections the mass-weighted conservation equations will be derived.

In comparison with unweighted averaging Favre- or mass-weighted averaging of the conservation equations yields a set of equations which is simpler in form and has a clearer physical meaning.

3.1. INTRODUCTION

Many flows occurring in combustion processes are turbulent. This is an essential feature because turbulence affects the combustion processes by a better mixing of the combustion reactants in comparison with laminar combustion.

It is difficult to give a precise definition of turbulence [13], and in most situations one suffices with giving some features, such as randomness or irregularity, high Reynolds numbers, dissipative, diffusive, to describe it.

In turbulent flows properties, for instance the velocity, are fluctuating in space and time and are therefore, at a given point and time, not predictable.

To get a mathematical description of turbulent flows, one has to use statistical methods. It is assumed that the values of a property are distributed according to some definite probability laws $p(\nu)$ where $\nu$ represents the distribution of the property along all the possible values this property can take [14]. Such probability relations must be determined experimentally. From the statistical description of properties one can derive statistical averages of these properties, and these averages are usually used in the description of turbulent flows based on the transport equations. An arbitrary property $\alpha$ may be written as the sum of its statistical average and a fluctuating part. There are two methods to decompose $\alpha$ which differ in the definition of the statistical average. The first method is based on conventional- or Reynolds-averaging, the second on mass-weighted or Favre-averaging.

With Reynolds-averaging the local value of a property $\alpha$ equals

$$\alpha (x_i, t, \nu) = \overline{\alpha} (x_i, t) + \alpha' (x_i, t, \nu) , \quad (3.1)$$

where

$$\alpha (x_i, t) = \int_{-\infty}^{+\infty} (x_i, t, \nu) f(\nu) \, d\nu . \quad (3.2)$$

The function $f(\nu)$ is the probability density function of the property $\alpha$. This function is defined such that $f(\nu) \, d\nu$ is the probability that the value of $\alpha$ at a fixed point $(x_i, t)$ lies in the range from $\nu$ to $\nu + d\nu$. Because $\nu$ represents all possible values that $\alpha$ can take at a given point $(x_i, t)$ it is clear that
\[
\int_{-\infty}^{+\infty} f(\nu) \, d\nu = 1 \quad .
\]

(3.3)

With Favre-averaging $\alpha$ may be written as

\[
\alpha \left( x_i, \, t, \, \nu \right) = \overline{\alpha} \left( x_i, \, t \right) + \alpha'' \left( x_i, \, t, \, \nu \right) \quad ,
\]

(3.4)

where

\[
\overline{\alpha} = \frac{\alpha x}{\rho} = \int_{-\infty}^{+\infty} \alpha \left( x_i, \, t, \, \nu \right) g_\alpha \left( \nu \right) \, d\nu \quad ,
\]

(3.5)

and

\[
\int_{-\infty}^{+\infty} g_\alpha \left( \nu \right) \, d\nu = 1 \quad ,
\]

(3.6)

with $g_\alpha \left( \nu \right)$ the mass-weighted probability density function of $\alpha$. The bar (̅) and prime (') are related to Reynolds-averaging, the tilde (̃) and double prime ("") are related to Favre-averaging.

If the probability density functions $f(\nu)$ and $g_\alpha(\nu)$ are known, it is possible to calculate the statistical averages and to derive a mathematical description of turbulent flows.

The probability density distribution of a property may be found from experiments. The question which arises by measuring turbulent properties is: are we measuring unweighted or mass-weighted properties? This question itself is directly related to the question which method of averaging possesses the clearest physical meaning. Unfortunately, a clear answer to this question doesn't exist. For example, if one measures the temperature with a thermocouple which is infinitely small, one will detect the unweighted instantaneous temperature, but if one uses a thermocouple of finite size one measures some kind of density-weighted temperature [15]. It may be argued that some measurements, such as measuring the velocity by pitot probes may be closer to Favre-averaging than to conventional averaging [8]. In general, however, the type of quantity (weighted or unweighted) obtained by many experimental techniques is still open to question and the choice of the averaging method is, with regard to measurements, rather arbitrary. An important advantage of using Favre-averaging instead of Reynolds-averaging is that the conservation equations describing the flow take simpler forms because they don't contain terms involving density fluctuations correlations. In addition Favre-averaging provides equations describing the variation of the mean values of those quantities which are conserved and have therefore a clearer physical meaning than Reynolds-averaging.

From Eq. (3.2), (3.3), (3.5) and (3.6) the following relations can be derived
\[
\bar{\alpha} = \int_{-\infty}^{+\infty} \bar{\alpha} (x, t) f(v) \, dv = \bar{\alpha} \int_{-\infty}^{+\infty} f(v) \, dv = \bar{\alpha}, \quad (3.7)
\]

\[
\bar{\alpha} = \int_{-\infty}^{+\infty} \bar{\alpha} (x, t) g_\alpha (v) \, dv = \bar{\alpha} \int_{-\infty}^{+\infty} g_\alpha (v) \, dv = \bar{\alpha}, \quad (3.8)
\]

\[
\bar{\alpha} = \int_{-\infty}^{+\infty} \bar{\alpha} (x, t) g_\alpha (v) \, dv = \bar{\alpha} \int_{-\infty}^{+\infty} g_\alpha (v) \, dv = \bar{\alpha}, \quad (3.9)
\]

\[
\bar{\alpha} = \int_{-\infty}^{+\infty} \bar{\alpha} (x, t) f(v) \, dv = \bar{\alpha} \int_{-\infty}^{+\infty} f(v) \, dv = \bar{\alpha} \quad (3.10)
\]

From the Eqs. (3.1) through (3.10) the following relations can be obtained:

Reynolds-averaging of Eq. (3.1) yields

\[
\bar{\alpha} = \bar{\alpha} + \bar{\alpha}' = \bar{\alpha} + \bar{\alpha}' \Rightarrow \bar{\alpha}' = 0 \quad (3.11)
\]

Reynolds-averaging of Eq. (3.4) yields

\[
\bar{\alpha} = \bar{\alpha} + \bar{\alpha}'' = \bar{\alpha} + \bar{\alpha}'' \Rightarrow \bar{\alpha}'' = 0 \quad (3.12)
\]

From these equations it can be concluded that the Reynolds-average of the unweighted fluctuating part of a property equals zero, while the Reynolds-average of the weighted fluctuating part doesn't. This is caused by the difference in definition of the unweighted and weighted average. Favre-averaging of Eq. (3.1 and 3.4) gives a similar result,

\[
\bar{\alpha} = \bar{\alpha} + \bar{\alpha}' = \bar{\alpha} + \bar{\alpha}' \Rightarrow \bar{\alpha}' = 0 \quad (3.13)
\]

and

\[
\bar{\alpha} = \bar{\alpha} + \bar{\alpha}'' = \bar{\alpha} + \bar{\alpha}'' \Rightarrow \bar{\alpha}'' = 0 \quad (3.14)
\]

Multiplying Eq. (3.4) with the density \(\rho\), and subsequent Reynolds-averaging yields
\[ \rho \tilde{\alpha} = \rho \bar{\alpha} + \rho \tilde{\alpha}' = \bar{\alpha} + \rho \tilde{\alpha}' = 0 \]  

where use has been made of the definition of the mass-weighted mean, Eq. (3.5). The relation between the unweighted fluctuating component \( \alpha' \) and the mass-weighted fluctuating component \( \alpha'' \), which will be used in Chapter 4, can be derived as follows. Decomposition of the density \( \rho \) and the property \( \alpha \) into a unweighted mean and a fluctuating component, and substitution of these properties into the definition of the mass-weighted mean (Eq. (3.5)) yields

\[ \bar{\alpha} = \frac{\rho \tilde{\alpha}}{\rho} = \frac{\bar{\rho} \bar{\alpha} + \rho \tilde{\alpha} + \rho \tilde{\alpha}'}{\bar{\rho}} = \bar{\alpha} + \rho \frac{\tilde{\alpha}'}{\rho}, \]  

where use has been made of Eqs. (3.7) and (3.11). Comparison with Eq. (3.13) yields

\[ \bar{\alpha}' = \frac{\rho \tilde{\alpha}'}{\rho}, \]  

and comparison with Eq. (3.12) yields

\[ \bar{\alpha}'' = -\frac{\rho \tilde{\alpha}'}{\rho}. \]  

From Eq. (3.11) it follows that \( \bar{\alpha}' \) equals zero, and Eq. (3.18) can be written as

\[ \bar{\alpha}'' = -\frac{\rho \tilde{\alpha}'}{\rho} = -\frac{\bar{\rho} \tilde{\alpha}'}{\rho} = -\frac{\rho \tilde{\alpha}'}{\rho}. \]  

Decomposing \( \alpha \) into a mass-weighted component and fluctuating component and substitution of Eqs. (3.10) and (3.11) yields

\[ \bar{\alpha}'' = -\frac{\rho \tilde{\alpha} + \rho \tilde{\alpha}''}{\bar{\rho}} = -\frac{\rho \tilde{\alpha}'}{\rho} \Rightarrow \rho \bar{\alpha}'' = -\rho \tilde{\alpha}''. \]  

From Eqs. (3.18), (3.19) and (3.20) it can be concluded that

\[ \rho \tilde{\alpha}' = \rho \tilde{\alpha} = \rho \tilde{\alpha}'' \].
By means of these relations one obtains the Favre-averaged conservation equations in a simple way. Note that in flows with constant density Favre-averaging equals Reynolds-averaging, as follows from Eq. (3.16). When using Favre-averaging one usually separates the pressure into a conventional mean and a fluctuating part. This is done because the pressure has a measurable unweighted average [12]. The temperature $T$ is in the equation of state associated with the density $\rho$ and is therefore often decomposed in a mass-weighted average and a fluctuating part. In some cases however the conventional decomposition is used.

3.2. THE FAVRE-AVERAGED EQUATION FOR CONSERVATION OF MASS

The continuity equation or law for conservation of mass as derived in [1] states

$$\frac{\partial}{\partial t} (\rho) + \frac{\partial}{\partial x_j} (\rho v_j) = 0 \quad (3.22)$$

Favre decomposition of the velocity gives

$$\frac{\partial}{\partial t} (\tilde{\rho}) + \frac{\partial}{\partial x_j} (\tilde{\rho} \tilde{v}_j) = 0 \quad (3.23)$$

and averaging upon using (3.15) yields

$$\frac{\partial}{\partial t} (\bar{\rho}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{v}_j) = 0 \quad (3.24)$$

If Eq. (3.16) is substituted into this equation, one finds the conventional or Reynolds-averaged continuity equation:

$$\frac{\partial}{\partial t} (\bar{\rho}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{v}_j + \bar{\rho} \bar{v}_i \bar{v}_j) = 0 \quad (3.25)$$

Comparising Eq. (3.25) with Eq. (3.24) shows that the Favre-averaged continuity equation is simpler in form because it contains no terms involving density fluctuations.

3.3. THE FAVRE-AVERAGED MOMENTUM EQUATION

The momentum equation states [1]

$$\frac{\partial}{\partial t} (\rho v_i) + \frac{\partial}{\partial x_j} (\rho v_i v_j) = \rho g_i - \frac{\partial}{\partial x_j} p + \frac{\partial}{\partial x_j} \tau_{ij} \quad (3.26)$$
where the stress tensor \( \tau_{ij} \) is given by

\[
\tau_{ij} = \mu \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) - \frac{2}{3} \mu \left( \frac{\partial V_i}{\partial x_i} \right) \delta_{ij} .
\] (3.27)

The coefficient of bulk viscosity is assumed to be negligible small. The coefficient of viscosity \( \mu \) for a multicomponent gas mixture depends on the temperature, pressure and the composition of the mixture [1]. It is assumed that the coefficient of viscosity can be decomposed in an unweighted averaged part and a fluctuating component, i.e.

\[
\mu = \mu_0 + \mu'.
\] (3.28)

Furthermore, it is assumed that the stress tensor \( \tau_{ij} \), just like the pressure \( p \), can be decomposed into a conventional mean and a fluctuating part. Decomposition of Eq. (3.27) and subsequent averaging yields

\[
\bar{\tau}_{ij} = \bar{\mu} \bar{\eta}_{ij} + \mu \hat{\eta}_{ij} - \frac{2}{3} \left( \bar{\mu} \frac{\partial \bar{V}_i}{\partial x_i} + \bar{\mu} \frac{\partial \bar{V}_j}{\partial x_j} + \mu \frac{\partial \bar{V}_i}{\partial x_i} \right) \delta_{ij} ,
\] (3.29)

where

\[
\hat{\eta}_{ij} = \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} ,
\] (3.30)

and

\[
\hat{n}_{ij} = \frac{\partial V_i''}{\partial x_j} + \frac{\partial V_j''}{\partial x_i} .
\] (3.31)

Fave-decomposition of Eq. (3.26) yields

\[
\frac{\partial}{\partial t} \left( \bar{\rho} ( \bar{\bar{V}}_i + V_i'' ) \right) + \frac{\partial}{\partial x_j} \left( \bar{\rho} ( \bar{\bar{V}}_i + V_i'' ) ( \bar{\bar{V}}_j + V_j'' ) \right) = \bar{\rho} g_i - \frac{\partial}{\partial x_i} ( \bar{p} + \rho')
\]

\[
+ \frac{\partial}{\partial x_j} ( \bar{\tau}_{ij} + \bar{\tau}_{ij}' )
\] (3.32)
where

$$\tau_{ij} = \mu \delta_{ij} - \frac{2}{3} \mu \left( \frac{\partial V_i}{\partial x_j} \right) \delta_{ij} .$$

(3.33)

Averaging yields

$$\frac{3}{\partial t} (\bar{\rho} \bar{V}_i) + \frac{3}{\partial x_j} (\bar{\rho} \bar{V}_j \bar{V}_i + \bar{\rho} \bar{V}_i \bar{V}_j) = \bar{\rho} g_i - \frac{3}{\partial x_i} \bar{\rho} + \frac{3}{\partial x_j} \bar{\tau}_{ij} ,$$

(3.34)

where $\bar{\tau}_{ij}$ is given by Eq. (3.29)

3.4. THE FAVRE-AVERAGED ENERGY EQUATION

The energy equation may be written as [1]

$$\frac{3}{\partial t} \rho (h - \frac{p}{\rho} + \frac{1}{2} V_i V_i) + \frac{3}{\partial x_j} \rho V_j (h - \frac{p}{\rho} + \frac{1}{2} V_i V_i) = \rho V_i g_i$$

$$- \frac{3}{\partial x_j} \rho P_{ij} V_i - \frac{3}{\partial x_i} q_i ,$$

(3.35)

where the total heat transfer vector for a multicomponent gas mixture may be written as

$$q_i = -\lambda \frac{3}{\partial x_i} T + \rho \sum_s V_s h_s V_{si} + q_i^D$$

(3.36)

The quantity $q_i^D$ represents the sum of the Dufour-heat flux and radiative heat flux.

The coefficient of thermal conductivity $\lambda$, and the diffusion velocity, $V_{si}$, depend, in a complicated way, on the temperature, pressure and composition of the mixture. Analogous to the coefficient of viscosity $\nu$, the coefficient of thermal conductivity $\lambda$ will be decomposed into a unweighted mean and a fluctuating part. The diffusion velocity will, analogous to the velocity, be decomposed into a mass-weighted mean and a fluctuating part. The term $q_i^D$ will be decomposed into an unweighted mean and a fluctuating component. This latter choice of decomposition is arbitrary.

The pressure tensor $P_{ij}$ may be written as

$$P_{ij} = \rho \delta_{ij} - \tau_{ij} ,$$

(3.37)
and the energy equation as

\[
\frac{\partial}{\partial t} \rho (h + \frac{1}{2} V_i V_i) + \frac{\partial}{\partial x_j} \rho \left( V_j (h + \frac{1}{2} V_i V_i) - \frac{\partial \rho}{\partial t} = \rho \left( V_i g_i + \frac{\partial}{\partial x_j} \tau_{ij} V_i - \frac{\partial}{\partial x_i} q_i \right) \right)
\]

(3.38)

Decomposition of Eq. (3.38) and Eq. (3.36) yields

\[
\frac{\partial}{\partial t} [\bar{h} + h''] + \frac{1}{2} \left( \bar{V}_i + V_i'' \right) \left( V_i + V_i'' \right) \] + \frac{\partial}{\partial x_j} \rho \left( \bar{V}_j + V_j'' \right) [\bar{h} + h'']
+ \frac{1}{2} \left( \bar{V}_i + V_i'' \right) \left( \bar{V}_i + V_i'' \right) - \frac{\partial}{\partial t} (\bar{p} + p') =

\rho (\bar{V}_i + V_i'') g_i + \frac{\partial}{\partial x_j} \left( \bar{\tau}_{ij} + \tau_{ij}' \right) (\bar{V}_i + V_i'') - \frac{\partial}{\partial x_i} (\bar{q}_i + q_i')
\]

(3.39)

where

\[
\bar{q}_i = - \left( \lambda \frac{\partial}{\partial x_i} \bar{T} + \lambda' \frac{\partial}{\partial x_i} T'' \right) + \rho \left( \bar{V}_s \bar{h}_s \bar{V}_s i + \bar{V}_s h'' \bar{V}_s i \right)
+ \bar{Y}_s h'' \bar{V}_s i + \bar{Y}_s h' h'' \bar{V}_s i') + \bar{q}_i^D
\]

(3.40)

and

\[
q_i' = - \lambda' \frac{\partial}{\partial x_i} \bar{T} + \rho \left( h'' \bar{V}_s \bar{V}_s i + \bar{V}_s h' \bar{V}_s i + \bar{V}_s h'' \bar{V}_s i \right) + q_i^D
\]

(3.41)

Averaging of Eq. (3.39) finally yields

\[
\frac{\partial}{\partial t} = \bar{\rho} (\bar{h} + \frac{1}{2} \bar{V}_i \bar{V}_i + \frac{1}{2} \bar{V}_i'' \bar{V}_i'') \] + \frac{\partial}{\partial x_j} \bar{\rho} \left( \bar{V}_j (\bar{h} + \frac{1}{2} \bar{V}_i \bar{V}_i + \frac{1}{2} \bar{V}_i'' \bar{V}_i'') \right)
+ \bar{\rho} \bar{V}_j h'' + \bar{\rho} \bar{V}_j \bar{V}_i'' \bar{V}_i + \bar{\rho} \bar{V}_j \bar{V}_i'' \bar{V}_i'') - \frac{\partial}{\partial t} \bar{\rho} \left( \bar{\tau}_{ij} \bar{V}_i + \bar{\tau}_{ij} \bar{V}_i'' \right)
+ \bar{\tau}_{ij} \bar{V}_i'' - \frac{\partial}{\partial x_i} \bar{q}_i
\]

(3.42)
where \( \tau_{ij} \) and \( \tau_{ij}' \) are given by Eq. (3.29) and (3.33) respectively.

### 3.5. THE FAIVRE-AVERAGED EQUATION FOR CONSERVATION OF ANGULAR MOMENTUM

Experiments with the hybrid-racket motor at PMLTNO, where the combustion has been filmed with a high-speed camera, clearly indicated that the flow through such a motor may possess strong vortices. It may therefore be advantageous to apply the equation for conservation of angular momentum instead of, or together with, the equation for conservation of linear momentum. The equation for conservation of angular momentum has been derived in ref. 2 and states:

\[
\frac{\partial}{\partial t} \left( \varepsilon_{ijk} r_{ij} r_{jkl} \rho V_k \right) + \varepsilon_{ijk} r_{ij} r_{jkl} \frac{\partial \rho}{\partial x_l} V_j = \varepsilon_{ijk} r_{ij} r_{jkl} \rho g_k - \varepsilon_{ijk} r_{ij} \frac{\partial p}{\partial x_k} + \varepsilon_{ijk} r_{ij} \frac{\partial}{\partial x_k} \tau_{ik},
\]

(3.43)

where \( r_0 \) is the position vector to an arbitrary reference point. Define the specific angular momentum \( b_i \) as

\[
b_i = \varepsilon_{ijk} r_{ij} V_k (= r_0 \times V) \quad .
\]

(3.44)

Equation (3.43) may now be written as

\[
\frac{\partial}{\partial t} \left( \rho b_i \right) + \varepsilon_{ijk} r_{ij} \frac{\partial V_j}{\partial x_l} = \varepsilon_{ijk} r_{ij} \rho g_k - \varepsilon_{ijk} r_{ij} \frac{\partial p}{\partial x_k} + \varepsilon_{ijk} r_{ij} \frac{\partial}{\partial x_k} \tau_{ik} \quad .
\]

(3.45)

Mass-averaging of the specific angular momentum yields

\[
\tilde{b}_i = \frac{\rho b_i}{\rho} = \frac{\rho \varepsilon_{ijk} r_{ij} V_k}{\rho} = \varepsilon_{ijk} r_{ij} \frac{\rho V_k}{\rho} \quad .
\]

(3.46)

Decomposition of Eq. (3.45) yields

\[
\frac{\partial}{\partial t} \rho (\tilde{b}_i + b_i^\prime) + \varepsilon_{ijk} \frac{\partial}{\partial x_l} \rho (\tilde{b}_i + b_i^\prime) (\tilde{V}_j + V_j^\prime) = \varepsilon_{ijk} r_{ij} \rho g_k - \varepsilon_{ijk} r_{ij} \frac{\partial (p + p')}{\partial x_k} + \varepsilon_{ijk} r_{ij} \frac{\partial}{\partial x_k} (\tilde{\tau}_{ik} + \tau_{ik}^L) \quad .
\]

(3.47)
Averaging of this equation yields

\[
\frac{\partial}{\partial t} \bar{\rho} \bar{b}_i + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{b}_i \bar{V}_j + \bar{\rho} \bar{b}_{ii} \bar{V}_j^2) = \varepsilon_{ijk} r_{o_j} \bar{\rho} g_k - \varepsilon_{ijk} r_{o_j} \frac{\partial}{\partial x_k} \bar{\rho} + \varepsilon_{ijk} r_{o_j} \frac{\partial}{\partial x_k} \bar{\tau}_{ik},
\]

(3.48)

where \( \bar{\tau}_{ik} \) is given by Eq. (3.29).

### 3.6. THE FAVRE-AVERAGED EQUATION FOR CONSERVATION OF SPECIES

The equation for conservation of species \( s \) states [1]

\[
\frac{\partial}{\partial t} (\rho \bar{Y}_s) + \frac{\partial}{\partial x_j} (\rho \bar{Y}_s \bar{V}_j) = - \frac{\partial}{\partial x_j} (\rho \bar{Y}_s \bar{V}_s) + \omega_s
\]

(3.49)

As already mentioned, the diffusion velocity \( \bar{V}_s \) depends in a complex way on the temperature, pressure and the composition of the mixture, and will be decomposed in a mass-weighted mean and a fluctuating part. The net mass rate of production of species \( s \) by chemical reactions, \( \omega_s \), depends in a complex way on the temperature, the composition of the mixture and the chemical reactions involving \( \omega_s \). Modeling of this term will be out of the scope of this report, but may be obtained from the available literature [8]. In this report this term is decomposed into a unweighted mean with a fluctuating component [8]. Decomposing Eq. (3.49) yields

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_s) + \frac{\partial}{\partial x_j} (\bar{\rho} (\bar{Y}_s + \bar{Y}_s^u) (\bar{V}_j + \bar{V}_j^u)) = - \frac{\partial}{\partial x_j} (\bar{\rho} (\bar{Y}_s + \bar{Y}_s^u) (\bar{V}_s + \bar{V}_s^u) + \omega_s + \omega_s^u
\]

(3.50)

Averaging yields

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_s) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{Y}_s \bar{V}_j + \bar{\rho} \bar{Y}_s \bar{V}_j^u) = - \frac{\partial}{\partial x_j} (\bar{\rho} \bar{Y}_s \bar{V}_s + \bar{\rho} \bar{Y}_s \bar{V}_s^u
\]

(3.51)

### 3.7. COMPILATION OF THE FAVRE-AVERAGED CONSERVATION EQUATIONS

The Favre-averaged conservation equations, as derived in this Chapter, are summarized below.
CONSERVATION OF MASS

\[ \frac{\partial}{\partial t} (\bar{\rho}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{V}_j) = 0 \quad , \] (3.52)

CONSERVATION OF MOMENTUM

\[ \frac{\partial}{\partial t} (\bar{\rho} \bar{V}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{V}_i \bar{V}_j + \bar{\rho} \bar{V}_i \bar{V}_j) = \bar{\rho} \bar{g}_i - \frac{\partial}{\partial x_i} \bar{\rho} + \frac{\partial}{\partial x_j} \bar{T}_{ij} \quad , \] (3.53)

CONSERVATION OF ENERGY

\[ \frac{\partial}{\partial t} \bar{h} [\bar{h} + \frac{1}{2} \bar{V}_i \bar{V}_i + \frac{1}{2} \bar{V}_i \bar{V}_i] + \frac{\partial}{\partial x_j} [\bar{h} \bar{V}_j (\bar{h} + \frac{1}{2} \bar{V}_i \bar{V}_i + \frac{1}{2} \bar{V}_i \bar{V}_i)] + \bar{\rho} \bar{V}_j \bar{h} + \bar{\rho} \bar{V}_i \bar{V}_j + \frac{1}{2} \bar{\rho} \bar{V}_j \bar{V}_i \bar{V}_i - \frac{\partial \bar{p}}{\partial t} = \bar{\rho} \bar{V}_i \bar{g}_i \]

\[ + \frac{\partial}{\partial x_j} (\bar{T}_{ij} \bar{V}_i + \bar{T}_{ij} \bar{V}_i + \bar{T}_{ij} \bar{V}_i) - \frac{\partial}{\partial x_i} \bar{q}_i \quad , \] (3.54)

CONSERVATION OF ANGULAR MOMENTUM

\[ \frac{\partial}{\partial t} (\bar{\rho} \bar{b}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{b}_i \bar{V}_j + \bar{\rho} \bar{b}_i \bar{V}_j) = \varepsilon_{ijk} \bar{r}_{ij} \bar{b}_k - \varepsilon_{ijk} \bar{r}_{ij} \frac{\partial}{\partial x_k} \bar{b}_i \]

\[ + \varepsilon_{ijk} \bar{r}_{ij} \frac{\partial}{\partial x_k} \bar{T}_{ik} \quad , \] (3.55)

CONSERVATION OF SPECIES

\[ \frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_s) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{Y}_s \bar{V}_j + \bar{\rho} \bar{Y}_s \bar{V}_j) = - \frac{\partial}{\partial x_j} (\bar{\rho} \bar{Y}_s \bar{V}_s \bar{V}_j + \bar{\rho} \bar{Y}_s \bar{V}_s \bar{V}_j) + \bar{\omega}_s \quad , \] (3.56)

where \( \bar{T}_{ij} \) is given by Eq. (3.29), \( \bar{\tau}_{ij} \) by Eq. (3.33) and \( \bar{q}_i \) by Eq. (3.40). These equations have to be supplemented with an equation of state which gives the relation between the dependent thermodynamic variables and the two independent thermodynamic variables. (Only two thermodynamic variables can be chosen independently.) The Favre-averaged equation of state for a multicomponent mix-
ture of perfect gases may be written as [8]

\[ \bar{\rho} = R_0 \bar{\rho} \left( \bar{\rho} \bar{T} \bar{\gamma}_s + \bar{\rho} \bar{T}'' \bar{\gamma}_s'' \right) \frac{1}{M_s} . \]  

(3.57)

Other relations that must be known to solve these equations in relation with their boundary conditions are expressions for the averaged and for the fluctuating part of the transport coefficients (viscosity, thermal conductivity, etc.), for the mass-averaged and fluctuating part of the diffusion velocities and for the averaged chemical production terms. Modeling of these terms requires a detailed knowledge of the composition of the mixture and is outside the scope of this report.

The Second Law of Thermodynamics states that for a closed and isolated system the entropy changes according to

\[ dS \geq \frac{dQ}{T} , \]  

(3.58)

where \( dQ \) is the heat supplied to the system by its surroundings.

The 'equal' sign is applied to reversible processes, and the 'greater' sign to irreversible processes. If chemical reactions are taken in account it is useful to use the entropy balance which can be derived from the energy equation and the momentum equation (see Appendix A). The Favre-averaged form of the Second Law of Thermodynamics is

\[ \bar{\rho} \bar{T} \frac{\partial}{\partial t} \bar{s} + \bar{T} \frac{\partial}{\partial x_1} \bar{s}'' + \bar{T} \frac{\partial}{\partial x_j} \bar{s}'' + \bar{\rho} \bar{T} \bar{V}_j \frac{\partial}{\partial x_j} \bar{s} + \bar{T} \bar{V}_j \frac{\partial}{\partial x_j} \bar{s}'' + \bar{\rho} \bar{T} \bar{V}_j'' \frac{\partial}{\partial x_j} \bar{s}'' + \bar{T} \bar{V}_j'' \frac{\partial}{\partial x_j} \bar{s}'' + \bar{\rho} \bar{T}'' \bar{V}_j'' \frac{\partial}{\partial x_j} \bar{s}'' \geq \]

\[ - \frac{\partial}{\partial x_1} \bar{q}_1 + \bar{\tau}_{ij} \frac{\partial}{\partial x_j} \bar{V}_1 + \bar{\tau}_{ij} \frac{\partial}{\partial x_j} \bar{V}_1'' + \bar{\tau}_{ij} \frac{\partial}{\partial x_j} \bar{V}_1'' \]  

(3.59)

To complete the set of equations presented in this Chapter, one has to adopt a turbulence closure model in which the terms involving turbulent fluctuations are modelled. Several turbulence closure models are available, and the particular choice of one of these will be discussed in the following Chapter.
4. TURBULENCE MODELLING

It was mentioned in Section 3.7 that a turbulence closure model has to be adopted to complete the set of conservation equations describing a turbulent reacting flow of a multicomponent mixture. Several turbulence closure models have been developed in the past. Four of them will be discussed in this chapter. In the first section a more general introduction to turbulence modelling is given. In the following sections, the \( k - \varepsilon \) model, a Reynolds-stress closure model, an Algebraic Stress Model (ASM) and a multiple-scale closure model are discussed. In the final section the particular choice of the \( k - \varepsilon \) model which will be applied in a computational model is explained.

4.1. INTRODUCTION

As follows from Section 3.7., the terms which must be modelled with a turbulence closure model are the Reynolds-stresses \(- \rho \ddot{V}_i \ddot{V}_j\) \((i, j = 1, 2, 3)\), the turbulent kinetic energy \( k = \frac{1}{2} \ddot{V}_i \ddot{V}_i\), the fluctuating velocity \( \ddot{V}_i \) and the turbulent heat- and mass-fluxes \(- \rho \ddot{V}_i \ddot{\varphi}\), where \( \varphi \) stands for the enthalpy \( h \) or the mass-fraction of species \( s \). In a turbulence closure model unknown correlations of turbulent quantities are approximated by lower order correlations to get a deterministic set of equations.

The very first attempt to turbulence modelling was made by Boussinesq in 1877 [16]. In analogy with the momentum transport by molecular motion, he suggested that the turbulent shear- or Reynolds-stress could be replaced by the product of the mean velocity gradient and a 'turbulent- or eddy-viscosity'. In general, Boussinesq's eddy-viscosity concept can be expressed by [15]

\[
- \rho \ddot{v}_i \ddot{v}_j = \mu_t \left( \frac{\partial \ddot{v}_i}{\partial x_j} + \frac{\partial \ddot{v}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left( \rho \ddot{k} + \mu_t \frac{\partial \ddot{v}_k}{\partial x_k} \right),
\]

(4.1)

where the turbulent- or eddy-viscosity is not a fluid property but depends on the local structure of the turbulence. Analogous to the eddy-viscosity concept for turbulent momentum transport, the turbulent heat- and mass-transport are also related to the product of a turbulent- or eddy-diffusivity \( \Gamma_t \) and the gradient of the transported quantity,

\[
- \rho \ddot{v}_i \ddot{\varphi} = \Gamma_t \frac{\partial \ddot{\varphi}}{\partial x_i} = \frac{\mu_t}{\tau_t} \frac{\partial \ddot{\varphi}}{\partial x_i},
\]

(4.2)

where \( \sigma \) is the turbulent Prandtl number (heat transport) or turbulent Schmidt number (mass-transport). Experiments have shown that in boundary layer flows the value of the turbulent Prandtl number lies in the range from 0.7 to 1.0, and varies only little across a flow [17]. The often made assumption of the Prandtl number equal to 1.0 is called the 'Reynolds analogy'. The Eqs. (4.1) and (4.2) only give a framework for constructing a turbulence closure model because the eddy viscosity \( \mu_t \) is still unknown. From a simplified analysis of momentum transport by molecular motion, it can be shown that the molecular viscosity is proportional to [4]
\[ \mu = \rho \ell V, \]  
\[ \text{(4.3)} \]

where \( \ell \) is the free-path and \( V \) the molecular velocity. Analogous to this equation, Prandtl supposed in 1925 that the eddy-viscosity equals

\[ \mu_t = \rho \lambda_t \bar{V}_t, \]  
\[ \text{(4.4)} \]

where \( \lambda_t \) is a turbulent length scale and \( \bar{V}_t \) the turbulent velocity. Both quantities vary strongly from place to place and are very difficult to determine accurately. Prandtl therefore proposed the second part of his hypothesis in which the turbulent velocity \( \bar{V}_t \) was related to the turbulent length scale and the mean velocity gradient as follows

\[ \bar{V}_t = \lambda_t \frac{\partial \bar{u}}{\partial y}. \]  
\[ \text{(4.5)} \]

The physical reasoning behind this assumption is the following [18]. Consider a turbulent shear flow along a wall. In a turbulent flow particles coalesce into 'lumps' or 'eddies' which move together over a distance \( \lambda_t \) before breaking up. Assume that such an eddy moves from \( y + \lambda_t \) to \( y \). The velocity difference between these two points then may be approximated by

\[ \Delta u = \bar{u} (y + \lambda_t) - \bar{u} (y) = \lambda_t \frac{\partial \bar{u}}{\partial y}. \]

This velocity difference is proportional to the turbulent velocity, and Prandtl took the proportionality constant unity. Substitution of Eq. (4.5) into Eq. (4.4) and averaging yields

\[ \mu_t = \rho \lambda_m \frac{\partial \bar{u}}{\partial y} \frac{\partial \bar{u}}{\partial y}. \]  
\[ \text{(4.6)} \]

The mean length-scale \( \lambda_m \), called the 'mixing-length' remains unknown and must be determined empirically. For many shear layers this can be done in a very simple way. Well known examples for boundary layers near a solid wall are

\[ \lambda_m = \kappa y, \]  
\[ \text{(4.7)} \]

where \( \kappa (= 0.43) \) is the Von Kármán constant and \( y \) is the distance to the wall, and the Van Driest hypothesis

\[ \lambda_m = \kappa y \left[ 1 - \exp \left( -\frac{y \tau_s^{1/2} \rho^{1/2}}{\mu} \right) \right], \]  
\[ \text{(4.8)} \]
where $A$ is a constant and $\tau_S$ is the shear stress at the solid wall. Other expressions for the mixing length are given in [16].

Although the mixing length model has some important advantages, i.e. it is simple and it gives for many boundary layer flows realistic predictions, it has some disadvantages. For instance, it does not account for transport and diffusion of turbulent quantities. The mixing-length hypothesis implies that at each point in the flow turbulence is dissipated at the same rate as it is produced, and that there is no influence of the remainder of the field [17]. The mixing-length model belongs to the class of 'zero-equation' models since no partial differential equations are used to model turbulence. To overcome the short comings of the mixing-length model turbulence models have been developed in which the turbulent velocity scale was obtained from solving a partial differential equation for the turbulent kinetic energy. These are the one-equation models [19]. The turbulent kinetic energy is found by solving a transport equation in the form

$$\frac{3}{\alpha} \frac{\partial \bar{k}}{\partial t} + \frac{3}{\alpha x_j} \frac{\partial \bar{V}_j \bar{k}}{\partial x_j} = \text{production} + \text{diffusion} + \text{dissipation} \quad (4.9)$$

rate of convection change

The eddy-viscosity equals the Kolmogorov - Prandtl expression [17]:

$$u_t = \rho \ C_{\mu} \sqrt{\bar{k}} \ \ell_1 \quad (4.10)$$

where $C_{\mu}$ is an empirical constant. The length scale $\ell_1$ must be determined from an empirical relation similar to the one for the mixing-length. In principle one-equation models are more general than the mixing-length model because they take into account the effects of transport and history on turbulence. The application of one-equation models however is limited to simple shear flows because in complex flows it is difficult to specify the length scale $\ell_1$ empirically. Therefore, and since in some flows the length scale is also affected by transport processes and its history, models which determine the length scale from a partial differential equation have been developed (two-equation models). Because the turbulent kinetic energy is known from a transport equation, it is not necessary to use the length scale $\ell_1$ as the dependent variable of the length scale transport equation. Any combination in the form $z = k^n \ell^m$ would do just as well [16], [17]. Several workers proposed values for the coefficients $m$ and $n$. Examples are [16] Kolmogorov who proposed $z = k^{3/2}$ and Rotta (1951) and Spalding (1967) who used $z = \bar{c}$. The most popular and widely used variable for determining the length scale is the dissipation rate $\varepsilon$, $\varepsilon = k^{3/2}/\ell$. The use of the dissipation rate $\varepsilon$ as variable for determining the length scale $\ell$ has the advantage that the transport equation for $\varepsilon$ requires no additional terms near the walls [17]. Substitution of $\ell = k^{3/2}/\varepsilon$ into Eq. (4.4) yields the eddy-viscosity

$$u_t = \rho \ C_{\mu} \ k^2/\varepsilon \quad (4.11)$$
where $C_u$ again is an empirical constant. The $k - \varepsilon$ model in the form as proposed by Jones and Launder [20] will be extensively discussed in the following section. The $k - \varepsilon$ model has been applied to a large number of different flows, and is one of the best tested turbulence models available. All turbulence models discussed in this Section so far are based upon the eddy viscosity/diffusivity concept, which is not valid under all circumstances. A severe limitation of this concept is the assumption of local isotropy, i.e. all the various $\delta V_i V_j$ $(i, j = 1, 2, 3)$ and $\delta V_i \omega_j$ $(i = 1, 2, 3)$ are using the same values for the eddy viscosity/diffusivity. Further it is assumed that the local state of turbulence can be characterized by a single velocity scale and that all the individual $\delta V_i V_j$ can be related to this scale. In reality however, the individual $\delta V_i V_j$ may develop quite differently, which is especially the case in complex flows.

To account for the different development of the individual stresses, turbulence models which solve transport equations for $\delta V_i V_j$ and $\delta V_i \omega_j$ have been developed (Stress/flux equation models). Models based on these equations are called second-order-closure schemes because they solve partial differential equations for the second order correlations $\delta V_i V_j$. This type of turbulence modelling will be discussed in Section 4.3. The disadvantage of Reynoldsstress modelling is that is it very complex and that the number of equations to be solved is very large. If a flow with $N$ species is considered, the number of equations to be solved for the mean flow equals $N + 4$, while for the turbulence model 6 (Reynoldsstresses) $+ 2(\varepsilon, k) + 3 \times N (\delta V_i \omega_j) + 3 (\delta V_i) \text{ equations are necessary.}$ Take $N = 4$, then the number of equations to be solved equals $8 + 23 = 31$. For practical applications, it would be desirable to use simplified models. Therefore turbulence models have been developed in which the partial differential transport equations are simplified to algebraic equations in a way that the model still retains most of its basic features. These Algebraic Stress/ Flux Models will be discussed in Section 4.4. The turbulence models discussed in this Section until now all use a single averaged length scale and a single averaged time scale. Turbulence however consists of a fluctuating motion with a continuous spectre of length- and time scales. The assumption of one averaged length scale implies that there is a constant relationship between the length scale for turbulence production and the length scale for turbulence dissipation. This assumption doesn't hold for all flows, and to overcome this a multiple-scale-model has recently been developed [21] which is a modified form of the two-equation $k - \varepsilon$ model. In a multiple-scale-model the turbulence production length scale and the turbulence dissipation length scale are seperately computed. One of the areas in which a multiple scale model seems to have great potential is in turbulence-chemistry interactions [22]. Therefore, the multiple scale model will be discussed in Section 4.5.

4.2. THE $k - \varepsilon$ MODEL

The $k - \varepsilon$ turbulence closure model is a two-equation model in which transport equations are solved for the turbulent kinetic energy $k$ and the dissipation rate $\varepsilon$ to determine an averaged turbulent velocity scale and an averaged turbulent length scale. These transport equations can be derived from the Navier-Stokes equations. This leads to unknown higher order correlations which must be approximated by lower order known quantities to close the set of equations. The $k - \varepsilon$ model involves the Boussinesq approximation (Eq. (4.1)) which assumes a linear relation between the Reynoldsstresses and the rate of strain. The turbulent viscosity is calculated from Eq. (4.11),

$$\mu_t = \rho \frac{C_u}{\varepsilon} \overline{k^2} / \overline{\varepsilon} \quad (4.11)$$
The equation for the turbulent kinetic energy can be derived as follows. The momentum equation states [1]

$$\frac{\partial}{\partial t} \rho V_i + \frac{\partial}{\partial x_j} \rho V_i V_j = \rho g_i - \frac{\partial}{\partial x_i} \rho + \frac{\partial}{\partial x_j} \tau_{ij}$$ \hspace{1cm} (4.12)$$

and the Favre-averaged momentum equation (Eq. (3.53))

$$\frac{\partial}{\partial t} \tilde{V}_i + \frac{\partial}{\partial x_j} \tilde{V}_i \tilde{V}_j = \tilde{\rho} g_i - \frac{\partial}{\partial x_i} \tilde{\rho} + \frac{\partial}{\partial x_j} \tau_{ij} - \frac{\partial}{\partial x_j} \tilde{V}_i \tilde{V}_j \tilde{V}_j \tau_{ij} \hspace{1cm} (4.13)$$

Multiplying Eq. (4.12) by $V_k$, and adding it to the same equation with subscripts $i$ and $k$ interchanged yields

$$V_k \frac{\partial}{\partial t} \rho V_i + V_i \frac{\partial}{\partial t} \rho V_k + V_k \frac{\partial}{\partial x_j} \rho V_i \tilde{V}_j + V_i \frac{\partial}{\partial x_j} \rho V_k \tilde{V}_j =$$

$$\rho V_k g_i + \rho V_i g_k - V_k \frac{\partial}{\partial x_i} \rho - V_i \frac{\partial}{\partial x_k} \rho + V_k \frac{\partial}{\partial x_j} \tau_{ij}$$

$$+ V_i \frac{\partial}{\partial x_j} \tau_{kj} \hspace{1cm} (4.14)$$

The left hand side of this equation may be written as

$$V_k \frac{\partial}{\partial t} \rho V_i + V_i \frac{\partial}{\partial t} \rho V_k + V_k \frac{\partial}{\partial x_j} \rho V_i \tilde{V}_j + V_i \frac{\partial}{\partial x_j} \rho V_k \tilde{V}_j =$$

$$\frac{\partial}{\partial t} \rho V_i \tilde{V}_k + \frac{\partial}{\partial x_j} \rho \tilde{V}_j \tilde{V}_i \tilde{V}_k \hspace{1cm} (4.15)$$

where the equation for conservation of mass multiplied with $V_i \tilde{V}_k$ has been added. Favre-decomposition and subsequent averaging yields

$$\frac{\partial}{\partial t} \left( \tilde{\rho} \tilde{V}_i \tilde{V}_k + \tilde{\rho} \tilde{V}_i \tilde{V}_k \right) + \frac{\partial}{\partial x_j} \left( \tilde{\rho} \tilde{V}_j \tilde{V}_i \tilde{V}_k + \tilde{\rho} \tilde{V}_j \tilde{V}_i \tilde{V}_k \right) = \tilde{\rho} \left( \tilde{V}_k g_i + \tilde{V}_i g_k \right) - \left( \frac{\partial}{\partial x_i} \tilde{\rho} + \frac{\partial}{\partial x_k} \tilde{V}_i \tilde{V}_j \tilde{V}_j \right)$$

$$+ \tilde{V}_k \frac{\partial}{\partial x_j} \tilde{V}_{ij} + \tilde{V}_i \frac{\partial}{\partial x_j} \tilde{V}_{kj} - \left( \frac{\partial}{\partial x_i} \tilde{V}_i \tilde{V}_j \tilde{V}_j \tilde{V}_i \tilde{V}_k + \frac{\partial}{\partial x_k} \tilde{V}_i \tilde{V}_j \tilde{V}_j \tilde{V}_i \tilde{V}_k \right)$$
Multiplying Eq. (4.13) by \( \tilde{v}_k \), and adding it to the same equation with subscripts \( i \) and \( k \) interchanged yields

\[
\frac{\partial}{\partial t} \rho \tilde{v}_i \tilde{v}_k + \frac{\partial}{\partial x_j} \rho \tilde{v}_j \tilde{v}_i \tilde{v}_k - \tilde{v}_k \left( \frac{\partial}{\partial x_i} \rho + \frac{\partial}{\partial x_k} \rho \right) + \tilde{v}_k \frac{\partial}{\partial x_j} \tau_{ij} = \tilde{v}_i \frac{\partial}{\partial x_j} \rho \tilde{v}_j + \tilde{v}_i \frac{\partial}{\partial x_k} \rho \tilde{v}_k \tilde{v}_j \quad (4.17)
\]

Subtracting Eq. (4.17) from Eq. (4.16) yields

\[
\frac{\partial}{\partial t} \rho \tilde{v}_i \tilde{v}_k + \frac{\partial}{\partial x_j} \rho \tilde{v}_j \tilde{v}_i \tilde{v}_k = \frac{\partial}{\partial x_j} \rho \tilde{v}_i \tilde{v}_j \tilde{v}_k + \frac{\partial}{\partial x_k} \rho \tilde{v}_k \tilde{v}_j \tilde{v}_i - \frac{\partial}{\partial x_j} \rho \tilde{v}_i \tilde{v}_j \tilde{v}_k - \frac{\partial}{\partial x_k} \rho \tilde{v}_k \tilde{v}_j \tilde{v}_i - \frac{\partial}{\partial x_j} \tau_{ij} + \frac{\partial}{\partial x_k} \tau_{kj} \quad (4.18)
\]

This is the equation for the transport of Reynolds stresses, which will be discussed in Section (4.3). Putting \( k = i \) in this equation yields

\[
\frac{\partial}{\partial t} \rho \tilde{v}_i \tilde{v}_i + \frac{\partial}{\partial x_j} \rho \tilde{v}_j \tilde{v}_i \tilde{v}_i = -2 \frac{\partial}{\partial x_j} \rho \tilde{v}_i \tilde{v}_j \tilde{v}_i - \frac{\partial}{\partial x_j} \rho \tilde{v}_j \tilde{v}_i \tilde{v}_i - \frac{\partial}{\partial x_j} \tau_{ij} + 2 \frac{\partial}{\partial x_j} \tau_{ij} \quad (4.19)
\]

The turbulent kinetic energy per unit mass \( \tilde{k} \) now is defined as

\[
\tilde{k} = \frac{\tilde{v}_i \tilde{v}_i}{2} \quad (4.20)
\]

and substituting this expression into Eq. (4.19) yields the equation for the transport of turbulent kinetic energy:
\[
\frac{\partial}{\partial t} \bar{\rho} \tilde{k} + \frac{\partial}{\partial x_j} \bar{\rho} \tilde{V}_j \tilde{k} = -\bar{\rho} \bar{V}_i'' \bar{V}_j'' \frac{\partial}{\partial x_j} \tilde{V}_i - \frac{1}{2} \frac{\partial}{\partial x_j} \bar{\rho} \bar{V}_j'' \bar{V}_i'' \bar{V}_i'' - \bar{V}_i'' \frac{\partial \bar{\rho}}{\partial x_j} 
\]
rate of convection production diffusion change dissipation

\[
(4.21)
\]

In order to obtain a closed equation, the diffusion and dissipation terms must be modelled. (The production term is given by the Boussinesq approximation.) The last three terms of Eq. (4.21) may be written as

\[
- \frac{1}{2} \frac{\partial}{\partial x_j} \bar{\rho} \tilde{V}_j \tilde{V}_i'' \bar{V}_i'' - \bar{V}_i'' \frac{\partial \bar{\rho}}{\partial x_j} \tau_{ij} + \bar{V}_i'' \frac{\partial}{\partial x_j} \tau_{ij} = - \frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{V}_j'' k'' + \bar{V}_j'' p' \right) 
\]

\[
- \bar{\rho} \frac{\partial}{\partial x_j} \bar{V}_i'' p' + \frac{\partial \bar{V}_i''}{\partial x_j} \tau_{ij} \bar{V}_i'' + \tau_{ij} \frac{\partial}{\partial x_j} \bar{V}_i'' , 
\]

(4.22)

where \(k'' = \frac{1}{2} \bar{V}_i'' \bar{V}_i''\). The first term on the right-hand side of this equation represents diffusion of turbulent kinetic energy, and can be modelled with the eddy-diffusivity concept (see Eq. (4.2)) [23]

\[
- \frac{\partial}{\partial x_j} \bar{\rho} \tilde{V}_j'' (k'' + \frac{p'}{\bar{\rho}}) = \frac{\partial}{\partial x_j} \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} , 
\]

(4.23)

where \(\sigma_k\) is the turbulent Prandtl number for the turbulent kinetic energy. The term \(- \bar{\rho} \frac{\partial}{\partial x_j} \bar{V}_i'' \bar{V}_i'' \bar{V}_i''\) occurs only in the Favre-averaged equation for the turbulent kinetic energy. This term may be modelled with the help of Eqs. (3.18) and (3.20),

\[
\bar{V}_i'' = \frac{\bar{\rho}'}{\bar{\rho}} \bar{V}_i'' = \frac{-\bar{\rho}'}{\bar{\rho}} (\bar{V}_i + \bar{V}_i') = -\frac{\rho'}{\bar{\rho}} \bar{V}_i'' = -\rho' \bar{V}_i'' .
\]

(4.24)

The term \(\rho' \bar{V}_i''\) can be approximated by and eddy-diffusivity concept [24] yielding

\[
\bar{\rho} \frac{\partial \bar{V}_i'}{\partial x_j} = - \mu_t \frac{\partial \bar{\rho}}{\partial t} ,
\]

(4.25)

Another kind of modelling of the term \(- \bar{\rho} \frac{\partial \bar{\rho}}{\partial x_j} \) was suggested by Kollmann and Vandramme [25] who approximated this term by
\[ - \nabla_i \frac{\delta \bar{\rho}}{\delta x_i} = - C_p \frac{1}{\rho} \left( \nabla_i \nabla_i V^n \right) \frac{1}{\beta} \frac{\delta \bar{\rho}}{\delta x_i} , \]  

(4.26)

where the density fluctuations \( \bar{\rho}^{ij} \) in a complicated way were determined from the equations for conservation of species \( s \). In this stage, we will use Eq. (4.25) to model \( - \nabla_i \frac{\delta \bar{\rho}}{\delta x_i} \) because it is simpler to use. The term

\[ \rho' \frac{\partial V_i^m}{\partial x_i} \]

in Eq. (4.22) is neglected \([25]\) because the divergence of the velocity fluctuations is much smaller than for instance the rate of strain. The last two terms in Eq. (4.22) can be written as

\[
\begin{align*}
\frac{\partial}{\partial x_j} \tau_{ij} V_i^m - \tau_{ij} \frac{\partial}{\partial x_j} V_i^m = \frac{\partial}{\partial x_j} \tau_{ij} V_i^m + \frac{\partial}{\partial x_j} \tau_{ij} V_i^m - \tau_{ij} \frac{\partial V_i^m}{\partial x_j} \\
= - \tau_{ij} \frac{\partial V_i^m}{\partial x_j} .
\end{align*}
\]  

(4.27)

In high Reynolds number flow the fluctuating stress tensor is much larger than the mean stress tensor, and terms involving the mean stress tensor may be neglected \([13]\). The second term on the right hand side represents molecular diffusion and is negligible small \([8]\). The remaining term on the right hand side represents the dissipation of turbulent kinetic energy, and will be calculated from a transport equation,

\[ \bar{\rho} \tilde{\varepsilon} = \tau_{ij} \frac{\partial V_i^m}{\partial x_j} . \]  

(4.28)

With these assumptions Eq. (4.21) holds

\[
\frac{\partial}{\partial t} \bar{\rho} \tilde{\varepsilon} + \frac{\partial}{\partial x_j} \bar{\rho} \tilde{V}_j \tilde{\varepsilon} = P_k + \frac{\partial}{\partial x_j} \mu \frac{\partial \tilde{\varepsilon}}{\partial x_j} - \frac{\mu}{\rho^2} \frac{\partial \bar{\rho}}{\partial x_i} \frac{\partial \bar{\rho}}{\partial x_i} - \bar{\rho} \tilde{\varepsilon} ,
\]  

(4.29)

where \( P_k \), the production of turbulent kinetic energy, equals

\[ P_k = - \bar{\rho} \nabla_i \nabla_j \frac{\partial}{\partial x_j} \tilde{V}_i . \]  

(4.30)
The exact equation for the dissipation rate of turbulent kinetic energy, $\tilde{\varepsilon}$, can be derived only in a special case. The general form of this equation may be written as

$$\frac{3}{\rho} \frac{\partial}{\partial t} \tilde{\varepsilon} + \frac{3}{\rho x_j} \frac{\partial}{\partial x_j} \tilde{\varepsilon} \tilde{V}_j \tilde{\varepsilon} = \text{Generation} + \text{Diffusion} + \text{Destruction}. \quad (4.31)$$

For high Reynolds number flow with constant density the exact equation for the dissipation rate can be derived from the Navier-Stokes equations. Modelling this equation gives an idea about the modelling of the dissipation equation for fluctuating density flows, and therefore this equation will be derived and modelled here. For constant density flows, the following relations holds

$$V''_j = V'_j, \quad (4.32)$$

$$\frac{\partial}{\partial x_j} V''_j = \frac{\partial}{\partial x_j} V'_j = 0, \quad (4.33)$$

and

$$\rho \tilde{\varepsilon} = \tau'_{ij} \frac{\partial}{\partial x_j} \tilde{V}'_{ij} = \mu \left( \frac{\partial V'_i}{\partial x_j} + \frac{\partial V'_j}{\partial x_i} \right) \frac{\partial V'_i}{\partial x_j} = \mu \left( \frac{\partial V'_i}{\partial x_j} \right)^2 + \mu \frac{\partial V'_i}{\partial x_i} \frac{\partial V'_j}{\partial x_j}. \quad (4.34)$$

The last term of this equation is small for high Reynolds number flows as encountered in combustion systems [26], and will therefore be omitted. Decomposing the velocity, pressure and stress tensor into mean- and fluctuating quantities in Eq. (4.12), and subtracting Eq. (4.13) from this equation yields a transport equation for the fluctuating velocity

$$\frac{\partial}{\partial t} V'_i + \frac{3}{\rho x_j} (V'_i V'_j + \tilde{V}_i V'_j + V'_i \tilde{V}_j) = - \frac{1}{\rho} \frac{\partial}{\partial x_i} \rho' + \frac{1}{\rho} \frac{3}{\rho x_j} \tau'_{ij}$$

$$+ \frac{3}{\rho x_j} \tilde{V}'_{ij} \tilde{V}'_{ij}. \quad (4.35)$$

Differentiating this equation with respect to $x_j$, multiplying with $2 \sqrt{\frac{\partial V'_i}{\partial x_j}}$ and subsequent averaging yields the transport equation for the dissipation of turbulent kinetic energy [19], [26]

$$\frac{\partial}{\partial t} \tilde{\varepsilon} + \tilde{V}_j \frac{\partial}{\partial x_j} \tilde{\varepsilon} = - 2 \sqrt{\frac{\partial \tilde{V}_i}{\partial x_k}} \left( \frac{\partial \tilde{V}_i}{\partial x_j} \frac{\partial \tilde{V}_i}{\partial x_j} + \frac{\partial V'_i}{\partial x_j} \frac{\partial V'_i}{\partial x_j} \right) - 2 \sqrt{V'_k} \left( \frac{\partial \tilde{V}_i}{\partial x_j} \frac{\partial \tilde{V}_i}{\partial x_j} \right) \frac{\partial V'_i}{\partial x_k} \frac{\partial V'_i}{\partial x_j}. \quad (4.36)$$
\[
2 \frac{\partial V_i}{\partial x_k} \frac{\partial V_j}{\partial x_j} - 2 \frac{\partial^2 V_i}{\partial x_k \partial x_j} = \frac{\partial^2}{\partial x_k \partial x_j} \left( \frac{\nu}{\partial x_i} \right)^2 - 2 \frac{\partial \nu}{\partial x_i} \frac{\partial V_i}{\partial x_k} \frac{\partial V_j}{\partial x_j} - \frac{\partial \nu}{\partial x_k} \frac{\partial V_i}{\partial x_i} \right) \quad (4.36)
\]

The terms \(a\) and \(b\) represent generation by the mean flow and are negligible small at high Reynolds number [13]. Term \(c\) represents generation by turbulence, term \(d\) destruction by viscous action and term \(e\) represents diffusion. These three terms all contain unknown correlations of fluctuating quantities, and closure assumptions are necessary to model these terms. It can be argued [27] that the generation and destruction term can't be modelled seperately because these terms become infinitely large as the Reynolds number approaches infinity, whereas their difference remains finite. These two terms are commonly modelled as [17]

\[
-2 \nu \frac{\partial V_i}{\partial x_k} \frac{\partial V_j}{\partial x_j} - 2 \left( \frac{\partial^2 V_i}{\partial x_k \partial x_j} \right)^2 = C_{e_1} \frac{\nu}{k} \frac{\partial^2}{\partial x_k \partial x_j} - C_{e_2} \frac{\nu}{k} \frac{\partial^2 V_i}{\partial x_k \partial x_j} \quad , \quad (4.37)
\]

where \(C_{e_1}\) and \(C_{e_2}\) are empirical constants and \(P_k\) is the production of turbulent kinetic energy. The first component of the diffusion term \(e\) in Eq. (4.36) is modelled with the eddy-diffusivity concept, yielding

\[
\frac{\partial}{\partial x_k} \nu \frac{\partial V_i}{\partial x_j} - \frac{\partial}{\partial x_k} \nu \frac{\partial V_i}{\partial x_j} \frac{\partial \nu}{\partial x_k} = -\frac{\partial}{\partial x_k} \frac{\nu}{\sigma_k} \frac{\partial \nu}{\partial x_k} \quad , \quad (4.38)
\]

where \(\sigma_k\) is an empirical constant. The second component of the diffusion term, the pressure-diffusion term can be neglected [26], and the equation for dissipation of turbulent kinetic energy for constant density flows finally yields

\[
\frac{\partial}{\partial t} \nu \frac{\partial \nu}{\partial x_j} + \frac{\partial}{\partial x_j} \frac{\partial V_i}{\partial x_j} = -C_{e_1} \frac{\nu}{k} \frac{\partial V_i}{\partial x_j} \frac{\partial V_j}{\partial x_j} \frac{\partial \nu}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\nu}{\sigma_k} \right) \frac{\partial e}{\partial x_j} \right] - C_{e_2} \frac{\nu}{k} \frac{\partial^2 \nu}{\partial x_j \partial x_j} \quad , \quad (4.39)
\]

Note that the term \(\frac{\partial^2 \nu}{\partial x_j \partial x_j}\) is often neglected.
The weakest point in the $k - \varepsilon$ closure model is(8,21),(994,994) the equation for the dissipation rate $\varepsilon$ because the modelling of this equation can't be determined from measurements. Therefore several modifications of this equation are proposed, for instance by Hanjalic and Launder [28] who suggested to extend the generation term with a component taking into account effects of irrotational straining, and by Sindir and Harsha [26] who suggested to replace the production term of turbulent kinetic energy $P_k$ by

$$P_k = C_{\mu} \frac{k}{\varepsilon} \left( \frac{\partial \tilde{V}_i}{\partial x_j} \right)^2.$$  (4.40)

Both these modifications seems to give better results in predicting turbulent flows, but should be tested better before using them in Eq. (4.39). The equation for the dissipation rate of turbulent kinetic energy for flows with variable density may now be written in a form analogous to Eq. (4.39) [29]. The only extension of this equation is a term taking into account the velocity-density correlation $\tilde{V} \bar{\rho}$ yielding [24]

$$\frac{\partial}{\partial t} \bar{\rho} \varepsilon + \frac{\partial}{\partial x_j} \bar{\rho} \tilde{V}_j \varepsilon = C_{\varepsilon 1} \frac{\bar{\rho}}{k} P_k - C_{\varepsilon 2} \frac{\bar{\rho}}{\bar{k}^2} \sigma_t \frac{\partial \bar{\rho}}{\partial x_i} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_t} \frac{\partial \varepsilon}{\partial x_j} \right] - C_{\varepsilon 2} \frac{\bar{\rho}}{k} \varepsilon^2.$$  (4.41)

The $\bar{k} - \bar{\varepsilon}$ turbulence closure model for flows with variable density may be summarized as

$$- \bar{\rho} \tilde{V}_i \tilde{V}_j = \mu_t \left( \frac{\partial \tilde{V}_i}{\partial x_j} + \frac{\partial \tilde{V}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left( \bar{\rho} \bar{k} + \mu_t \frac{\partial \tilde{V}_k}{\partial x_k} \right),$$  (4.42)

$$- \bar{\rho} \tilde{V}_i \varphi'' = \mu_t \frac{\partial \tilde{\varphi}}{\partial x_i},$$  (4.43)

$$\mu_t = \bar{\rho} C_{\mu} \bar{k} \tilde{\gamma} \bar{\varepsilon},$$  (4.44)

$$\bar{k} = \frac{\tilde{\varphi}}{2},$$  (4.45)

$$P_k = - \bar{\rho} \tilde{V}_i \tilde{V}_j \frac{\partial \tilde{V}_j}{\partial x_i},$$  (4.46)
\[
\frac{\partial}{\partial t} \bar{\rho} \bar{k} + \frac{\partial}{\partial x_j} \bar{\rho} \bar{V}_j \bar{k} = \bar{P}_k + \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_k} \frac{\partial \bar{k}}{\partial x_j} \right] - \frac{\mu_t}{\rho^2} \frac{\partial \bar{\rho}}{\partial x_i} \frac{\partial \bar{\rho}}{\partial x_i} - \bar{\rho} \bar{\varepsilon}, \quad (4.47)
\]

\[
\frac{\partial}{\partial t} \bar{\rho} \bar{\varepsilon} + \frac{\partial}{\partial x_j} \bar{\rho} \bar{V}_j \bar{\varepsilon} = C_{\varepsilon_1} \frac{\bar{\varepsilon}}{k} \bar{P}_k - C_{\varepsilon_2} \bar{\varepsilon} \frac{\mu_t}{\rho^2} \frac{\partial \bar{\rho}}{\partial x_i} \frac{\partial \bar{\rho}}{\partial x_i} +
\]

\[
\frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_k} \frac{\partial \bar{\varepsilon}}{\partial x_j} \right] - C_{\varepsilon_2} \bar{\rho} \frac{\bar{\varepsilon}^2}{k} \quad (4.48)
\]

The constants appearing in these equations have assigned to the values given in Table 4.1 [15]

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$C_{\varepsilon_1}$</th>
<th>$C_{\varepsilon_2}$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\varepsilon$</th>
<th>$\sigma_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
<td>1.0</td>
<td>1.30</td>
<td>0.7</td>
</tr>
</tbody>
</table>

Table 4.1: Values for the constants appearing in the $\bar{k} - \bar{\varepsilon}$ model

Note however that some authors use slightly different values for these constants.

4.3. REYNOLDS-STRESS CLOSURE MODELS

The $\bar{k} - \bar{\varepsilon}$ model is based on the eddy viscosity/diffusivity concept in which it is assumed that the eddy viscosity/diffusivity are isotropic. This means that the various Reynolds stresses

\[
\bar{\rho} \bar{V}_i'' \bar{V}_j'' \quad \text{and the fluxes} \quad \bar{\rho} \bar{V}_i'' \bar{V}_j''
\]

are all taking similar forms. This assumption is certainly not true for complex flows [29]. To overcome this problem, transport equations for the various Reynolds stresses and scalar fluxes must be derived from the Navier-Stokes equations. These equations contain higher order correlations which have to be approximated by lower order correlations to obtain a deterministic set of equations. As already mentioned in Section 4.1, the application of a Reynolds stress/flux turbulence closure model is limited because, especially in flows with a large number of species, the number of equations to be solved is large. Therefore this section has to be regarded as an introduction to Algebraic Stress Modelling which will be discussed in the next section. The transport equation for the Reynolds stresses has been derived in Section 4.2 and states

\[
\frac{\partial}{\partial t} \bar{\rho} \bar{V}_i'' \bar{V}_j'' + \frac{\partial}{\partial x_k} \bar{\rho} \bar{V}_k V_i'' V_j'' = - \bar{\rho} V_i'' V_k'' \frac{\partial}{\partial x_k} \dot{V}_j'' - \bar{\rho} V_j'' V_k'' \frac{\partial}{\partial x_k} \dot{V}_i'' -
\]

\[a\]
\[
\frac{\partial}{\partial x_i} \left( \rho V_i \frac{\partial \rho}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left( \rho V_i \frac{\partial p}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left( \frac{K_{ij}}{\rho} \frac{\partial \rho}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left( \frac{\partial p}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left( \frac{\partial \tau_{ij}}{\partial x_i} \right) \quad (4.49)
\]

The transport equations for the scalar fluxes may be derived as follows. In general, the scalar conservation equation may be written as

\[
\frac{\partial}{\partial t} \rho \phi + \frac{\partial}{\partial x_j} \rho V_j \phi = - \frac{\partial}{\partial x_j} D_j(\phi) + \rho S(\phi) \quad (4.50)
\]

where \( \phi \) represents the scalar, \( D_j \) the diffusion of \( \phi \) and \( S(\phi) \) a source term. For instance, if \( \phi \) represents the mass fraction of species \( s \), \( Y_s \), then \( D_j \) equals \( \rho Y_s V_{sj} \) and \( S(\phi) \) equals \( \rho \omega_s \). The Favre-averaged scalar conservation equation yields

\[
\frac{\partial}{\partial t} \bar{\rho} \bar{\phi} + \frac{\partial}{\partial x_j} \bar{\rho} V_j \bar{\phi} = - \frac{\partial}{\partial x_j} \bar{D_j} - \frac{\partial}{\partial x_j} \bar{V}_j^\prime \bar{\phi} + \bar{\rho} \bar{S} - \frac{\partial}{\partial x_j} \bar{\rho} V_j^\prime \bar{\phi}'' \quad (4.51)
\]

Multiplying the momentum equation (4.12) by \( \bar{\phi} \) and adding this equation to the scalar conservation equation (4.50) multiplied by \( V_i \) yields

\[
\frac{\partial}{\partial t} \rho V_i \phi + \frac{\partial}{\partial x_j} \rho V_i V_j \phi = \rho g_i \phi - \phi \frac{\partial p}{\partial x_i} + \phi \frac{\partial \tau_{ij}}{\partial x_i} - V_i \frac{\partial}{\partial x_j} D_j + \rho V_i S \quad (4.52)
\]

Favre-decomposition and subsequent averaging yields

\[
\frac{\partial}{\partial t} \left( \bar{\rho} \bar{V}_i \bar{\phi} + \bar{\rho} \bar{V}_i^\prime \bar{\phi}' \right) + \frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{V}_i \bar{V}_j \bar{\phi} + \bar{\rho} \bar{V}_i \bar{V}_j^\prime \bar{\phi}' + \bar{\rho} \bar{V}_i \bar{V}_j^\prime \bar{\phi}'' + \bar{\rho} \bar{V}_i \bar{V}_j \bar{\phi}'' \right) \]
\[
\bar{\rho} \bar{\phi} \bar{V}_i \bar{V}_j + \bar{\rho} \bar{V}_i \bar{V}_j^\prime \bar{\phi}' \right) = \bar{\rho} g_i \bar{\phi} - \bar{\phi} \frac{\partial \bar{p}}{\partial x_i} - \bar{\phi} \frac{\partial \tau_{ij}}{\partial x_i} + \bar{\rho} \bar{V}_i \bar{S} + \bar{\rho} \bar{V}_i \bar{S}'' \quad (4.53)
\]

Multiplying the Favre-averaged momentum equation (4.13) by \( \bar{\phi} \), adding it to the Favre averaged scalar conservation equation (4.51) multiplied by \( \bar{V}_i \) and subtracting this equation from Eq. (4.53) yields the scalar flux equation
The Eqs. (4.49) and (4.54) have analogous forms, and the meaning of the various terms is

a. represents generation of stresses and fluxes. These terms don't require modelling because they are expressed in terms of stresses and fluxes;

b. represents diffusion;

c. represents the pressure strain rate (Eq. (4.49)) and the pressure-flux correlation (Eq. (4.54));

d. represents dissipation and;

e. is the source term correlation.

The diffusion term in Eq. (4.49) may be modelled as [25]

\[
\frac{\partial}{\partial x_k} \rho \bar{V}_i^n \bar{V}_j^n = - \frac{\partial}{\partial x_k} \left[ C_s \rho \frac{k}{\varepsilon} \left( \bar{V}_i^n \bar{V}_j^n \frac{\partial}{\partial x_k} \bar{V}_j^n + \bar{V}_j^n \frac{\partial}{\partial x_k} \bar{V}_i^n \right)^2 \right],
\]

where \( C_s \) is an empirical constant. This equation is quite complicated and possess a large number of terms, and therefore Jones [29] suggested to use

\[
\frac{\partial}{\partial x_k} \rho \bar{V}_i^n \bar{V}_j^n = - \frac{\partial}{\partial x_k} \left[ C_s \rho \frac{k}{\varepsilon} \bar{V}_j^n \frac{\partial}{\partial x_k} \bar{V}_i^n \bar{V}_j^n \right].
\]

where \( C_s \) is a constant, equal to 0.22 (\( C_s^2 \) equals 0.11). Calculations showed that the difference in predictions with these two models is small [26], and therefore we will use Eq. (4.56) to model the diffusion term in Eq. (4.49). The diffusion term in the scalar-flux equation is modelled in an analogous way as [29]

\[
\frac{\partial}{\partial x_j} \rho \bar{V}_i^n \bar{V}_j^n \phi^n = - \frac{\partial}{\partial x_j} \left[ C_s \rho \frac{k}{\varepsilon} \left( \bar{V}_i^n \bar{V}_j^n \frac{\partial}{\partial x_k} \bar{V}_j^n \phi^n + \bar{V}_j^n \frac{\partial}{\partial x_k} \bar{V}_i^n \phi^n \right) \right].
\]
\[ \begin{align*}
\bar{V}_j \frac{\partial \bar{V}_i}{\partial x_j} + \bar{V}_i \frac{\partial \bar{V}_j}{\partial x_i} &= \bar{V}_j \frac{\partial \bar{p}}{\partial x_j} + \bar{V}_i \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{p}}{\partial x_j} \frac{\partial \bar{V}_i}{\partial x_j} + \frac{\partial \bar{p}}{\partial x_i} \frac{\partial \bar{V}_j}{\partial x_i} - \\
\rho' \left( \frac{\partial \bar{V}_i}{\partial x_j} + \frac{\partial \bar{V}_j}{\partial x_i} \right) & \quad . \quad (4.58)
\end{align*} \]

The two diffusion terms in this equation are negligible in high Reynolds number flows [26] and are omitted. The first two terms can be modelled by deriving and modelling equations for the fluctuating velocity components, yielding [25]

\[ \begin{align*}
\frac{\partial}{\partial t} \bar{V}_i + \frac{\partial}{\partial x_j} \bar{p} \bar{V}_j \bar{V}_i &= - \bar{p} \bar{V}_j \frac{\partial}{\partial x_j} \bar{V}_i + \left[ \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial}{\partial x_k} \bar{V}_i \right] + \\
\bar{V}_j \bar{V}_k \frac{\partial}{\partial x_k} \bar{V}_i \bar{V}_j + \left[ C_1 \frac{\bar{V}_i \bar{V}_j \bar{V}_k}{k} \frac{\partial}{\partial x_k} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial}{\partial x_k} \bar{V}_i \right] - \\
C_2 \frac{\bar{V}_i \bar{V}_j \bar{V}_k}{k} \frac{\partial}{\partial x_k} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial}{\partial x_k} \bar{V}_i - \\
C_3 \frac{\bar{V}_i \bar{V}_j \bar{V}_k}{k} \frac{\partial}{\partial x_k} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial}{\partial x_k} \bar{V}_i - \\
C_4 \frac{\bar{V}_i \bar{V}_j \bar{V}_k}{k} \frac{\partial}{\partial x_k} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial}{\partial x_k} \bar{V}_i - \quad (4.59)
\end{align*} \]

where \( C_1 = 0.22, C_2 = 4.3, C_3 = 3.2, C_4 = 0.5 \) and \( C_4 = 1.0 \). (Jones [29] gives a slightly different modelling of this equation.) The remaining two terms in Eq. (4.58) are called the 'redistribution' terms because they redistribute turbulent energy among the normal stresses. The modelling of this term is extensively discussed by Sindir and Harsha [26] and by Jones [29], yielding

\[ \begin{align*}
\rho' \left( \frac{\partial \bar{V}_i}{\partial x_j} + \frac{\partial \bar{V}_j}{\partial x_i} \right) &= - C_1 \bar{p} \frac{\bar{V}_i \bar{V}_j \bar{V}_k}{k} \left( \frac{2}{3} \delta_{ij} \bar{k} \right) + \frac{C_2 + 8}{11} \left( \bar{p} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial \bar{V}_j}{\partial x_k} \right) + \\
\frac{6C_2 + 4}{11} \left( \bar{p} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial \bar{V}_j}{\partial x_k} \right) + \delta_{ij} \bar{p} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial \bar{V}_j}{\partial x_k} - \\
\frac{2 - 8C_2}{11} \left( \bar{p} \bar{V}_i \bar{V}_j \bar{V}_k \frac{\partial \bar{V}_j}{\partial x_k} + \bar{p} \bar{V}_j \bar{V}_k \frac{\partial \bar{V}_i}{\partial x_j} \right) - \\
\frac{40C_2 + 12}{55} \delta_{ij} \bar{V}_i \bar{V}_j \bar{V}_k \bar{p} \bar{k} \quad . \quad (4.60)
\end{align*} \]

The constants \( C_1 \) and \( C_2 \) appearing in this equation have a value of 1.5 and 0.4 respectively. This equation is derived with the assumption of small density fluctuations [25], [29], and it is indicated that the constants \( C_1 \) and \( C_2 \) .
should depend on the variation of the density fluctuations [25]. The pressure-flux correlation term in Eq. (4.54) can be split up into two parts

$$\rho \frac{\partial \tilde{\psi}}{\partial x_i} = \bar{\omega} \rho \frac{\partial \tilde{p}}{\partial x_i} + \bar{\omega} \rho \frac{\partial \tilde{p}'}{\partial x_i}$$

(4.61)

Modelling of the first term requires an expression for \(\bar{\omega}\). Jones [29] assumes that this term will be given by the combustion model. Combustion modelling will be discussed in a following report, and until then we assume that \(\bar{\omega}\) is known. The second term in Eq. (4.61) is modelled as [29]

$$\rho \frac{\partial \tilde{p}'}{\partial x_i} = C_{\omega_1} \bar{\psi} \frac{\rho}{k} \frac{\partial}{\partial x_i} \bar{\omega} + C_{\omega_2} \bar{\psi} \frac{\rho}{k} \left( \frac{\partial \bar{V}_i \bar{V}_j}{\partial x_k} \right) \bar{V}_j \bar{\omega} +$$

$$\frac{1}{5} \left( \delta_{ij} \frac{\partial}{\partial x_k} \bar{V}_i \bar{\omega} + \delta_{ik} \frac{\partial}{\partial x_j} \bar{V}_j \bar{\omega} \right) \bar{V}_j \bar{\omega} - \frac{4}{5} \bar{\omega} \bar{V}_j \bar{\omega} \frac{\partial \bar{V}_i}{\partial x_j},$$

(4.62)

where \(C_{\omega_1} = 4.3\) and \(C_{\omega_2} = 3.2\). The dissipation term in Eq. (4.49) can be related to the dissipation function \(\varepsilon\). As already mentioned in Section 4.2, terms involving the mean stress tensor, and terms involving diffusion of stresses are negligible small, and the dissipation term may be approximated by [29]

$$\bar{V}_j \frac{\partial}{\partial x_k} \tau_{ik} + \bar{V}_i \frac{\partial}{\partial x_k} \tau_{jk} = - \left( \tau_{ik} \frac{\partial}{\partial x_k} \bar{V}_j + \tau_{ik} \frac{\partial}{\partial x_k} \bar{V}_i \right) = - \frac{2}{3} \varepsilon \delta_{ij}$$

(4.63)

It is hereby assumed that the small scale dissipative turbulent motion is isotropic, which is the case in high Reynolds number flows. When this assumption is applied to the dissipation term in the scalar flux equation, it leads to the disappearance of this term. The term which remains to be modelled is the source term in Eq. (4.54). The modelling of this term must be given by a combustion model, which will be discussed in a following report. The Reynolds-stress closure model must be completed with equations for the turbulent kinetic energy \(k\) and the dissipation rate \(\varepsilon\). These equations are derived and modelled in Section 4.2, but when using a Reynolds stress closure model it is customary to model the diffusion terms with a general gradient flux model with tensorial transport coefficients, i.e.

$$\tilde{p} \bar{V}_i \bar{\psi} = C_{\psi} \frac{k}{\varepsilon} \tilde{p} \bar{V}_i \bar{V}_j \frac{\partial \bar{\psi}}{\partial x_i}$$

(4.64)

The Reynolds stress/flux closure model can now be summarized as
\[
\frac{3}{3t} \rho \bar{v}_i^e \bar{v}_j^e + \frac{3}{3x_k} \rho \bar{v}_k \bar{v}_i^e \bar{v}_j^e = p_{ij} + \frac{3}{3x_k} \left[ c_s \frac{\kappa}{\varepsilon} \left( \bar{v}_k \bar{v}_i^e \frac{3}{3x_k} \bar{v}_i^e \bar{v}_j^e \right) \right] - \\
C_1 \frac{\bar{v}_i^e}{k} \left( \bar{v}_j^e \bar{v}_j^e - \frac{2}{3} \delta_{ij} \right) + \frac{C_2 + 8}{11} p_{ij} - \frac{6C_2 + 4}{11} \left( \bar{v}_i^e \bar{v}_j^e \frac{3}{3x_k} \bar{v}_k + \delta_{ij} p_k \right) - \\
\frac{2 - 8C_2}{11} \left( \bar{v}_i^e \bar{v}_k \frac{3}{3x_j} \bar{v}_k + \bar{v}_i^e \bar{v}_j^e \frac{3}{3x_k} \bar{v}_k + \delta_{ij} \frac{3}{55} \left( \bar{v}_i^e \frac{3}{3x_j} + \frac{3}{3x_k} \bar{v}_i^e \right) \bar{v}_k + \\
\frac{40C_2 + 12}{55} \delta_{ij} \frac{3}{3x_k} \bar{v}_k + \frac{2}{3} \bar{v}_k \right] = 0. \\
(4.65)
\]

\[
P_{ij} = - \rho \bar{v}_i^e \frac{3}{3x_k} \bar{v}_i^e \bar{v}_j^e = \bar{v}_j^e - \rho \bar{v}_i^e \frac{3}{3x_k} \bar{v}_i^e, \\
(4.66)
\]

\[
P_k = \frac{1}{2} P_{ii} = - \rho \frac{3}{3x_j} \bar{v}_i^e \bar{v}_i^e \bar{v}_i^e - \rho \bar{v}_i^e \frac{3}{3x_j} \bar{v}_i^e; \\
(4.67)
\]

\[
\frac{\bar{v}_i^e}{\Delta t} \bar{v}_i^e + \frac{3}{3x_j} \rho \frac{3}{3x_j} \bar{v}_j^e \bar{v}_i^e \bar{v}_j^e = - \rho \bar{v}_i^e \frac{3}{3x_j} \bar{v}_i^e - \rho \bar{v}_i^e \frac{3}{3x_j} \bar{v}_j^e \frac{3}{3x_j} \bar{v}_i^e + \frac{3}{3x_j} \bar{v}_i^e \bar{v}_j^e + \frac{3}{3x_j} \bar{v}_j^e \frac{3}{3x_j} \bar{v}_j^e + \frac{3}{3x_j} \bar{v}_j^e \frac{3}{3x_j} \bar{v}_i^e \\
\]
\[ C_4 \left( \frac{\rho V_i^2}{\rho^2} \right) \frac{\partial}{\partial x_j} \rho \frac{V_i V_j}{x_i} \]  

(4.69)

\[ \frac{\partial}{\partial t} \rho \frac{k}{\rho} + \frac{\partial}{\partial x_j} \rho \frac{V_j}{x_j} \frac{\partial k}{\partial x_j} = P_k + \frac{3}{\partial x_j} \left[ C_s \frac{k}{\rho} \frac{\partial}{\partial x_j} \left( \frac{V_i V_j}{x_i} \frac{\partial \rho}{\partial x_i} \right) \right] - \left( \frac{\partial}{\partial x_i} \frac{\rho V_i}{x_i} \frac{\partial k}{\partial x_i} \right) \]  

(4.70)

\[ \frac{3}{\partial t} \rho \frac{\partial}{\partial x_j} \rho \frac{V_j}{x_j} \frac{\partial k}{\partial x_j} = C_{\varepsilon_1} \frac{\rho}{k} \left( P_k - \frac{\partial}{\partial x_i} \frac{\partial k}{\partial x_i} \right) + \frac{\partial}{\partial x_j} \left[ C_{\varepsilon_2} \frac{\partial k}{\partial x_j} \frac{\partial V_i}{x_i} \frac{\partial \varepsilon}{\partial x_i} \right] \]  

(4.71)

The values of the different constants appearing in these equations are summarized in Table 4.2.

<table>
<thead>
<tr>
<th></th>
<th>Ref. 25</th>
<th>Ref. 29</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_s )</td>
<td>0.22</td>
<td>0.22</td>
</tr>
<tr>
<td>( C_1 )</td>
<td>8.5*</td>
<td>1.5</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>( C_{\varepsilon_1} )</td>
<td>-</td>
<td>4.3</td>
</tr>
<tr>
<td>( C_{\varepsilon_2} )</td>
<td>-</td>
<td>3.2</td>
</tr>
<tr>
<td>( C_{1_1} )</td>
<td>4.3</td>
<td>4.3</td>
</tr>
<tr>
<td>( C_{2_2} )</td>
<td>3.2</td>
<td>3.2</td>
</tr>
<tr>
<td>( C_{3_3} )</td>
<td>0.5</td>
<td>0.8</td>
</tr>
<tr>
<td>( C_{4_4} )</td>
<td>1.0</td>
<td>~1.0</td>
</tr>
<tr>
<td>( C_{\varepsilon_1} )</td>
<td>1.28</td>
<td>1.45</td>
</tr>
<tr>
<td>( C_{\varepsilon_2} )</td>
<td>2.2</td>
<td>1.90</td>
</tr>
<tr>
<td>( C_\varepsilon )</td>
<td>0.18</td>
<td>0.18</td>
</tr>
</tbody>
</table>

(* This value of \( C_1 \) may be doubtful, ref. 27 for instance also gives \( C_1 = 1.5 \))

Table 4.2.: Values for the Constants appearing in the Reynolds Stress/Flux Equations.
From the Eqs. (4.65) to (4.71), it can concluded that the Reynolds Stress/Flux turbulence closure model is complicated, and that the number of equations to be solved is large.

4.4. ALGEBRAIC STRESS/FLUX MODELS

Reynolds Stress/Flux modelling is one of the most general turbulence closure models that can be applied to all kind of flows. Disadvantages of this method however are the large number of differential equations that have to be solved and the complexity of this model. To overcome these problems so called Algebraic Stress Models have been developed in which the transport equations for the stresses and fluxes are simplified to algebraic equations, whereby the model still retains the most of its basis features, such as for instance the non-isotropic eddy viscosity/diffusivity concept.

It can be seen from Eq. (4.65) that the only terms which contain gradients of \( \rho \overline{V_i^V V_j^V} \) are the local rate of change, the convective transport and the diffusive transport. These terms need to be modelled to obtain an algebraic model.

The simplest approach is neglecting these terms, but this leads to the inconsistency that the sum of the normal stresses \( V_i^V V_j^V \) is equal to \( 2k \) only in the case that the production of turbulent kinetic energy equals the dissipation [30].

In general, this is not the case.

A more general approximation has been proposed by Rodi [31] who related the transport of Reynolds stresses \( V_i^V V_j^V \) to the transport of turbulent kinetic energy \( k \) by noting that

\[
-\frac{\partial}{\partial t} \overline{V_i^V V_j^V} = \frac{\partial}{\partial t} \overline{V_i^V V_j^V} \frac{Dk}{D\bar{t}} + \frac{1}{k} \frac{Dk}{Dt} \frac{\overline{V_i^V V_j^V}}{k} \quad .
\]  

(4.72)

Furthermore, he assumed that the material change of \( \overline{V_i^V V_j^V} / k \) is small compared with the material change of \( V_i^V V_j^V \), and Eq. (4.72) can be approximated by

\[
-\frac{\partial}{\partial t} \overline{V_i^V V_j^V} = \frac{\partial}{\partial t} \overline{V_i^V V_j^V} \frac{Dk}{D\bar{t}} .
\]

(4.73)

The diffusion term in the Reynolds stress transport equation (4.65) may be written as

\[
\text{Diff} \left( \overline{V_i^V V_j^V} \right) = \frac{3}{\partial x_k} \left( B \frac{3}{\partial x_k} \overline{V_i^V V_j^V} \right) ,
\]

(4.74)

where

\[
B = C_s \frac{\rho}{k} \overline{k \overline{V_i^V V_j^V}} \quad .
\]

(4.75)
The diffusion term in the equation for the turbulent kinetic energy \( \tilde{k} \) (4.70) may be written as

\[
\text{Diff} (\tilde{k}) = \frac{\partial}{\partial x_k} \left( B \frac{\partial}{\partial x_k} \tilde{k} \right) .
\]  
(4.76)

Eqs. (4.76) and (4.74) have similar forms and, analogous to Eq. (4.73), it is therefore assumed that

\[
\text{Diff} (V_i'' V_j'') = \frac{\tilde{V}_i'' \tilde{V}_j''}{k} \text{Diff} (\tilde{k}) .
\]  
(4.77)

From Eq. (4.70) it follows that

\[
\bar{\rho} \frac{D}{Dt} \tilde{k} - \text{Diff} (\tilde{k}) = P_k - \sum_i \frac{\partial \tilde{p}}{\partial x_i} - \tilde{\rho} \tilde{\varepsilon}
\]  
(4.78)

where use has been made of the equation for conservation of mass. Subtracting Eq. (4.77) from Eq. (4.73), and substitution of Eq. (4.78) yields

\[
\bar{\rho} \frac{D}{Dt} \tilde{V}_i'' \tilde{V}_j'' \left( \text{Diff} (\tilde{V}_i'' \tilde{V}_j'') \right) = \frac{\tilde{V}_i'' \tilde{V}_j''}{k} \left( P_k - \sum_i \frac{\partial \tilde{p}}{\partial x_i} - \tilde{\rho} \tilde{\varepsilon} \right)
\]  
(4.79)

From Eq. (4.65) it follows that the Reynolds stresses equals the following algebraic expression

\[
\tilde{V}_i'' \tilde{V}_j'' = \frac{\tilde{k}}{(P_k + \sum_i \frac{\partial \tilde{p}}{\partial x_i})} \left\{ P_{ij} - C_1 \tilde{\rho} \tilde{\varepsilon} \left( \tilde{V}_i'' \tilde{V}_j'' - \frac{2}{3} \delta_{ij} \tilde{k} \right) - \frac{C_2 + 8}{11} \frac{6C_2 + 4}{11} \left( \tilde{\rho} \tilde{V}_i'' \tilde{V}_j'' \frac{\partial}{\partial x_k} \tilde{V}_k + \delta_{ij} P_k \right) - \frac{2 - 8C_2}{11} \right\} + \\
\left( \tilde{\rho} \frac{\partial}{\partial x_j} \tilde{V}_j'' \frac{\partial}{\partial x_k} \tilde{V}_k + \tilde{\rho} \frac{\partial}{\partial x_j} \tilde{V}_j'' \frac{\partial}{\partial x_k} \tilde{V}_k \right) - \frac{30C_2 - 2}{55} \left( \frac{\partial \tilde{V}_i''}{\partial x_j} + \frac{\partial \tilde{V}_j''}{\partial x_i} \right) \tilde{\rho} \tilde{k} + \frac{40C_2 + 12}{55} \delta_{ij} \frac{\partial}{\partial x_k} \tilde{V}_k - \frac{2}{3} \tilde{\varepsilon} \delta_{ij} \right\}
\]  
(4.80)
Simplyfing the scalar flux equations to algebraic expressions is difficult because both velocity and scalar fluctuations contribute to this term. Analogous to Eq. (4.73), the local and spatial transport of the scalar flux \( \overline{V_i \varphi} \) is written as [29]

\[
- \frac{\rho}{\partial t} \overline{V_i \varphi} = - \frac{\rho}{\partial t} \left( \frac{\overline{V_i \varphi}}{\sqrt{k \overline{\varphi^{\prime 2}}}} \right) \approx - \frac{\overline{V_i \varphi}}{\sqrt{k \overline{\varphi^{\prime 2}}}} \frac{D}{\partial t} \sqrt{k \overline{\varphi^{\prime 2}}},
\]

(4.81)

The property \( \sqrt{k \overline{\varphi^{\prime 2}}} \) cannot be calculated from a transport equation, and therefore Gibson and Launder [32] proposed to model the transport terms (i.e., local-, spatial- and diffusive transport) in the scalar flux equations as

\[
- \frac{\rho}{\partial t} \overline{V_i \varphi} - \text{Diff (} \overline{V_i \varphi} \text{)} = \frac{\overline{V_i \varphi}}{2 \overline{k}} \left( p_{k} - \frac{\overline{V_i \varphi}}{\partial x_i} - \rho \varepsilon \right),
\]

(4.82)

where the contribution of the scalar fluctuation \( \overline{\varphi^{\prime 2}} \) to \( \overline{V_i \varphi} \) is assumed to be negligible small. Substitution of Eq. (4.68) into Eq. (4.82) yields the algebraic flux equation

\[
\overline{V_i \varphi} = \frac{2 \overline{k}}{\left( p_{k} - \overline{V_i \varphi} \frac{\partial \rho}{\partial x_i} - \rho \varepsilon \right)} \left\{ - \rho \overline{V_j \varphi} \frac{\partial}{\partial x_i} \overline{V_i} - \frac{\overline{V_j \varphi}}{\partial x_j} + \frac{\rho \varepsilon}{\overline{k}} \left( \frac{\overline{V_i \varphi}}{\overline{k}} - \frac{2}{3} \delta_{ij} \right) \overline{V_j \varphi} - \frac{1}{5} \left( \delta_{jk} \rho \overline{V_i \varphi} \varphi'' + \delta_{ik} \rho \overline{V_j \varphi} \varphi'' \right) \frac{\partial \overline{V_i \varphi}}{\partial x_k} + \frac{4}{5} \rho \overline{V_i \varphi} \overline{V_j \varphi} \frac{\partial \overline{V_j \varphi}}{\partial x_j} + \rho \overline{V_i \varphi} \overline{S''} \right\}.
\]

(4.83)

The simplest way to model the transport terms in the equation for the fluctuating velocity components (4.69) is neglecting these terms [29] yielding

\[
- \rho \overline{V_j} \frac{\partial \overline{V_i \varphi}}{\partial x_j} + \overline{V_i \varphi} \frac{\rho}{\partial x_j} - C_{1} \frac{\rho}{k} \overline{V_i \varphi} + C_{2} \frac{\rho}{k} \overline{V_j \varphi} \left( \frac{\overline{V_i \varphi}}{k} - \frac{2}{3} \delta_{ij} \right) - \rho \overline{V_j} \frac{\partial \overline{V_i \varphi}}{\partial x_j},
\]

\[
C_{3} \frac{\rho}{\partial x_j} - C_{4} \frac{\rho^{2}}{\partial x_j} \overline{V_i \varphi} = 0.
\]

(4.84)

Another, rather crude approximation of the fluctuating velocity components, which is possibly of limited value, is to approximate these terms by a gradient flux model [29], i.e.
\[
V_j = \frac{1}{c} \frac{k}{\varepsilon} \left( \nabla V_i \nabla V_j - \frac{2}{3} \delta_{ij} \nabla \cdot V \right)
\]

(4.85)

This expression may be derived from Eq. (4.84) by assuming that the mean rate of strain can be ignored, and by putting the constants \( C_2 \) to \( C_4 \) equal to zero. The Algebraic Stress/Flux Model consists of the Eqs. (4.80), (4.83) and (4.84), whereby \( k \) and \( \varepsilon \) are determined from Eqs. (4.70) and (4.71) respectively. The values of the different constants appearing in these equations are summarized in Table 4.2.

4.5. MULTIPLE-SCALE TURBULENCE MODELLING

Turbulence consists of fluctuating motions with a continuous spectrum of length (and time) scales. The largest length scales or eddies have the dimension of the flowfield, while the smallest length scales are related to the diffusive action of the molecular viscosity [13]. Turbulent energy production is related to the largest eddies, while dissipation of turbulent energy is primarily related to the smallest eddies. Turbulence closure models which employ just a single length scale therefore are very simplistic because they neglect the fact that production- and dissipation of turbulent energy occurs at different length scales. The fact that single-scale models yield successful predictions of many flowfields reflects more that these flows are close to spectral equilibrium, i.e. the dissipation of turbulent energy of the large eddies equals the dissipation of the small eddies (\( \varepsilon_p = \varepsilon_T = \varepsilon \)), than that the single-scale model is adequate [21].

Because turbulent energy production occurs at large length scales and dissipation of turbulent energy mainly takes place at small length scales, there must be a region of length scales (the transfer region) in which turbulent energy is transferred from the largest eddies to the smallest. This transfer can introduce a lag phenomenon, i.e. turbulent energy production and turbulent energy dissipation do not both decrease or increase in the same regions of the flow, as for instance the \( k - \varepsilon \) model implies. Figure 3 [21] shows the energy spectre of turbulent energy in a shear flow at high Reynolds number as function of the wave number \( k \) (\( k^{-1} \) is proportional to the length scale).

![Figure 3: Spectral Division of Turbulent Energy and Dissipation Rate](image-url)
To introduce a model which takes into account the different processes at different length scales (or wave numbers), Hanjalic et al. [21] divided the energy spectrum in three parts, as is shown in Figure 3. They assumed that production of turbulent energy takes place at wave numbers below \( K_1 \), characterized by \( k_p \) and \( \varepsilon_p \), that transfer of turbulent energy takes place in the wave number range from \( K_1 \) to \( K_2 \), characterized by \( k_T \) and \( \varepsilon_T \) and that at wave numbers above \( K_2 \) turbulent energy is dissipated as heat. The division of the energy spectrum in more parts is the key feature of the multiple-scale-model, and may be carried out as many times as necessary. In practice however, a division in three regions appears to be sufficient [22]. This requires two sets of transport equations. The exact value of \( K_1 \), in the wave number spectrum at which the energy spectrum is divided seems to have little influence on the results, except in the limiting cases \( K_1 = K_2 \) and \( K_1 = 0 \); however the choice of \( K_1 \) seems to affect the determination of the initial condition according to Fabris et al. [22]. The equations for the production and transfer of turbulent energy \( k \) and dissipation rate \( \varepsilon \) are similar to the single point \( k \) and \( \varepsilon \) equations, derived in Section 4.2, because they describe similar processes. Until now however, equations for \( k_p \), \( k_T \), \( \varepsilon_p \) and \( \varepsilon_T \) had only been derived in the case of constant density flows. In the case of fluctuating density flows, the equations for the turbulent kinetic energy \( k \) and the dissipation rate \( \varepsilon \) are extended with a term containing gradients of mean pressure and mean density. Mean quantities vary slowly across a flow (except near walls), and are therefore connected with the large length scales or small wave number. It is assumed that these terms only are important at low wave numbers, i.e. in the production region. The \( k - \varepsilon \) equations for the production region may now be written as

\[
\frac{\partial}{\partial t} \overline{\rho} \overline{k_p} + \frac{\partial}{\partial x_j} \overline{\rho} \overline{\nabla_j} \overline{k_p} = P_k - \frac{\mu_t}{\sigma_t} \frac{\partial \overline{\rho}}{\partial x_i} \frac{\partial \overline{\rho}}{\partial x_i} + \frac{\partial}{3x_j} \left[ \frac{\mu_t}{\sigma_k} \frac{\partial \overline{k_p}}{\partial x_j} \right] - \overline{\rho} \overline{\varepsilon_p}, \quad (4.86)
\]

and

\[
\frac{\partial}{\partial t} \overline{\rho} \overline{\varepsilon_p} + \frac{\partial}{\partial x_j} \overline{\rho} \overline{\nabla_j} \overline{\varepsilon_p} = \frac{C_p}{k_p} \frac{\overline{\rho}}{k_p} \frac{\overline{\varepsilon_p}}{P_k} - \frac{C_p}{k_p} \frac{\overline{\rho}}{k_p} \frac{\mu_t}{\sigma_t} \frac{\partial \overline{\rho}}{\partial x_i} \frac{\partial \overline{\rho}}{\partial x_i} + \frac{\partial}{3x_j} \left[ \frac{\mu_t}{\sigma_k} \frac{\partial \overline{\varepsilon_p}}{\partial x_j} \right] - \frac{C_p}{k_p} \frac{\overline{\rho}}{k_p} \overline{\varepsilon_p}^2, \quad (4.87)
\]

where \( P_k \), the production of turbulent kinetic energy is given by Eq. (4.67). The \( k - \varepsilon \) equations for the transfer region can be written in a similar form whereby the production of turbulent kinetic energy in this region is equal to the dissipation of turbulent kinetic energy from the production region, i.e.

\[
\frac{\partial}{\partial t} \overline{\rho} \overline{k_T} + \frac{\partial}{\partial x_j} \overline{\rho} \overline{\nabla_j} \overline{k_T} = \overline{\rho} \overline{\varepsilon_p} + \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_k} \frac{\partial \overline{k_T}}{\partial x_j} \right] - \overline{\rho} \overline{\varepsilon_T}, \quad (4.88)
\]

and

\[
\frac{\partial}{\partial t} \overline{\rho} \overline{\varepsilon_T} + \frac{\partial}{\partial x_j} \overline{\rho} \overline{\nabla_j} \overline{\varepsilon_T} = \overline{\rho} \overline{\varepsilon_p} + \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_k} \frac{\partial \overline{\varepsilon_T}}{\partial x_j} \right] - \overline{\rho} \overline{\varepsilon_T},
\]
\[
\frac{\partial}{\partial t} \rho \tilde{c}_T + \frac{\partial}{\partial x_j} \rho \tilde{v}_j \tilde{c}_T = C_{T_1} \frac{\tilde{c}_T}{k_T} \frac{\partial \tilde{c}_p}{\partial k_T} + \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_t} \frac{\partial \tilde{c}_T}{\partial x_j} \right] - C_{T_2} \frac{\tilde{c}_T}{k_T} \tilde{c}_p^2. \tag{4.89}
\]

The multiple-scale approach discussed here can be described with a 'tank and tube' analogy, as is shown in Figure 4. Turbulent energy is fed into the production 'tank' at a rate \(P_k\).

![Tank-and-Tube analogy of spectral transfer of energy](image)

Figure 4: Tank-and-Tube analogy of spectral transfer of energy.

The dissipation rate \(\varepsilon_p\) serves as a 'valve' controlling the transfer of turbulent energy from the production 'tank' to the transfer 'tank'. The transfer 'tank' loses energy at a rate \(\varepsilon_T\) which is converted into thermal energy by viscous actions. It is clear from this picture that the dissipation rate \(\varepsilon_p\) must be connected with the turbulent energy in the production region and with the turbulent energy in the transfer region. If, for instance, \(k_T\) becomes larger then \(k_p\), the dissipation rate will be negative. Therefore the constant \(C_{T_2}\) occurring in the equation for the dissipation rate \(\varepsilon_p\) depends on the difference between \(k_p\) and \(k_T\). Analogously, it may be argued that the dissipation rate in the transfer region \(\varepsilon_T\) depends on the energy supplied to this region, i.e. depends on the dissipation rate \(\varepsilon_p\). The constant \(C_{T_1}\) occurring in Eq. (4.89) therefore depends on the ratio \(\varepsilon_p/\varepsilon_T\). Note that if \(\varepsilon_p = \varepsilon_T = \varepsilon\), which is the case for simple flows, these is no energy storage in the transfer region and the multiple-scale model changes to the basis \(k - \varepsilon\) model. The constants appearing in the Eqs. (4.86), (4.87), (4.88) and (4.89) may be assigned to the following values [21]

\[
C_{p_1} = 2.2 \quad C_{p_2} = 1.8 - 0.3 \left( \frac{k_p}{k_T} - 1 \right) / \left( \frac{k_p}{k_T} + 1 \right)
\]

\[
C_{T_1} = 1.08 \frac{\varepsilon_p}{\varepsilon_t} \quad C_{T_2} = 1.15 \quad \sigma_k = 1.0 \quad \sigma_\varepsilon = 1.30 \quad \sigma_T = 0.7.
\]

The Reynolds-stresses and scalar fluxes can be modelled with the Boussinesq approximation.
\[ - \tilde{\rho} V_i V_j^{''} = \mu_t \left( \frac{\partial \tilde{V}_i}{\partial x_j} + \frac{\partial \tilde{V}_j}{\partial x_i} \right) - 2 \frac{2}{3} \delta_{ij} \left( \tilde{\rho} \tilde{k} + \mu_t \frac{\partial \tilde{V}_k}{\partial x_k} \right), \]  

(4.90)

in which the turbulent viscosity may be determined from [22]

\[ \mu_t = \tilde{\rho} C_\mu \tilde{k} \frac{\tilde{k}}{\tilde{e}} = \tilde{\rho} C_\mu (\tilde{k}_p + \tilde{k}_T) \frac{\tilde{k}_p}{\tilde{e}} \]  

(4.91)

where \( C_\mu = 0.09 \). The scalar fluxes are approximated by

\[ - \tilde{\rho} V_i \varphi^{''} = \mu_t \frac{\partial \tilde{\varphi}}{\partial x_i} \]  

(4.92)

It is also possible to use the multiple-scale model in combination with a Reynolds stress closure model [21] or an algebraic stress model.

### 4.6. SELECTING A TURBULENCE CLOSURE MODEL FOR USE IN A COMPUTATIONAL MODEL

In the previous Sections four turbulence closure models which seems to be capable of predicting turbulent reacting flows, are discussed. One of these models will have to be used in a computational model describing the turbulent flow of a multicomponent chemical reacting mixture in a Solid Fuel Combustion chamber. The choice of this model is discussed in this Section. The advantages and disadvantages of these four models may be summarized as follows:

**\( \tilde{k} - \tilde{e} \) model**

- **Advantages:** simple to use
  - widely tested with good results in combustion problems [15]

- **Disadvantages:** assumption of isotropic eddy viscosity/diffusivity concept. This concept fails in complex flow problems.

**Reynolds-Stress model**

- **Advantages:** very general and applicable to almost all flow problems.

- **Disadvantages:** a very large number of partial differential equations to be solved, especially for multicomponent mixtures
  - very complex
  - hardly tested in combustion problems

**Algebraic Stress Model**

- **Advantages:** very general

- **Disadvantages:** very complex
  - hardly tested in combustion problems

**Multiple-Scale-Model**

- **Advantages:** accounts for different processes taking place at different length scales in turbulent flows, i.e. its physical background is better than that of the 3 previous
models.
- simple when used with the eddy-viscosity concept

disadvantages: - not tested in combustion problems

From these list it may be concluded that, at the present state of development of turbulence models

1) The $k - \varepsilon$ model is the most widely tested model for combustion problems.
2) The Reynolds-stress model, though very general, is impractical for combustion problems.
3) The Algebraic-Stress Model has potential for combustion problems, but is not well tested.
4) The multiple-scale model seems to have great potential in predicting turbulent reacting flows, but is not tested until now.

In our computational model, we will therefore use the $k - \varepsilon$ turbulence closure model, while the multiple scale model, in combination with the Algebraic Stress Model, will be kept in mind.

5. FUTURE INVESTIGATIONS

In the following period a computational model describing a steady state 2 dimensional rotationally symmetric turbulent flow will be developed. In the first stage of development chemical reactions will not be taken in account. In developing the model, the following topics are of interest.

i ) Simplifying the conservation equations to equations for a 2 D rotationally symmetric flow without chemical reactions.

ii ) Deriving the boundary conditions. In turbulent flows, the Reynolds number near solid walls is low because velocities are small, and low Reynolds number effects must be taken in account in the turbulence model.

iii ) Selecting a numerical scheme. This scheme may not introduce numerical instabilities because this affects the turbulence and combustion and unrealistic solutions may result.

iv ) Deriving the numerical boundary conditions.

v ) Deriving an optimal and general structure of the computational model in which components, e.g. the turbulence model, can be replaced in a simple way.
6. REFERENCES

The equations for a 3 Dimensional Transient Flow of a Multicomponent gas-
mixture with Chemical Reactions
Dep. of Aerospace Engineering, Delft University of Technology/Prins
Maurits Laboratory TNO, Report LR 362/PML 1982-149, SFCC Publication
no. 2, Delft/Rijswijk 1982

Radiation and Reentry

Introduction to Physical Gas Dynamics
John Wiley and Sons, New York 1965

Thermodynamik und Statistik
Akademische Verlagsgesellschaft, Geest & Portig K.-G, Leipzig 1965

[5] M. Planck
Ueberdas Gesetz der Energieverteilung im Normalspectrum, Annalen der
Physik, vol. 4, no. 3, 1901, p. 553

Analysis of Heat and Mass Transfer

The Coupling of Radiative Transfer and Gas Motion

Turbulent Reacting Flows
Springer Verlag, Berlin - Heidelberg 1980

Radiative Heat Transfer

[10] J. de Ris
Fire Radiation - a Review
17th Symposium (Int.) on Combustion
The Combustion Institute, Pittsburgh 1979

Modeling Solid - Fuel Ramjet Combustion Including Radiation Heat
Transfer to the Fuel Surface
NPS report no. NPS 67-81-012, Monterey 1981

[12] A. Favre
 Statistical Equations of Turbulent Gases
in: Problems of Hydrodynamics and Continuum Mechanics
SIAM, Philadelphia 1969
A. first Course in Turbulence
MIT Press, Cambridge 1972

[14] G.K. Batchelor
The Theory of Homogeneous Turbulence
University Press, Cambridge 1953

Calculation Methods for Reacting Turbulent Flow: a Review

[16] B.E. Launder and D.B. Spedding
Lectures in Mathematical Models of Turbulence
Academic Press, London 1972

[17] W. Rodi
Turbulence Models for Environmental Problems
in: Prediction Methods for Turbulent Flows
ed. W. Kollmann

[18] H. Schlichting
Boundary Layer Theory

Calculation of Turbulent Flows
in: Turbulence
ed. P. Bradshaw
Springer - Verlag. Berlin 1976

The Prediction of Laminarization with a Two-Equation Model of Turbulence

Multiple-Time-Scale Concepts in Turbulent Transport Modelling
in: Turbulent Shear Flows 2
ed. L.J.S. Bradbury, F. Durst, B.E. Launder, F.W. Schmidt and J.H. Whitelaw
Springer - Verlag, Berlin 1980

Multiple-Scale Turbulence Modeling of Boundary Layer Flows for
Scramjet Applications
NASA Contractor Report 3433, may 1981

[23] K.N.C. Bray
The Interaction Between Turbulence and Combustion
17th Symposium (Int.) on Combustion
The Combustion Institute, Pittsburgh 1979

Engineering Calculation Methods for Turbulent Flow
[25] W. Kollmann and D. Vandromme  
Turbulent Shear Flow with Fluctuating Density  
AIAA-79-1485, 1979

[26] M.M. Sindir and P.T. Harsha  
Assessment of Turbulence Models for Sramjet Flowfields  
NASA Contractor Report 3643, November 1982

[27] B.E. Launder, G.J. Reece and W. Rodi  
Progress in the Development of a Reynolds Stress Turbulence Closure  
J. of Fluid Mechanics, vol. 68, 1975, p. 537

[28] K. Hanjalic and B.E. Launder  
Preferential Spectral Transport by Irrotational Straining  
in: Turbulent Boundary Layers  
ed.: H.E. Weber  
ASME, New York 1979

[29] W.P. Jones  
Models for Turbulent Flows with Variable Density and Combustion  
in: Prediction Methods for Turbulent Flows  
ed. W. Kollmann  

Calculation of Turbulent Wall Jetts with an Algabraic Reynolds Stress Model  
in: Turbulent Boundary Layers  
ed.: H.E. Weber  
ASME, New York 1979

[31] W. Rodi  
A New Algabraic Relation for calculating the Reynolds Stresses  
ZAMM 56, 1976, T 219 - 221

[32] M.M. Gibson and B.E. Launder  
On the Calculation of Horizontal, Turbulent Free Shear Flow under Gravitational Influence  
J. Heat Transfer, 98C, 1976, p. 81

Non-Equilibrium Thermodynamics  
North-Holland Publishing Company, Amsterdam 1962

[34] R.B. Bird, W.E. Stewart and E.N. Lightfoot  
Transport Phenomena  
John Wiley & Sons, New York 1960
APPENDIX A: THE DERIVATION OF THE EQUATION FOR ENTROPY BALANCE

The second law of thermodynamics states that for a closed and isolated system the variation of the entropy $S$ equals

$$\text{d} \ S = \frac{\text{d} Q}{T} \quad \text{(A.1)}$$

for reversible processes and

$$\text{d} \ S > \frac{\text{d} Q}{T} \quad \text{(A.2)}$$

for irreversible processes. $\text{d} Q$ denotes the heat added to the system. It may be advantageous, especially if chemical reactions are taken into account, to use the equation for conservation of entropy in addition to the equation for conservation of energy. In this Appendix the equation for conservation of entropy will be derived.

The second law of thermodynamics for a closed and isolated system states [33]

$$\text{d} \ S > \frac{\text{d} Q}{T} \quad \text{(A.3)}$$

The first law of thermodynamics states

$$\text{d} Q = \text{d} U + p \ \text{d} V \quad \text{(A.4)}$$

and Eq. (A.3) may therefore be written as

$$T \ \text{d} \ S > \text{d} U + p \ \text{d} V \quad \text{(A.5)}$$

Terms involving the viscous effects and the total heat flux are assumed to be implicitly taken into account by the internal energy.

The time rate of change of the entropy $s$ per unit mass may be written as

$$T \ \frac{\text{D}}{\text{D} t} \ s \geq \frac{\text{D}}{\text{D} t} \ u + p \ \frac{\text{D}}{\text{D} t} \ \frac{1}{\rho} \quad \text{(A.6)}$$

or

$$\rho \ T \ \frac{\text{D}}{\text{D} t} \ s \geq \rho \ \frac{\text{D}}{\text{D} t} \ u - \frac{p}{\rho} \ \frac{\text{D}}{\text{D} t} \ \rho \quad \text{(A.7)}$$
With the help of the energy- and momentum equation this equation may be rewritten. The energy equation states [1]

\[
\frac{\partial}{\partial t} \rho (U + \frac{1}{2} V_i V_i) + \frac{\partial}{\partial x_j} \rho V_j (U + \frac{1}{2} V_i V_i) = \rho V_i q_i - \frac{\partial}{\partial x_j} (p \delta_{ij} - \tau_{ij}) V_i - \frac{\partial}{\partial x_i} \tau_{ij} \quad ,
\]

(A.8)

where \( q_i \), the total heat transfer vector, is given by Eq. (3.36)

Substitution of the equation for conservation of mass yields

\[
\frac{\partial}{\partial t} u + \frac{\partial}{\partial x_j} \rho V_i V_j = \rho V_i g_i - \frac{\partial}{\partial x_i} p V_i + \frac{\partial}{\partial x_j} \tau_{ij} V_i - \frac{\partial}{\partial x_i} q_i \quad .
\]

(A.9)

The momentum equation may be written as

\[
\frac{\partial}{\partial t} \rho V_i + \frac{\partial}{\partial x_j} \rho V_i V_j = \rho V_i g_i - \frac{\partial}{\partial x_i} p + \frac{\partial}{\partial x_j} \tau_{ij} \quad ,
\]

(A.10)

or

\[
\frac{\partial}{\partial t} V_i = \rho V_i g_i - \frac{\partial}{\partial x_i} p + \frac{\partial}{\partial x_j} \tau_{ij} \quad .
\]

(A.11)

Scalar multiplying of this latter equation with \( V_i \) yields [34]

\[
\frac{\partial}{\partial t} \frac{1}{2} V_i V_i = \rho V_i g_i - V_i \frac{\partial}{\partial x_i} p + V_i \frac{\partial}{\partial x_j} \tau_{ij} \quad ,
\]

(A.12)

or

\[
\frac{\partial}{\partial t} \frac{1}{2} V_i V_i = \rho V_i g_i - \frac{\partial}{\partial x_i} p V_i + p \frac{\partial}{\partial x_i} V_i + \frac{\partial}{\partial x_j} \tau_{ij} V_i - \tau_{ij} \frac{\partial}{\partial x_j} V_i \quad .
\]

(A.13)

Subtracting of Eq. (A.13) from Eq. (A.9) yields
\[ \rho \frac{Du}{Dt} = -\frac{2}{3x_i} q_i - p \frac{2}{3x_i} V_i = \tau_{ij} \frac{3}{3x_j} V_i \]  

(A.14)

The equation for conservation of mass may be written as

\[ \frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_i} \rho V_i = \frac{\partial}{\partial t} \rho + \rho \frac{\partial}{\partial x_i} V_i + V_i \frac{\partial}{\partial x_i} \rho = 0 \Rightarrow \]

\[ \frac{1}{c} \frac{D}{Dt} \rho = -\frac{3}{3x_i} V_i \]  

(A.15)

Multiplying this equation with \( p \) and subtracting it from Eq. (A.14) finally yields

\[ \rho \frac{Du}{Dt} - p \frac{D}{Dt} \rho = -\frac{3}{3x_i} q_i + \tau_{ij} \frac{3}{3x_j} V_i \]  

(A.16)

or

\[ \rho \frac{D}{Dt} s \geq -\frac{3}{3x_i} q_i + \tau_{ij} \frac{3}{3x_j} V_i \]  

(A.17)

where use has been made of Eq. (A.7). Equation (A.17) is the equation for entropy balance.

Favre-decomposition of this equation gives

\[ \rho(\bar{T} + T'') \frac{3}{3x_i} (\bar{s} + s'') + (\bar{V}_j + V''_j) \frac{3}{3x_j} (\bar{s} + s'') \geq -\frac{3}{3x_i} (\bar{q}_i + q_i') + \]

\[ (\tau_{ij} + \tau_{ij}') \frac{3}{3x_j} (\bar{V}_i + V''_i) \]  

(A.18)

and averaging finally yields

\[ \bar{\rho} \bar{T} \frac{D}{Dt} \bar{s} + \bar{T} p \frac{3}{3x_i} s'' + \bar{T} T'' \frac{3}{3x_i} s'' + \bar{T} \bar{V}_j \frac{3}{3x_j} \bar{s} + \bar{T} V''_j \frac{3}{3x_j} s'' \geq -\]

\[ \frac{3}{3x_i} \bar{q}_i + \bar{T} \tau_{ij} \frac{3}{3x_j} \bar{V}_i + \bar{T} \tau_{ij} \frac{3}{3x_j} V''_i + \bar{T} \tau_{ij} \frac{3}{3x_j} V''_i \]  

(A.19)
where $\tau_{ij}$ is given by Eq. (4.39), $\tau_{ij}'$ by Eq. (3.33) and $\bar{q}_i$ by Eq. (3.40).