Delft University of Technology
Department of Aerospace Engineering

Prins Maurits Laboratory TNO
Rijswijk

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THE EQUATIONS FOR A 3 DIMENSIONAL TRANSIENT FLOW OF A MULTICOMPONENT GASMIXTURE WITH CHEMICAL REACTIONS.

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Summary

This report gives a general description of the basic equations for the 3-dimensional transient flow of a multicomponent gas mixture with chemical reactions. The number of assumption made is small.

Next to the equation of momentum, the equation of angular momentum is introduced. It could in the future be advantageous to use the latter equation instead of the first because the flow may possess vortices which introduce an angular momentum.

In the first chapter of this report, the conservation equations are introduced. In the next chapters, the processes which occur on microscale are described. In the last chapter, the conservation equations are modelled for turbulence. This is done with Reynolds' decomposition and time-averaging of the subsequent equations.

This report occurs within the framework of the investigation of the flow and combustion in a solid fuel combustion chamber (SFCC). This investigation is supported by the Netherlands Foundation for Technical Research (STW) under projectnumber DLR 11.0120 and is carried out by the Department of Aerospace Engineering of the Delft University of Technology and the Prins Maurits Laboratory TNO.

Contents

Nomenclature

A - Frequency factor in the Arrhenius expression

B - Constant in the Arrhenius expression

$\underline{B}$ - Angular momentum

c_p - Specific heat at constant pressure

C_p - Molar heat capacity at constant pressure

C - Molar concentration

c_v - Specific heat at constant volume

C_v - Molar heat capacity at constant volume

D_{sr} - Diffusion coefficient between species s and r

D^T_s - Thermal diffusion coefficient

e - Emissive power

E - Activation energy

$\underline{g}$ - Acceleration due to gravity = 9.80665 m/sec^2

h - Specific enthalpy

H - Molar enthalpy

Ie - Boltzmann's constant = 1.3805 10^{-23} eV/molecule K

k - Specific reaction rate constant

K_c - Equilibrium constant

m - Mass of a molecule

M - Molar mass

$\underline{M}_e$ - Moment caused by external forces

n - Number density

$\underline{n}$ - Unit normal vector

N_A - Avogadro's number = 6.023 10^{23} moleculs/mole

p - Hydrostatic pressure

$\underline{\underline{P}}$ - Pressure tensor

$\underline{q}$ - Heat transfer vector

$\underline{r}_o$ - Position vector

R^o - Universal gas constant = 8.314.4 kgm^2/sec^2 kmole

R - Gas constant

S - Surface

t - Time

T - Temperature

u - Specific internal energy

U - Molar internal energy

$\underline{v}$ - Velocity

$\underline{V}$ - Diffusion velocity

$\mathcal{V}$ - Volume
X - Molar fraction
Y - Mass fraction

α - Constant in the Arrhenius expression
γ - Molar rate of production
ε - Emissivity
η - Second coefficient of viscosity
κ - Coefficient of bulk viscosity
κ_r - Absorption coefficient
λ - Thermal conductivity
Λ_r - Photon mean path length
μ - Coefficient of viscosity
ν - Stoichiometric coefficient
ρ - Density
σ - Stefan-Boltzmann constant = $5.6697\ 10^{-8}\ W/(m^2K^4)$
σ - Collision diameter
$\underline{\underline{\tau}}^D$ - Diffusion stress tensor
$\underline{\underline{\tau}}^V$ - Viscous stress tensor
ω - Mass rate of production
Ω - Collision integral

Subscripts

b - backward
f - forward
k - reaction k
mix - mixture
r - species r
s - species s

Superscripts

a - reactants
b - products
$-$ - averaged
$'$ - fluctuating
$\sim$ - mean

1. Introduction

In a solid fuel combustion chamber (SFCC) an efficient and complete combustion may be realized. Because the combustion temperatures are high (from 2000 to 3000 K), the thermal efficiency is high and the combustion gases are relatively clean.

An SFCC consists of a solid fuel with an inner bore. The gaseous oxidizer is fed into this bore, and at the interface between the pyrolyzing fuel and the oxidizer a turbulent boundary layer is formed. In this turbulent boundary layer, combustion takes place.

The scope of the SFCC-project is to obtain a thorough understanding of the processes which occur in a turbulent boundary layer involving chemical reactions, and to obtain a mathematical description of the combustion and flow processes in a SFCC.

In this report, the basic equations for a 3 dimensional transient flow of a multicomponent gas mixture with chemical reactions are presented. From the equations presented in this report, computational models of the 1-dimensional transient flow, the 2-dimensional and the 2-dimensional transient flow trough a SFCC will be derived in the future.

2. Conservation Equations

In this chapter, the conservation equations for a 3-dimensional transient flow of a multicomponent gas mixture with chemical reactions are introduced. The equation of conservation of angular momentum is derived because it may be adventageous to apply this equation instead of or together with the equation of linear momentum when vortices are taken in account.

2.1 Conservation of Mass

Consider an orbitrairy control volume $\mathcal{V}$, enclosed by a surface S (figure 1). Assume that there are no discontinuities in this volume and that the gas can flow through this volume.
The amount of mass in this volume changes by transport of mass through the surfaces. The law of conservation of mass is written as [1].

$$\underbrace{\int_{\mathcal{V}} \frac{\partial \rho}{\partial t}\, d\mathcal{V}}_{\text{local change}} = \underbrace{- \int_{S} \rho \underline{v} . \underline{n}\, dS}_{\text{transport}} \qquad (2.1)$$

The surface integral can be converted into a volume integral, yielding

$$\int_{\mathcal{V}} \left(\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot \rho \underline{v} \right) d\mathcal{V} = 0 \qquad (2.2)$$

This equation is valid for any orbitrairy control volume $\mathcal{V}$ and (2.2) may therefore replaced by

$$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot \rho \underline{v} = 0 \qquad (2.3)$$

This equation is the differential form of the law of conservation of mass, frequently called the continuity equation.

2.2 Conservation of Momentum

The amount of momentum in a material control volume $\mathcal{V}$ (figure 1) changes by forces which are acting on this volume. These forces can be divided into two groups, body forces which act on the entire mass in the volume, and surface forces which act on the boundaries of the system by virtue of their contact with the surroundings.
The law of conservation of momentum is written as [1]

$$\frac{D}{Dt}\int_{\mathcal{V}} (\rho\underline{v})\ d\mathcal{V} = \int_{\mathcal{V}} \rho\underline{g}\ d\mathcal{V} - \int_{S} \underline{\underline{P}}.\underline{n}\ dS$$

or

$$\underset{\text{local change}}{\int_{\mathcal{V}} \frac{\partial}{\partial t}(\rho\underline{v})\ d\mathcal{V}} + \underset{\text{transport}}{\int_{S} (\rho\underline{v})\ \underline{v}.\underline{n}\ dS} = \underset{\text{body forces}}{\int_{\mathcal{V}} \rho\underline{g}\ d\mathcal{V}} - \underset{\text{surface forces}}{\int_{S} \underline{\underline{P}}.\underline{n}\ dS} \tag{2.4}$$

The surface integrals in eq. (2.4) can be converted into volume integrals, yielding

$$\int_{\mathcal{V}} \left[\frac{\partial}{\partial t}(\rho\underline{v}) + \underline{\nabla}\ .\ \rho\underline{v}\,\underline{v}\right] d\mathcal{V} = \int_{\mathcal{V}} \left[\rho\underline{g} - \underline{\nabla}\ .\ \underline{\underline{P}}\right] d\mathcal{V} \tag{2.5}$$

Since the material volume $\mathcal{V}$ is chosen arbitrairy, and as on the other hand equation (2.5) is always valid, it follows that the integral equation (2.5) may be replaced by

$$\frac{\partial}{\partial t}\ \rho\underline{v} + \underline{\nabla}\ .\ \rho\,\underline{v}\,\underline{v} = \rho\underline{g} - \underline{\nabla}\ .\ \underline{\underline{P}} \tag{2.6}$$

A multicomponent mixture possesses several species s.
In general, the pressure tensor for species s is defined as [2]

$$\underline{\underline{P}}_s = p_s\delta_{ij} - \underline{\underline{\tau}}_s^V - \underline{\underline{\tau}}_s^D \tag{2.7}$$

where p_s denotes the hydrostatic pressure of species s, $\underline{\underline{\tau}}_s^V$ denotes the viscous stress tensor for species s and $\underline{\underline{\tau}}_s^D$ denotes the diffusion stress tensor for species s. The viscous stress tensor is caused by the different velocities of each particle of species s through which they exercise forces on each other. The diffusion stress tensor is caused by transport of species s with velocity $\underline{V}_S$ with respect to the mass-averaged velocity of the entire mixture.
The diffusion stress tensor for species s may be written as [5]

$$\underline{\underline{\tau}}_s^D = \rho\, Y_s\, \underline{V}_s\, \underline{V}_s \tag{2.8}$$

where Y_s is the mass fraction of species s (see section 2.5).
The total pressure tensor $\underline{\underline{P}}$ is the sum of the partial pressure tensors $\underline{\underline{P}}_s$ for the different species s,

$$\underline{\underline{P}} = \sum_s p_s \delta_{ij} - \sum_s \underline{\underline{\tau}}_s^V - \sum_s \underline{\underline{\tau}}_s^D \tag{2.9}$$

The mean hydrostatic pressure may be defined as

$$p = \sum_s p_s \tag{2.10}$$

and the stress tensor for the entire mixture as [5]

$$\underline{\underline{\tau}} = \sum_s \underline{\underline{\tau}}_s^V + \sum_s \underline{\underline{\tau}}_s^D \tag{2.11}$$

The total stress tensor $\underline{\underline{\tau}}$ is usually written as

$$\underline{\underline{\tau}} = \tau_{ij} = \mu \left[\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right] - \eta \left(\frac{\partial v_i}{\partial x_i} \right) \delta_{ij} \tag{2.12}$$

where μ is the coefficient of viscosity for the multicomponent mixture and η is the second viscosity coefficient, commonly written as

$$\eta = \frac{2}{3} \mu - \kappa \tag{2.13}$$

where κ is the coefficient of bulk viscosity.
Combining equations (2.9), (2.10), (2.11), (2.12) and (2.13) yields

$$\underline{\underline{P}} = P_{ij} = p\delta_{ij} - \mu \left[\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right] - \left(\frac{2}{3}\mu - \kappa \right) \left(\frac{\partial v_i}{\partial x_i} \right) \delta_{ij} \tag{2.14}$$

The momentum equation may be written as

$$\frac{\partial}{\partial t} \rho \underline{v} + \underline{\nabla} \cdot \rho \underline{v}\underline{v} = \rho \underline{g} - \underline{\nabla} p - \underline{\nabla} \cdot \underline{\underline{\tau}} \tag{2.15}$$

where $\underline{\underline{\tau}}$ is given by the equations (2.12) and (2.13).

2.3 Conservation of Energy

For a material control volume $\mathcal{V}$ (figure 1), the first law of thermodynamics states that the rate of increase of internal plus kinetic energy equals the rate of which work is done by the body forces and the surface forces plus the rate of heat transferred into the volume. This gives the following equation, also called the energy equation [1]

$$\frac{D}{Dt}\int_{\mathcal{V}} \rho\;(u+\frac{1}{2}\,\underline{v}.\underline{v})\;d\mathcal{V} = \int_{\mathcal{V}} \rho\,\underline{v}\;.\;\underline{g}d\mathcal{V} - \int_{S} (\underline{v}.\underline{\underline{P}}).\underline{n}dS - \int_{S} \underline{q}.\underline{n}dS$$

or

$$\int_{\mathcal{V}} \frac{\partial}{\partial t}\,\rho(u+\frac{1}{2}\,\underline{v}.\underline{v})\;d\mathcal{V} + \int_{S} \rho\;(u+\frac{1}{2}\,\underline{v}.\underline{v})\underline{v}.\underline{n}\;dS = \int_{\mathcal{V}} \rho\underline{v}.\underline{g}\;d\mathcal{V}\;+$$

local change — transport — work from body forces done by the medium

$$-\int_{S} (\underline{v}.\underline{\underline{P}}).\underline{n}\;dS - \int_{S} \underline{q}.\underline{n}\;dS \qquad (2.16)$$

work from surface forces done by the medium — heat transfer into the volume

The differential form of the energy equations is given by

$$\frac{\partial}{\partial t}\,\rho(u+\frac{1}{2}\,\underline{v}.\underline{v}) + \underline{\nabla}\;.\;\rho\underline{v}\;(u+\frac{1}{2}\,\underline{v}.\underline{v}) = \rho\underline{v}.\underline{g} - \underline{\nabla}\;.\;(\underline{\underline{P}}.v) - \underline{\nabla}.\underline{q} \qquad (2.17)$$

In a multicomponent mixture, the heat transfer vector may be caused by conduction, by diffusion of species s through the mixture and by radiation. The heat transfer by conduction may be described by Fourier's law [6]

$$\underline{q}_c = -\,\lambda\underline{\nabla}\;T \qquad (2.18)$$

where λ is the thermal conductivity of the mixture.
In a multicomponent mixture, the average velocity of species s differs from the mass-averaged velocity $\underline{v}$ of the entire mixture. This gives rise to an enthalpy transport, equal to

$$\rho_s\;h_s\;\underline{V}_s$$

Summation for all species s gives

$$\rho\;\sum_s\;Y_s\;h_s\;\underline{V}_s \qquad (2.19)$$

where h_s is the enthalpy of species s, defined by

$$h_s = h_s^o (T_o) + \int_{T_o}^{T} c_{p,s}^o \, dT \qquad (2.20)$$

h_s^o is the enthalpy of species s at reference temperature T_o and at standard conditions [6]. $c_{p,s}^o$ is the specific heat at constant pressure at a reference pressure of 1 atmosphere.
If temperature gradients give rise to diffusion velocities (thermal diffusion) then concentration gradients must produce a heat flux. This process is known as the Dufour effect. The Dufour heat flux may be written as [7], [8]

$$R^o T \sum_s \sum_r \frac{X_r D_s^T}{M_s D_{sr}} (\underline{V}_s - \underline{V}_r) \qquad (2.21)$$

where D_s^T is the coefficient of thermal diffusion and D_{sr} is the coefficient of concentration diffusion for species s and r (see Chapter 3). Combining equations (2.19) and (2.21) gives the heat transfer caused by diffusion

$$\underline{q}_d = \rho \sum_s Y_s h_s \underline{V}_s + R^o T \sum_s \sum_r \frac{X_r D_s^T}{M_s D_{sr}} (\underline{V}_s - \underline{V}_r) \qquad (2.22)$$

Heat transfer by radiation may be thought of as transport of energy by photons. These photons are released from excited molecules or atoms, and travel through the medium until they are absorbed by other molecules or atoms, or, alternatively, it can be visualized as energy transport in the form of electromagnetic waves.

The heat transfer by radiation may be written as [11]

$$\underline{q}_r = - \frac{4}{3} \Lambda_r \underline{\nabla} e \qquad (2.23)$$

where e is the emissie power of the gas and Λ_r is the photon mean path length, defined as

$$\Lambda_r = \frac{1}{\rho \kappa_r} \qquad (2.24)$$

where ρ is the density of the gas and κ_r is the absorption coefficient of the gas. According to Stefan-Boltzmann's law, the emissie power of a black body radiating gas may be written as

$$e_b = \sigma T^4 \qquad (2.25)$$

where the Stefan-Boltzmann constant σ equals

$$\sigma = 5.6697 \; 10^{-8} \; W/m^2K^4 \tag{2.26}$$

In most cases, the emissie power may be written as

$$e = \varepsilon \, \sigma \, T^4 \tag{2.27}$$

where ε is the emissivity, $\varepsilon < 1$.
Combining equations (2.23) and (2.27) gives the heat transfer by radiation

$$\underline{q}_r = - \frac{16}{3} \Lambda_r \, T^3 \, \underline{\nabla} \, \varepsilon \, T \tag{2.28}$$

The total heat transfer may be written as

$$\underline{\underline{q}} = - \lambda \, \underline{\nabla} \, T + \rho \sum_s Y_s \, h_s \, \underline{V}_s + R^o T \sum_s \sum_r \frac{X_r \, D_s^T}{M_s D_{sr}} (\underline{V}_s - \underline{V}_r) - \frac{16}{3} \Lambda_r \, \sigma T^3 \, \underline{\nabla} \, \varepsilon \, T \tag{2.29}$$

It is convenient to use the enthalpy h instead of the internal energy u in the energy equation. The enthalpy h of a multicomponent mixture equals

$$h = \sum_s Y_s \, h_s \tag{2.30}$$

where h_s is given by (2.20). The relation between the enthalpy h and the internal energy u is given by

$$u = h - \frac{p}{\rho} \tag{2.31}$$

The energy equation may now be written as

$$\frac{\partial}{\partial t} \rho \left(h - \frac{p}{\rho} + \frac{1}{2} \underline{v} \cdot \underline{v}\right) + \underline{\nabla} \cdot \rho \underline{v} \left(h - \frac{p}{\rho} + \frac{1}{2} \underline{v} \cdot \underline{v}\right) = \rho \underline{v} \cdot \underline{g} - \underline{\nabla} \cdot (\underline{\underline{P}} \cdot \underline{v}) - \underline{\nabla} \cdot \underline{q} \tag{2.32}$$

2.4 Conservation of angular momentum

Consider an arbitrairy material volume $\mathcal{V}$, enclosed by a surface S. Take an arbitrairy reference point O at a distance $\underline{r}_o$ of the volume (figure 2). The amount of angular momentum in this material volume equals [6]

$$\underline{B} = \int_{\mathcal{V}} \underline{r}_o \times (\rho \underline{v}) \, d\mathcal{V} \tag{2.33}$$

Consider a system of particles and assume that no particles can enter or leave this system, then, the change of angular momentum equals the moment caused by the external forces.

$$\frac{D\underline{B}}{Dt} = \sum_{e} \underline{M}_e \tag{2.34}$$

The left hand side of this equation may be written as

$$\frac{D\underline{B}}{Dt} = \int_{\mathcal{V}} \frac{\partial}{\partial t}\left[\underline{r}_o \times (\rho\underline{v})\right] d\mathcal{V} + \int_{S}\left[\underline{r}_o \times (\rho\underline{v})\right] \underline{v}.\underline{n}\; d\,S$$

While the right hand side equals

$$\sum_{e} \underline{M}_e = \int_{\mathcal{V}} \underline{r}_o \times \rho\underline{g}\; d\mathcal{V} - \int_{S} \underline{r}_o \times \underline{\underline{P}}.\underline{n}\; d\,S$$

Combining these equations gives the law of conservation of angular momentum

$$\underbrace{\int_{\mathcal{V}} \frac{\partial}{\partial t}(\underline{r}_o \times \rho\underline{v})\; d\mathcal{V}}_{\text{Local change}} + \underbrace{\int_{S}(\underline{r}_o \times \rho\underline{v})\underline{v}.\underline{n}\; d\,S}_{\text{transport}} = \underbrace{\int_{\mathcal{V}} \underline{r}_o \times \rho\underline{g}\; d\mathcal{V}}_{\text{moment by body forces}} - \underbrace{\int_{S} \underline{r}_o \times \underline{\underline{P}}.\underline{n}\; d\,S}_{\text{moment by surface forces}}$$

The differential form of this conservation equation is given by

$$\frac{\partial}{\partial t}\, \underline{r}_o \times \rho\underline{v} + \underline{\nabla}.(\underline{r}_o \times \rho\underline{v})\underline{v} = \rho\underline{r}_o \times \underline{g} - \underline{r}_o \times (\underline{\nabla}.\underline{\underline{P}}) \tag{2.36}$$

where the pressure tensor $\underline{\underline{P}}$ is given by (2.14).

2.5 Conservation of Species

For each of the species s in a multicomponent gasmixture with chemical reactions a conservation law of the form: the local change of mass fraction of species s in a control volume $\mathcal{V}$ equals the transport of mass fraction of species s plus net mass rate production of species s by chemical reactions may be defined.
Before writing down this conservation law, it is usefull to define and to give the dimensions of the following variables [2], [3]

C_s = moles of species s per unit volume (moles/m^3)

M_s = molar mass of species s (kg/mole)

$\overline{M}$ = molar mass of the entire mixture (kg/mole)

n_s = number of species s per unit volume (/m^3)

n = total number of species per unit volume (/m^3) = $\sum_s n_s$

m_s = mass of 1 species s (kg)

$\overline{m}$ = averaged mass of 1 species (kg) = $\dfrac{\sum_s n_s m_s}{n}$

$\underline{v}$ = mass-averaged velocity of the mixture (m/s)

$\underline{v}_s$ = mass-averaged velocity of species s (m/s)

$\underline{V}_s$ = diffusion velocity of species s (m/s)

ω_s = net mass rate of production of species s per unit volume by chemical reactions (kg/m^{3}s)

From these definitions the following quantities may be derived.

$X_s = \dfrac{n_s}{n} = \dfrac{n_s}{N_A} / \dfrac{n}{N_A}$ = mole fraction of species s

$\rho_s = n_s m_s$ = partial density of species s (kg/m^3)

$\rho = n\,\overline{m}$ = density of the mixture (kg/m^3)

$Y_s = \dfrac{\rho_s}{\rho} = \dfrac{n_s m_s}{n\overline{m}} = X_s \dfrac{m_s}{\overline{m}}$ = mass fraction of species s

From these definitions, it is apparent that

$$\overline{M} = \sum_s X_s M_s$$
$$\sum_s X_s = 1$$
$$\sum_s Y_s = 1$$
$$\underline{v} = \sum_s Y_s \underline{v}_s = \sum_s \frac{\rho_s \underline{v}_s}{\rho_s}$$
$$\underline{V}_s = \underline{v}_s - \underline{v}$$
$$\sum_s \omega_s = 0$$

The law of conservation of the mass fraction of species s may now be written as

$$\int_{\mathcal{V}} \frac{\partial}{\partial t} \rho Y_s \, d\mathcal{V} + \int_S \rho Y_s \underline{v}_s \cdot \underline{n} \, dS = \int_{\mathcal{V}} \omega_s \, d\mathcal{V} \qquad (2.37)$$

local change transport net production by chemical reactions

In differential form this yields

$$\frac{\partial}{\partial t} \rho Y_s + \underline{\nabla} \cdot \rho Y_s \underline{v}_s = \omega_s \qquad (2.38)$$

or

$$\frac{\partial}{\partial t} \rho Y_s + \underline{\nabla} \cdot \rho Y_s \underline{v} = - \underline{\nabla} \cdot \rho Y_s \underline{V}_s + \omega_s \qquad (2.39)$$

The overall continuity equation for the mixture can be obtained by summation over all species s.
An expression for the diffusion velocity may be obtained from the moleculer theory of gases [7], [10] yielding

$$\underline{V}_s = \frac{n}{\rho X_s} \sum_r m_r D_{sr} \left(\underline{\nabla} X_r + (X_r - Y_r) \underline{\nabla} \ln p \right) - \frac{1}{\rho_s} D_s^T \underline{\nabla} \ln T \qquad (2.40)$$

This equation indicates that there are three diffusion mechanisms, namely concentration diffusion, pressure diffusion and thermal diffusion.

The conservation equations are completed by an equation of state.
This equation gives the relation between the dependent and independent thermodynamic variables. Only two thermodynamic variables can be choosen independently, for instance the pressure p and the temperature T. It follows than that

$$u = u(p,T) \; ; \; h = h(p,T) \; , \; \rho = \rho\,(p,T) \text{ etc.}$$

For a perfect gas, the equation of state is given by

$$\frac{p}{\rho} = RT$$

where R is the gasconstant for the mixture ($R = R^{o}/\overline{M}$).

3. Transport Coefficients

In the equations of the pressure tensor $\underline{\underline{P}}$, the heat flux vextor $\underline{q}$ and the diffusion velocity $\underline{V}_s$, there appear the transport coefficients μ, κ, λ, D_{sr} and D_s^T. Equations for these coefficients have, to a first approximation, been derived by the Chapman-Enshoy theory [7], [10]. In this Chapter, the results of this derivation are presented.

3.1 The Coefficient of Viscosity

The coefficient of viscosity for a multicomponent gas mixture may be written as [10]

$$\mu_{mix} = \sum_s X_s \left[\frac{X_s^{z}}{\mu_s} + \sum_{\substack{r=1 \\ r \neq s}} 1.385 \, X_r X_s \frac{R^{o} T}{p M_s D_{sr}} \right]^{-1} \qquad (3.1)$$

where the faktor 1.385 is an empirical constant. The theoretical value of this constant is 2 [10]. Note that the pressure p has to be given in atmospheres.
The coefficient of viscosity for species s may be approximated by [8], [10], [11]

$$\mu_s = \frac{5}{16} \frac{\sqrt{\pi M_s R^o T}}{\pi \sigma_s^2 \, \Omega_s^{(2,2)*} \, N_A} \qquad (3.2)$$

where σ_s is the collision diameter for collisions between species s and species s and $\Omega^{(2,2)*}$ is a collision integral which depends on the temperature and on the interaction energy ε between the molecules.
It follows from equation (3.2) that

$$\mu_s = \frac{266.93 \; 10^{-7} \sqrt{M_s T}}{\sigma_s^2 \; \Omega_s^{(2,2)*}} \qquad (3.3)$$

where σ_s is given in angstroms.

3.2 The Coefficient of Bulk-Viscosity

The coefficient of bulk viscosity depends on a characteristic time for the conversion of translation energy into internal energy in an atom or molecule [10]. An atom or molecule possesses several internal degrees of freedom ℓ, and each of them has its own characteristic time τ_ℓ. The expression for the coefficient of bulk viscosity yields [10]

$$\kappa = \frac{n \, k^2 T}{c_v} \; \Sigma_\ell \; c_v^{(\ell)} \; \tau_\ell \qquad (3.4)$$

where $c_v^{(\ell)}$ is the contribution of the internal degree of freedom ℓ to the specific heat at constant volume. The expression for the characteristic time τ_ℓ is very complicated and can be found in [10].
In most cases of practical interest, the coefficient of bulk viscosity is negligeble [2].

3.3 The Coefficient of Thermal Conductivity

The expression for the coefficient of thermal conductivity for a multicomponent gasmixture can be derived from the kinetic theory of gases, but it is a rather complicated expression [10]. An usefull approximation is given by [8]

$$\lambda_{mix} = \sum_s \lambda_s' \left(1 + 1.065 \sum_{\substack{r \\ r \neq s}} G_{sr}' \frac{X_r}{X_s}\right)^{-1} \qquad (3.5)$$

where

$$\lambda_s' = \lambda_s \; (0.115 + 0.354 \frac{C_{p,s}}{R_s}) \qquad (3.6)$$

and

$$G'_{sr} = \frac{\left[1 + \left(\lambda_s/\lambda_r\right)^{\frac{1}{2}} \left(M_s/M_r\right)^{1/4}\right]^2}{2^{3/2}\left[1 + \left(M_s/M_r\right)\right]^{\frac{1}{2}}} \tag{3.7}$$

λ_s is the thermal conductivity for monatomic species s, while λ'_s is the thermal conductivity for polyatomic species. The faktor between these termal conductivities is a modification of the Eucken relation.
The thermal conductivity for monatomic species s is given by [10]

$$\lambda_s = 1989.1 \, \frac{10^{-7}\sqrt{T/M_s}}{\sigma_s^{\,2}\;\Omega_s^{(2,2)*}} \tag{3.8}$$

For an ideal gas, the thermal conductivity for monatomic species s may be written as

$$\lambda_s = \frac{15}{4} R_s \mu_s \tag{3.9}$$

where $R_s = R^o/M_s$.

3.4 The Coefficient of Diffusion

The coefficient of (concentration) diffusion may be obtained from the molecular theory of gases, and is approximated by [8]

$$D_{sr} = \frac{3}{16}\,\frac{\left[2\pi kT\ (m_s+m_r)/m_s m_r\right]^{\frac{1}{2}}}{n\pi\,\sigma_{sr}^2\;\Omega_{sr}^{(1,1)*}} \tag{3.10}$$

where σ_{sr} is a collision diameter for collisions between species s and r and $\Omega_{sr}^{(1,1)*}$ is a collision integral which depends on the temperature and on the intermolecular forces between molecules s and r.
Equation (3.10) may be rewritten to

$$D_{sr} = \frac{262.80\ 10^{-5}\left[T^3\,(M_s + M_r)/2M_s M_r\right]^{\frac{1}{2}}}{p\sigma_{sr}^2\;\Omega_{sr}^{(1,1)*}} \tag{3.11}$$

where the collision diameter, σ_{sr}, is given in angstroms and the pressure p in atmospheres. In some cases it is important to estimate the temperature and pressure dependence of the diffusion coefficient. For this purpose the following relation is used [3]

$$D_{12} = D^o_{12}\left(\frac{T}{T^o}\right)^{\nu}\left(\frac{p^o}{p}\right) \qquad 1.5 \leq \nu \leq 2$$

3.5 The Coefficient of Thermal Diffusion

The coefficient of thermal diffusion for species s, D_s^T, in general depends on the pressure, temperature and concentration. The expression of the thermal diffusion for species s is very complicated and may be found in [10]. In most cases, the contribution of thermal diffusion to the heat-flux vector and to the diffusion velocity is negligeble [2].

4. Chemical Kinetics

In this Chapter a general description of chemical reactions will be given.

An arbitrary single step chemical reaction may be written in the form [2]

$$\sum_s \nu_s^a A_s \rightarrow \sum_s \nu_s^b A_s \tag{4.1}$$

where A_s is the chemical symbol for species s and ν_s^a and ν_s^b are the stoichiometric coëfficients for species s appaering as a reactant and as a product respectively. The meaning of this equation may be demonstrated by the following example

$$H_2 + \tfrac{1}{2}\, O_2 \rightarrow H_2O$$

Here, $A_1 = H_2$, $A_2 = O_2$ and $A_3 = H_2O$. Further, $\nu_1^a = 1$, $\nu_2^a = \tfrac{1}{2}$, $\nu_3^b = 1$ and $\nu_3^a = \nu_1^b = \nu_2^b = 0$.
In general, the stoichiometric coefficients are defined in such a way that 1 mole of products is formed by ν_s^a moles of reactants.
For the reaction in Eq. (4.1), there exists a relationship between changes in concentrations C_s (moles per unit volume) of all species s. Consider an arbitrary pair of species s and r. If γ_s and γ_r (moles per unit volume per second) denotes the time rate of increase of the concentration of species s and r, then equation (4.1) states that

$$\frac{\gamma_s}{\nu_s^b - \nu_s^a} = \frac{\gamma_r}{\nu_r^b - \nu_r^a} \tag{4.2}$$

Because this relation is valid for every pair of species s and r, we may define a reaction rate for reaction in Eq. (4.1) as

$$\gamma = \frac{\gamma_1}{\nu_1^b - \nu_1^a} \tag{4.3}$$

where species 1 may be taken te be any species for which $\nu_1^b - \nu_1^a \neq 0$.
The time rate of increase of the concentration of species s may now be written as

$$\gamma_s = (\nu_s^b - \nu_s^a)\, \gamma \tag{4.4}$$

According to the phenomenological law of mass action, the reaction rate is proportional to the product of the concentration of the reactants [2], [5]

$$\gamma = k \prod_s (C_s)^{\nu_s^a} \qquad (4.5)$$

where the proportionality factor k is called the specific reaction rate constant for reaction (4.1). Combining the equations (4.4) and (4.5) yields

$$\gamma_s = \frac{dC_s}{dt} = (\nu_s^b + \nu_s^a)\, k \prod_s (C_s)^{\nu_s^a} \qquad (4.6)$$

Since most chemical processes involve a number of simultaneous and successive chemical reactions, the net rate of production of species s equals a sum of terms, each term of which corresponds to the production rate in one of the reaction steps. An arbitrary number m of single-step chemical reactions may be written as

$$\sum_s \nu_{s,k}^a A_s \rightarrow \sum_s \nu_{s,k}^b A_s \qquad k = 1, \ldots\ldots m \qquad (4.7)$$

where the subscript k identify's the chemical reaction.

The rate of increase of the concentration of species s by reaction k may be written as

$$\gamma_{s,k} = \dot{C}_{s,k} = (\nu_{s,k}^b - \nu_{s,k}^a)\, k_k \prod_s C_s^{\nu_{s,k}^a} \qquad (4.8)$$

and the net rate of increase of the concentration of species s in the whole proces is given by

$$\dot{C}_s = \sum_k \dot{C}_{s,k} = \sum_k (\nu_{s,k}^b - \nu_{s,k}^a)\, k_k \prod_s C_s^{\nu_{s,k}^a} \qquad (4.9)$$

In general, chemical reactions can proceed both in the forward direction and in the reverse direction. The general set of opposing chemical reactions may be written in the form

$$\sum_s \nu_{s,k}^a A_s \underset{k_{f,k}}{\overset{k_{b,k}}{\rightleftarrows}} \sum_s \nu_{s,k}^b A_s \qquad k = 1, \ldots\ldots m \qquad (4.10)$$

or

$$\left\{\begin{array}{ll} \sum_s \nu_{s,k}^a A_s \xrightarrow[k_{f,k}]{} \sum_s \nu_{s,k}^b A_s & k = 1,\ldots\ldots m \\ \sum_s \nu_{s,k}^b A_s \xrightarrow[k_{b,k}]{} \sum_s \nu_{s,k}^a A_s & k = 1,\ldots\ldots m \end{array}\right.$$

The rate of increase of the concentration of species s by reaction k may now be written as

$$\dot{C}_{s,k} = \left(\nu_{s,k}^b - \nu_{s,k}^a\right) k_{f,k} \prod_s C_s^{\nu_{s,k}^a} + \left(\nu_{s,k}^a - \nu_{s,k}^b\right) k_{b,k} \prod_s C_s^{\nu_{s,k}^b}$$

$$= \left(\nu_{s,k}^b - \nu_{s,k}^a\right) k_{f,k} \prod_s C_s^{\nu_{s,k}^a} \left[1 - \frac{k_{b,k}}{k_{f,k}} \prod_s C_s^{(\nu_{s,k}^b - \nu_{s,k}^a)}\right]$$

(4.11)

At thermodynamic equilibrium, there is no net change in the composition of the system and the reaction rate constants $k_{f,k}$ and $k_{b,k}$ can be related to an equilibrium constant $K_{c,k}$.
From equation (4.11), it follows that at thermodynamic equilibrium holds

$$1 - \frac{k_{b,k}}{k_{f,k}} \prod_s C_s^{(\nu_{s,k}^b - \nu_{s,k}^a)} = 0 \quad ,$$

or

$$\frac{k_{f,k}}{k_{b,k}} = \prod_s C_s^{(\nu_{s,k}^b - \nu_{s,k}^a)} = K_{c,k} \; . \qquad (4.12)$$

The net rate of increase of the concentration of species s in a chemical system with opposing chemical reactions now can be expressed by

$$\dot{C}_s = \sum \left(\nu_{s,k}^b - \nu_{s,k}^a\right) k_{f,k} \prod_s C_s^{\nu_{s,k}^a} \left[1 - \frac{1}{K_{c,k}} \prod_s C_s^{\left(\nu_{s,k}^b - \nu_{s,k}^a\right)}\right].$$

(4.13)

By the following expressions, the net mass rate of production of species s may be derived from (4.13)

$$\omega_s = \dot{C}_s M_s \; , \qquad (4.14)$$

and

$$C_s = \frac{n_s}{N_A} = y_s \frac{\rho}{M_s} \quad . \tag{4.15}$$

Hence,

$$\omega_s = M_s \left\{ \sum_k \left(\nu_{s,k}^b - \nu_{s,k}^a \right) k_{f,k} \, \rho^{m_1} \prod_s \left(\frac{Y_s}{M_s} \right)^{\nu_{s,k}^a} \left[1 - \frac{1}{K_{c,k}} \rho^{m_2} \prod_s \left(\frac{Y_s}{M_s} \right)^{\left(\nu_{s,k}^b - \nu_{s,k}^a \right)} \right] \right\} , \tag{4.16}$$

where

$$m_1 = \sum_s \nu_{s,k}^a \quad ,$$

and

$$m_2 = \sum_s \left(\nu_{s,k}^b - \nu_{s,k}^a \right) \quad .$$

The reaction rate constant $k_{f,k}$ is given by the Arrhenius expression [2]

$$k_{f,k} = A_k \, e^{-E_k/R^o T} \quad , \tag{4.17}$$

where E_k represents the activation energy and A_k is the frequency factor for reaction k, which may be approximated by

$$A_k = B_k \, T^{\alpha_k} \quad , \tag{4.18}$$

where B_k and α_k $(0 \leq \alpha_k \leq 1)$ are constants which belong to the reaction k. If the detailed reaction mechanism of the reaction k were known, it were possible to determine B_k and α_k from the kinetic theory of gases. In most cases, however, the constants B_k and α_k have to be determined empirically. Note that the reaction rate constants also depend on the definition of the stoichiometric coefficients.

5. Turbulence Modelling of the Conservation Equation.

In this Chapter, the conservation equations which have been derived in Chapter 2 are modelled for turbulence. This involves Reynolds decomposition of the dependent variables and time averaging of the resulting equations.

5.1 Conservation of Mass.

The law of conservation of mass, Eq. (2.3), states

$$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot \rho\underline{v} = 0 \quad . \tag{2.3}$$

The Reynolds decomposition procedure implies that each instantaneous variable is replaced by the sum of its mean- and fluctuating components. For instance [12]

$$\rho = \tilde{\rho} + \rho' \quad , \tag{5.1}$$

where the tilde and prime denote mean and fluctuating quantities respectively. Time averaging implies that

$$\bar{\rho} = \lim_{T\to\infty} \frac{1}{T} \int_0^T \rho \, dt \quad . \tag{5.2}$$

where the bar denotes the average value of the quantity ρ over an interval T which is sufficiently long with respect to the time scale of the turbulent fluctuations.
In most cases of interest, the mean quantity of a variable is said to be equal to the average value, so

$$\tilde{\rho} = \bar{\rho} \quad . \tag{5.3}$$

From equation (5.2) it follows that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \rho' \, dt = 0 \quad . \tag{5.4}$$

Hence

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \bar{\rho}\, \rho' \, dt = \bar{\rho} \lim_{T\to\infty} \frac{1}{T} \int_0^T \rho' \, dt = 0 \; . \tag{5.5}$$

Reynolds' decomposition of the law of conservation of mass holds

$$\frac{\partial}{\partial t} (\bar{\rho} + \rho') + \underline{\nabla} \cdot (\bar{\rho} + \rho')\;(\bar{\underline{v}} + \underline{v}') = 0 \quad ,$$

or

$$\frac{\partial}{\partial t}\bar{\rho} + \frac{\partial}{\partial t}\rho' + \underline{\nabla} \cdot (\bar{\rho}\,\bar{\underline{v}} + \bar{\rho}\underline{v}' + \rho\,\bar{\underline{v}} + \rho\,\underline{v}') = 0 \; .$$

Time averaging yields

$$\frac{\partial}{\partial t}\bar{\rho} + \underline{\nabla} \cdot (\bar{\rho}\,\bar{\underline{v}} + \overline{\rho'\underline{v}'}) = 0 \quad . \qquad (5.6)$$

5.2 Conservation of Momentum.

The law of conservation of momentum Eq. (2.6) states

$$\frac{\partial}{\partial t}\rho\underline{v} + \underline{\nabla} \cdot \rho\underline{v}\underline{v} = \rho\underline{g} - \underline{\nabla} \cdot \underline{\underline{P}} \; . \qquad (2.6)$$

Reynolds decomposition of this equation yields

$$\frac{\partial}{\partial t}(\bar{\rho} + \rho')(\bar{\underline{v}} + \underline{v}') + \underline{\nabla} \cdot \left[(\bar{\rho} + \rho')(\bar{\underline{v}} + \underline{v}')(\bar{\underline{v}} + \underline{v}')\right] =$$

$$= (\bar{\rho} + \rho')\,\underline{g} - \underline{\nabla} \cdot (\bar{\underline{\underline{P}}} + \underline{\underline{P}}') \quad ,$$

or

$$\frac{\partial}{\partial t}(\bar{\rho}\bar{\underline{v}} + \bar{\rho}\underline{v}' + \rho'\bar{\underline{v}} + \rho'\underline{v}') + \underline{\nabla} \cdot (\bar{\rho}\bar{\underline{v}}\bar{\underline{v}} + \bar{\rho}\bar{\underline{v}}\underline{v}' + \rho\underline{v}'\bar{\underline{v}} + \bar{\rho}\underline{v}'\underline{v}' + \rho'\bar{\underline{v}}\bar{\underline{v}} +$$

$$+ \rho'\bar{\underline{v}}\underline{v}' + \rho'\underline{v}'\bar{\underline{v}} + \rho'\underline{v}'\underline{v}') = (\bar{\rho} + \rho')\,\underline{g} - \underline{\nabla} \cdot (\bar{\underline{\underline{P}}} + \underline{\underline{P}}') \; .$$

Time averaging yields

$$\frac{\partial}{\partial t}\bar{\rho}\bar{\underline{v}} + \underline{\nabla} \cdot (\bar{\rho}\bar{\underline{v}}\bar{\underline{v}} + \bar{\rho}\,\overline{\underline{v}'\underline{v}'} + \overline{\rho'\underline{v}\underline{v}'} + \overline{\rho'\underline{v}'}\,\bar{\underline{v}} + \overline{\rho'\underline{v}'\underline{v}'}) = \rho\underline{g} - \underline{\nabla} \cdot \underline{\underline{P}} \; . \qquad (5.7)$$

5.3 Conservation of Energy

The law of conservation of energy, Eq. (2.17), is given by

$$\frac{\partial}{\partial t}\rho\,(u + \frac{1}{2}\,\underline{v}\cdot\underline{v}) + \underline{\nabla} \cdot \rho\,\underline{v}\,(u + \frac{1}{2}\,\underline{v}\cdot\underline{v}) = \rho\,\underline{v}\cdot\underline{g} - \underline{\nabla}\cdot(\underline{\underline{P}}\cdot\underline{v}) - \underline{\nabla}\cdot\underline{q} \; . \qquad (2.17)$$

Reynolds decomposition yields

$$\frac{\partial}{\partial t}\left\{(\bar{\rho} + \rho')\left[\bar{u} + u' + \frac{1}{2}\,(\bar{\underline{v}} + \underline{v}') \cdot (\bar{\underline{v}} + \underline{v}')\right]\right\} +$$

$$\underline{\nabla} \cdot \left\{ (\bar{\rho} + \rho')(\underline{\bar{v}} + \underline{v}') \left[\bar{u} + u' + \frac{1}{2} (\underline{\bar{v}} + \underline{v}') \cdot (\underline{\bar{v}} + \underline{v}') \right] \right\} =$$

$$(\bar{\rho} + \rho')(\underline{\bar{v}} + \underline{v}') . \underline{g} - \underline{\nabla} \cdot \left[(\underline{\underline{\bar{P}}} + \underline{\underline{P}}') . (\underline{\bar{v}} + \underline{v}') \right] - \underline{\nabla} \cdot (\underline{\bar{q}} + \underline{q}') .$$

Time averaging yields

$$\frac{\partial}{\partial t} \bar{\rho}\ (\bar{u} + \frac{1}{2} \underline{\bar{v}} . \underline{\bar{v}}) + \underline{\nabla} . \left[\bar{\rho}\underline{\bar{v}}\bar{u} + \overline{\rho' u'}\, \underline{\bar{v}} + \bar{\rho}\ \overline{\underline{v}' u'} + \overline{\rho' \underline{v}'}\, \bar{u} + \overline{\rho' \underline{v}' u'} + \right.$$

$$\frac{1}{2} \bar{\rho}\underline{\bar{v}}\ (\underline{\bar{v}} . \underline{\bar{v}}) + \frac{1}{2} \bar{\rho}\underline{\bar{v}}\ \overline{(\underline{v}' . \underline{v}')} + \frac{1}{2} \overline{\rho'\ \underline{\bar{v}}\ (\underline{v}' . \underline{v}')} + \bar{\rho}\ \overline{\underline{v}'\ (\underline{\bar{v}} . \underline{v}')} +$$

$$\left. \frac{1}{2} \bar{\rho}\ \overline{\underline{v}' (\underline{v}' . \underline{v}')} + \frac{1}{2} \overline{\rho' \underline{v}'}\ (\underline{\bar{v}} . \underline{\bar{v}}) + \overline{\rho' \underline{v}'\ (\underline{\bar{v}} . \underline{v}')} + \overline{\frac{1}{2} \rho' \underline{v}'\ (\underline{v}' . \underline{v}')} \right] =$$

$$(\bar{\rho}\ \underline{\bar{v}} + \overline{\rho'\ \underline{v}'}) . \underline{g} - \underline{\nabla} . (\underline{\underline{\bar{P}}} . \underline{\bar{v}} + \overline{\underline{\underline{P}}' . \underline{v}'}) - \underline{\nabla} \cdot \underline{q} . \qquad (5.8)$$

5.4 Conservation of Angular Momentum

The law of conservation of angular momentum holds

$$\frac{\partial}{\partial t} (\underline{r}_o \times \rho\underline{v}) + \underline{\nabla} \cdot (\underline{r}_o \times \rho\underline{v})\underline{v} = \rho\underline{r}_o \times \underline{g} - \underline{r}_o \times (\underline{\nabla} \cdot \underline{\underline{P}}) \qquad (2.36)$$

Reynolds decomposition applied to this equation yields

$$\frac{\partial}{\partial t} \left[\underline{r}_o \times (\bar{\rho} + \rho')(\underline{\bar{v}} + \underline{v}') \right] + \underline{\nabla} \cdot \left[(\bar{\rho} + \rho') \left\{ \underline{r}_o \times (\underline{\bar{v}} + \underline{v}') \right\} (\underline{\bar{v}} + \underline{v}') \right] =$$

$$= (\bar{\rho} + \rho')\ \underline{r}_o \times \underline{g} - \underline{r}_o \times \underline{\nabla} \cdot (\underline{\underline{\bar{P}}} + \underline{\underline{P}}') ,$$

or

$$\frac{\partial}{\partial t} \left[\underline{r}_o \times (\bar{\rho}\ \underline{\bar{v}} + \bar{\rho}\ \underline{v}' + \rho' \underline{\bar{v}} + \rho' \underline{v}') \right] + \underline{\nabla} \cdot \left[\bar{\rho}\ (\underline{r}_o \times \underline{\bar{v}})\underline{\bar{v}} + \bar{\rho}\ (\underline{r}_o \times \underline{v}')\underline{\bar{v}} \right.$$

$$+ \bar{\rho}\ (\underline{r}_o \times \underline{\bar{v}})\underline{v}' + \bar{\rho}\ (\underline{r}_o \times \underline{v}')\underline{v}' + \rho'(\underline{r}_o \times \underline{\bar{v}})\underline{\bar{v}} + \rho'(\underline{r}_o \times \underline{v}')\underline{\bar{v}} +$$

$$\left. \rho'(\underline{r}_o \times \underline{\bar{v}})\underline{v}' + \rho'(\underline{r}_o \times \underline{v}')\underline{v}' \right] =$$

$$(\bar{\rho} + \rho') \, \underline{r}_o \times \underline{g} - \underline{r}_o \times (\underline{\nabla} \cdot \bar{\underline{\underline{P}}}) - \underline{r}_o \times (\underline{\nabla} \cdot \underline{\underline{P}}') \quad .$$

Time averaging yields

$$\frac{\partial}{\partial t} (\underline{r}_o \times \bar{\rho}\bar{\underline{v}}) + \underline{\nabla} \cdot \Big[\bar{\rho}(\underline{r}_o \times \bar{\underline{v}})\bar{\underline{v}} + \bar{\rho}\,\overline{(\underline{r}_o \times \underline{v}')\underline{v}'} + \overline{\rho'(\underline{r}_o \times \underline{v}')\bar{\underline{v}}} +$$

$$\overline{\rho'(\underline{r}_o \times \bar{\underline{v}})\underline{v}'} + \overline{\rho'(\underline{r}_o \times \underline{v}')\underline{v}'} \Big] = \rho\underline{r}_o \times \underline{g} - \underline{r}_o \times (\underline{\nabla} \cdot \bar{\underline{\underline{P}}}) \quad . \qquad (5.9)$$

5.5 Conservation of Species

The law of conservation of the mass fraction of species s, Eq. (2.39) states

$$\frac{\partial}{\partial t} \rho Y_s + \underline{\nabla} \cdot \rho Y_s \underline{v} = - \underline{\nabla} \cdot \rho Y_s \underline{V}_s + \omega_s \quad . \qquad (2.39)$$

Reynolds' decomposition yields

$$\frac{\partial}{\partial t} (\bar{\rho} + \rho')(Y_s + Y_s') + \underline{\nabla} \cdot \Big[(\bar{\rho} + \rho')(\bar{Y}_s + Y_s')(\bar{\underline{v}} + \underline{v}') \Big] =$$

$$- \underline{\nabla} \cdot \Big[(\bar{\rho} + \rho')(\bar{Y}_s + Y_s')(\bar{\underline{V}}_s - \underline{V}_s') \Big] + \bar{\omega}_s + \omega_s' \quad ,$$

or

$$\frac{\partial}{\partial t} (\bar{\rho}\bar{Y}_s + \bar{\rho}Y_s' + \rho'\bar{Y}_s + \rho'Y_s') + \underline{\nabla} \cdot \Big[\bar{\rho}\bar{Y}_s\bar{\underline{v}} + \bar{\rho}\bar{Y}_s\underline{v}' + \bar{\rho}Y_s'\underline{v}' +$$

$$\bar{\rho}Y_s'\underline{v}' + \rho'\bar{Y}_s\bar{\underline{v}} + \rho'\bar{Y}_s\underline{v}' + \rho'Y_s'\bar{\underline{v}} + \rho'Y_s'\underline{v}' \Big] =$$

$$- \underline{\nabla} \cdot \Big[\bar{\rho}\bar{Y}_s\bar{\underline{V}}_s + \bar{\rho}\bar{Y}_s V_s' + \bar{\rho}Y_s'\bar{\underline{V}}_s + \bar{\rho}Y_s'\underline{V}_s' + \rho'\bar{Y}_s\bar{\underline{V}}_s + \rho'\bar{Y}_s\bar{\underline{V}}_s +$$

$$\rho'\bar{Y}_s\underline{V}_s' + \rho'Y_s'\underline{V}_s' \Big] + \bar{\omega}_s + \omega_s' \quad .$$

Time averaging yields

$$\frac{\partial}{\partial t} \bar{\rho}\bar{Y}_s + \underline{\nabla} \cdot \Big[\bar{\rho}\bar{Y}_s\bar{\underline{v}} + \bar{\rho}\,\overline{Y_s'\underline{v}'} + \overline{\rho'\underline{v}'}\,\bar{Y}_s + \overline{\rho'Y_s'}\,\bar{\underline{v}} + \overline{\rho'Y_s'\underline{v}'} \Big] =$$

$$- \underline{\nabla} \cdot \left[\bar{\rho}\, \bar{Y}_s \bar{\underline{V}}_s + \bar{\rho}\, \overline{Y_s{}' \underline{V}_s{}'} + \overline{\rho' \underline{V}_s{}'}\, \bar{\underline{Y}}_s + \overline{\rho' Y_s{}'}\, \bar{\underline{V}}_s + \overline{\rho' Y_s{}' \underline{V}_s{}'} \right] + \bar{\omega}_s \; .$$

(5.10)

The conservation equations are supplemented by an equation of state (see Chapter 2). Furthermore, a turbulence closure model must be adopted to model the several turbulence terms in the conservation equations. Is is also necessary to derive expression for $\underline{\underline{P}}'$ and $\underline{V}_s{}'$.

6. Further Investigations

Following these basic derivations, which form the theoretical basis for these studies, the following subjects will have to be studied:

(i) 'Faire'-averaging of the turbulent conservation equations.
It seems to be advantageous to use 'Favre'-averaging when modelling the conservation equations for turbulence [9].

(ii) Radiative heat transfer
A more detailed investigation of the expression for radiative heat transfer is necessary.

(iii) Simplifying the conservation equations to the equations for a 2 dimensional transient flow.

(iv) Description of the processes which occur on the boundaries, heat and mass transport in a turbulent boundary layer with chemical reactions.

(v) Selecting a turbulence closure model. A commonly used model is for instance the k-e model proposed by Harlow and Nakyama.

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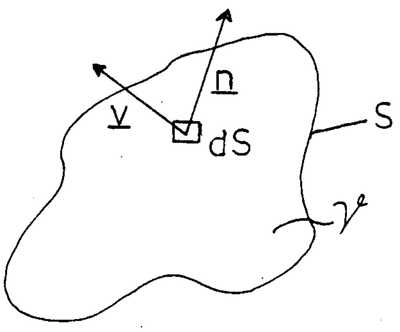

figure 1: an arbitrairy control volume

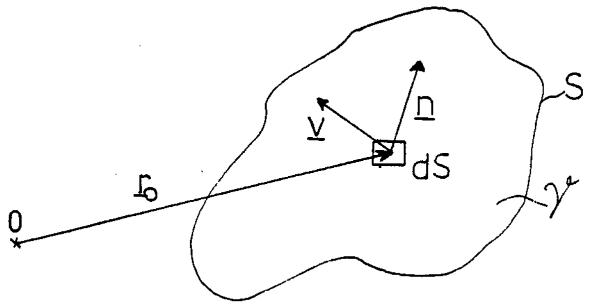

figure 2: an arbitrairy control volume at a distance $\underline{r}_0$ from 0